A subset solution to the sign problem in simulations at non-zero chemical potential

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Abstract. At nonzero quark chemical potential lattice QCD simulations with dynamical quarks are hampered by the sign problem caused by the complex fermion determinant. In this talk we discuss the relation between QCD and random matrix theory and present a novel solution to the sign problem in dynamical random matrix simulations. The sign problem is solved by gathering matrices in subsets, whose sums of complex determinants are real and positive. Markov chains of relevant subsets were generated in Monte Carlo simulations and various observables, like the chiral condensate and quark number, were accurately computed. The subset formula, which is at the basis of the positivity proof for the subset weights, also provides a simple solution to the Silver Blaze puzzle.

1. Introduction
The main motivation for this work is the study of the phases of QCD as a function of temperature and chemical potential. Although the phase diagram is believed to resemble Fig. 1, QCD has in fact only been studied extensively at nonzero temperature $T$ for zero chemical potential $\mu$ while very little is known about its behavior when $\mu$ is nonzero. It is therefore of utmost importance to make progress in the study of QCD at nonzero chemical potential.

The major reason for this deficit is that dynamical lattice simulations of QCD at nonzero chemical potential are prohibitively expensive due to the sign problem caused by the complex fermion determinant \[1\]. This complex nature prohibits the inclusion of the fermion determinant

![Figure 1. Conjectured QCD phase diagram.](image-url)
in the importance sampling weight of Monte Carlo simulations. The methods developed so far to circumvent this problem, e.g., reweighting using auxiliary ensembles, continuation from imaginary $\mu$ and Taylor series expansion around $\mu = 0$, typically require an amount of work that increases exponentially with growing volume and chemical potential in order to produce reliable results, and are therefore only usable at small $\mu$.

Note that the sign problem also occurs in theories other than QCD, and for some of these simpler models alternative methods, like complex Langevin or world-line and loop formulations, were able to simulate the model without encountering a sign problem [2,3].

In this talk we will present a subset solution to the sign problem in a random matrix model, which is equivalent to QCD in the $\varepsilon$-regime [4,5]. In Sec. 2 we introduce QCD at nonzero chemical potential and its relation to random matrix theory. In Sec. 3 we explain the subset method for dynamical simulations of the random matrix model. In Sec. 4 we present various numerical results computed with the method. Finally, we conclude with a summary in Sec. 5.

2. QCD and random matrix theory

2.1. QCD at nonzero quark chemical potential

After integration over the fermion fields the QCD partition function for $N_f$ dynamical fermions is given by

$$Z_{\text{QCD}} = \int DA_\mu e^{-S_G} \prod_{f=1}^{N_f} \det[D(m_f, \mu)].$$

(1)

with gauge fields $A_\mu$, gauge action $S_G$ and Dirac operator $D(m, \mu) = m + \gamma_\mu \partial_\mu + \mu \gamma_4$ for a quark of mass $m$ with quark chemical potential $\mu$. Because of the hermiticity and chirality properties of the Dirac operator its determinant satisfies

$$\det[D(m_f, \mu)] \text{ is } \begin{cases} \text{real and } \geq 0 & \text{for } \mu = 0 \\ \text{complex} & \text{for } \mu \neq 0 \end{cases}.$$  

(2)

At nonzero chemical potential QCD has a sign problem as the fermion determinant cannot be interpreted as a probabilistic weight in Monte Carlo simulations.

2.2. The random matrix model

To investigate the sign problem in QCD one can make use of the equivalence between QCD in the $\varepsilon$-regime ($m_\pi, \mu \ll \frac{1}{\varepsilon} \ll \Lambda$) and random matrix theory (RMT), which was derived from chiral perturbation theory (\chiPT) and holds both at zero and nonzero chemical potential.

One matrix model which was shown to satisfy this equivalence in its universal limit is the two-matrix model of Osborn [6]. In this model, $\phi_1$ and $\phi_2$ are complex $(N + \nu) \times N$ matrices distributed according to partition function

$$Z^{N_f}_\nu(\mu; \{m_f\}) = \int d\phi_1 d\phi_2 w(\phi_1) w(\phi_2) \prod_{f=1}^{N_f} \det D_{\mu,m_f}(\phi_1, \phi_2),$$  

(3)

with Gaussian weights $w(\phi) \propto \exp(-N \text{ tr } \phi^\dagger \phi)$ and Dirac matrix (with $\nu$ zero modes):

$$D_{\mu,m}(\phi_1, \phi_2) = \begin{pmatrix} m & i\phi_1^\dagger + \mu \phi_2^\dagger \\ i\phi_1^\dagger + \mu \phi_2^\dagger & m \end{pmatrix}.$$  

(4)
Figure 2. Three cuts of the microscopic spectral density over the overlap operator at chemical potential $\mu = 0.1$ on a 4$^4$ lattice using 8703 quenched configurations at $\beta = 5.1$. The curves clearly distinguish between topological sectors $\nu = 0$ and 1 [18].

The equivalence with QCD holds in the microscopic limit of RMT, where $N \to \infty$ while $m = 2N m = \Sigma V m_{\text{QCD}}$ and $\hat{\mu}^2 = 2N \mu^2 = F^2 V \mu_{\text{QCD}}^2$ are kept fixed.

Similarly to QCD, the Dirac matrix in the matrix model becomes non-Hermitian for $\mu \neq 0$. Its massless spectrum no longer lies on the imaginary axis, but spreads in the complex plane and is contained in a strip along the imaginary axis with width $\approx 4 \mu^2$. Its determinant is generically complex and dynamical simulations of the random matrix model also suffer from a sign problem.

Much information was gathered about the QCD Dirac operator and the sign problem using RMT. There are analytical solutions for the microscopic spectral densities [6, 7] and individual eigenvalue distributions [8]. There are also analytical results for the average phase of the fermion determinant [9–13], which characterizes the severity of the sign problem.

At finite $\mu$ the Banks-Casher relation ($\Sigma \propto \rho(0)$) is no longer valid and a new mechanism was uncovered relating the strong oscillations in the Dirac spectrum when $\mu > m_\pi/2$ with the discontinuity of $\Sigma$ at $m = 0$ [14, 15]. This mechanism also explains the Silver Blaze puzzle, i.e. the fact that the thermodynamical quantities are independent of $\mu$ up to $m_\pi N / 3$ in the full theory, while the quenched and phase-quenched approximations violate the Silver Blaze for $\mu > m_\pi/2$. An analogous scenario was recently found explaining the Silver Blaze for the quark number density [16].

2.3. Matching QCD to RMT

The equivalence between RMT and QCD in the $\varepsilon$-regime can be used to determine the low energy constants $\Sigma$ and $F$ of $\chi$PT by fitting Dirac spectra of lattice QCD to RMT predictions. Because of the sign problem in dynamical simulations of QCD, RMT predictions with real chemical potential $\mu$ were only verified for quenched QCD. The agreement of the microscopic spectral density was successfully verified for staggered fermions [17] and for overlap fermions [8, 18], which have the additional peculiarity of distinguishing between different topological sectors. A typical result is shown in Fig. 2. In a study of the overlap operator with imaginary chemical potential realistic values of $\Sigma$ and $F$ were computed [19].

2.4. Dynamical simulations and sign problem in RMT

As the Dirac operator $D_{\mu,m}$ is non-Hermitian for $\mu \neq 0$ its determinant $\det[D_{\mu,m}] = Re^{i\theta}$ is generically complex. The average phase factor $\langle e^{2i\theta} \rangle$ reflects the fluctuations of the fermion determinant and characterizes the strength of the sign problem in dynamical simulations:

$$
\langle e^{2i\theta} \rangle_{N_f} = \left\langle \frac{\det[D_{\mu,m}]}{\det[D_{\mu,m}^\dagger]} \right\rangle_{N_f} = \frac{Z_{\nu}^{N_f+1}(\mu, m_m)}{Z_{\nu}^{N_f}(\mu, m_f)},
$$

(5)
where the numerator in the right-hand side is the partition function with $N_f + 1$ quarks and one conjugate bosonic quark. The dependence of the average phase on the chemical potential is shown in Fig. 3. In dynamical simulations the sign problem will show up when the statistical sampling is flooded by the strong fluctuations of the phase.

Dynamical simulations of the random matrix partition function at nonzero $\mu$ can be used to probe the sign problem numerically and can serve as a playground for algorithmic developments. Standard reweighting methods only work at small $\mu$. In the next section we will introduce a subset method which performs partial resummations of configurations to overcome the sign problem.

3. Subset method

In the subset method [4,5] the random matrix configurations are gathered in subsets using the following principle: For of any given configuration $\Phi = (\phi_1, \phi_2)$ consider the set of matrices

$$\Omega(\Phi) = \left\{ \Psi(\Phi; \theta_n) : \theta_n = \frac{\pi n}{N_s} \wedge n = 0, \ldots, N_s - 1 \right\}, \quad (6)$$

containing $N_s$ orthogonal rotations $\Psi = (\psi_1, \psi_2)$ of $\Phi$ defined by:

$$\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}. \quad (7)$$

The Gaussian weights $W(\Omega) \equiv w(\psi_1)w(\psi_2)$ in the partition function are independent of $\theta$ such that all $\Psi(\Phi; \theta)$ in a subset $\Omega$ belong to the RMT ensemble and have the same Gaussian weights. If we factorize out the Gaussian weight, the remaining weight for the subset is given by the sum of fermion determinants, which we denote as fermionic subset weight:

$$\sigma_\Omega(\mu, m) = \sum_{n=0}^{N_s-1} \det^{N_f} D_{\mu,m}[\Psi(\Phi; \theta_n)]. \quad (8)$$

It is easy to see that the integral over all subsets $\Omega$,

$$Z = \int d\Omega W(\Omega) \sigma_\Omega(\mu, m), \quad (9)$$

is an $N_s$-fold covering of the original RMT partition function such that both formulations are equivalent. In the subset formulation, the observables of the original RMT ensemble are computed as:

$$\langle O \rangle = \frac{1}{Z} \int d\Omega W(\Omega) \sigma_\Omega(\mu, m) \langle O \rangle_\Omega \quad (10)$$
with subset measurements

\[
\langle O \rangle_\Omega = \frac{1}{\sigma_\Omega} \sum_{n=0}^{N_s-1} \det^{N_f} D(\Psi_n) O(\Psi_n), \quad \Psi_n \in \Omega. \tag{11}
\]

Of course, rewriting the partition function in terms of subsets does not a priori improve on the sign problem. What does cure the sign problem is that the special construction of the subsets satisfies the following positivity theorem: For any such subset \( \Omega \) the fermionic subset weight \( \sigma_\Omega(\mu, m) \) is real and positive if \( N_s > N_f N \) (for arbitrary \( m \) and \( \mu < 1 \)). This theorem immediately follows from the subset formula:

\[
\sigma_\Omega(\mu, m) = (1 - \mu^2)^{N_f (N_s + \frac{1}{2})} \sigma_\Omega(0, \frac{m}{\sqrt{1 - \mu^2}}) \quad \text{if} \quad N_s > N_f N, \tag{12}
\]

which was proven in Ref. [5]. As \( \sigma_\Omega(0, m) \) is real and positive for any \( m \in \mathbb{R} \), the left-hand side \( \sigma_\Omega(\mu, m) \) is real and positive for \( \mu < 1 \). Note that for \( m = 0 \) and \( \mu = 1 \) we have \( \sigma_\Omega(1, 0) = 0 \), i.e., the sum of determinants is exactly zero for all subsets and the system is maximally non-Hermitian.

4. Simulations and results

We use the positive subset weights \( W(\Omega)\sigma_\Omega \) to sample the ensemble of subsets using the Metropolis algorithm and generate a Markov chain with \( N_{MC} \) relevant subsets of random matrix configurations. The subset size is set to its minimum value required to ensure real positivity, i.e., \( N_s = N_f N + 1 \). Fermionic subset weights are computed by numerical evaluation of their constituent determinants using an LU decomposition. The sample average \( \overline{O} \) of an observable \( O \) in the RMT ensemble is computed as:

\[
\overline{O} = \frac{1}{N_{MC}} \sum_{k=1}^{N_{MC}} \langle O \rangle_{\Omega_k}, \tag{13}
\]

with the subset measurements \( \langle O \rangle_{\Omega_k} \) defined in Eq. (11).

4.1. Chiral condensate and quark number density

We used the subset method to compute the chiral condensate

\[
\Sigma = \frac{1}{2N} \int dZ = \left\langle \frac{1}{2N} \text{tr} D^{-1} \right\rangle \tag{14}
\]

and the quark number density

\[
n = \frac{1}{2N} \int d\mu = \left\langle \frac{1}{2N} \text{tr} \left[ \begin{pmatrix} 0 & \phi_2 \\ \phi_1 & 0 \end{pmatrix} D^{-1} \right] \right\rangle, \tag{15}
\]

and compare our results with those obtained with standard reweighting methods. For the latter we generate \( N_{MC} \times N_s \) random matrices so that we use the same total number of matrices as in subset method. We also compare the results with known analytical expressions.

We performed simulations for matrix sizes \( N = 2, \ldots, 34 \) with \( N_f = 1 \) and \( m = 0.1/2N \), i.e., the mass is small with respect to the magnitude of the smallest eigenvalue. The number of Monte Carlo samples was \( N_{MC} = 100,000 \). The statistical errors displayed in the figures take into account the autocorrelations.
Figure 4. Chiral condensate $\Sigma$ vs $\mu^2$ for $N = 2, 4, 8$. The top row displays the data for the subset method (blue bullets), the phase-quenched reweighting method (red squares) and the analytic curve (solid line). The bottom row displays the relative statistical error $\varepsilon$ on the data.

In Fig. 4 we show the chiral condensate $\Sigma$ as a function of the chemical potential for $N = 2, 4, 8$. The results computed with the phase-quenched reweighting method clearly suffer from the sign problem, which sets in for smaller and smaller $\mu$ as $N$ is increased. In contrast, the results of the subset method agree with the analytical curve from Ref. [15] over the complete $\mu$-range. This is confirmed by the statistical error which is stable for all values of $\mu$.

Similarly, Fig. 5 shows the results for the average quark number density (15). Again, the subset method agrees extremely well with the analytical curve, while the reweighting data are clearly plagued by the sign problem. Note that the relative error for the subset method is extremely small in this case; a peculiarity which can be understood from Eq. (21).

As the sign problem gets stronger with increasing volume, it is also interesting to look at the behavior of the error as a function of $N$; see Fig. 6 for the chiral condensate. For the subset method the $N$ dependence is mild and almost independent of $\mu$, however, for the reweighting method the error increases very rapidly with $N$ until the method breaks down altogether.

Figures 4-6 very much show the power of the subset method to solve the sign problem in these dynamical random matrix simulations.

4.2. Understanding the chiral condensate

At $\mu = 0$ the Banks-Casher formula relates the nonzero chiral condensate to the spectral density of the Dirac operator at the origin. At $\mu \neq 0$ this relation no longer holds and an alternative mechanism was uncovered by Osborn, Splittorff and Verbaarschot [14], which relates $\Sigma$ to extreme, microscopic oscillations in the eigenvalue spectrum of the Dirac operator when $m < 2\mu^2$ (see Fig. 7). As this region of parameter space exactly coincides with the sign problem the mechanism cannot be studied numerically with standard simulation methods. However, as can be seen in Fig. 8 the subset method seems to be insensitive to the large spectral oscillations and very nicely reproduces the analytical predictions for the dynamical chiral condensate when the quark mass moves into the cloud of eigenvalues: the reliability of the method remains unchanged when $m$ crosses the $2\mu^2$ threshold.
Figure 5. Quark number density $n$ vs $\mu^2$ for $N = 2, 4, 8$. The top row displays the data for the subset method (blue bullets), the phase-quenched reweighting method (red squares) and the analytic curve (solid line). The bottom row displays the relative statistical error $\varepsilon$ on the data.

Figure 6. Relative statistical error on the chiral condensate as a function of the matrix size $N$ for the subset method (left) and for phase-quenched reweighting (right) for chemical potential $\mu^2 = 0.1, 0.2, 0.3, 0.4, 0.5$.

Figure 7. Spectral density $\rho(x + iy)$ of the Dirac operator for $N = 16$ and $\mu^2 = 0.6$. From left to right the quark mass is $m = 0.1, 0.4, 1.2$. 

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4.3. Derivatives from the subset weight formula

4.3.1. At the ensemble level Using the subset formula, the partition function and thermodynamic observables at chemical potential \( \mu \) can be related to those at \( \mu = 0 \). For the \( N_f = 1 \) partition function we find

\[
Z_{N_f=1}(\mu; m) = (1 - \mu^2)^{N_f/2} Z_{N_f=1}(0; \frac{m}{\sqrt{1 - \mu^2}}).
\]

(16)

The derivatives with respect to the mass and chemical potential yield relations for the chiral condensate:

\[
\Sigma(\mu; m) = \frac{1}{\sqrt{1 - \mu^2}} \Sigma(0; \frac{m}{\sqrt{1 - \mu^2}}),
\]

(17)

and the quark number density:

\[
n(\mu; m) = -\frac{\mu}{1 - \mu^2} \left[ 1 + \frac{\nu}{2N} - m\Sigma(\mu; m) \right].
\]

(18)

These relations immediately show that the Silver Blaze is satisfied in the microscopic limit, as

\[
\Sigma(\hat\mu, \hat m) \to \Sigma(0; \hat m), \quad n(\hat\mu, \hat m) \to 0.
\]

(19)

4.3.2. At the subset level The subset formula also allows us to relate the subset measurements of the thermodynamical observables at \( \mu \) and \( \mu = 0 \) on individual subsets. The chiral condensate on a subset \( \Omega \) obeys

\[
\Sigma_{\Omega}(\mu; m) = \frac{1}{\sqrt{1 - \mu^2}} \Sigma_{\Omega}(0; \frac{m}{\sqrt{1 - \mu^2}}),
\]

(20)

and the quark number density on a subset \( \Omega \) satisfies

\[
n_{\Omega}(\mu; m) = -\frac{\mu}{1 - \mu^2} \left[ 1 + \frac{\nu}{2N} - m\Sigma_{\Omega}(\mu; m) \right].
\]

(21)
Note that the main contribution is exactly reproduced by each subset, which explains why the relative error on \( n \) is so small (see Fig. [5]).

It is interesting to note that the Silver Blaze is already solved on each individual subset:

\[
\Sigma_{\Omega}(\hat{\mu}, \hat{m}) \rightarrow \Sigma_{\Omega}(0; \hat{m}), \quad n_{\Omega}(\hat{\mu}, \hat{m}) \rightarrow 0.
\] (22)

4.4. Sign problem in reweighting methods

In this section we take a closer look at the sign problem in reweighting methods. The ensemble average of \( y \) in an ensemble with weight \( w \) is given by

\[
\langle y \rangle_w = \frac{\int dx w(x)y(x)}{\int dx w(x)}.
\] (23)

In reweighting an auxiliary ensemble with positive weight \( w_0 \) is introduced and the ensemble average is rewritten as

\[
\langle y \rangle_w = \frac{\int dx w_0(x) \left[ \frac{w(x)}{w_0(x)} y(x) \right]}{\int dx w_0(x) \left[ \frac{w(x)}{w_0(x)} \right]} = \frac{\langle \frac{w}{w_0} y \rangle_{w_0}}{\langle \frac{w}{w_0} \rangle_{w_0}}.
\] (24)

The auxiliary distribution \( w_0 \) can be sampled using importance sampling, and the observables in the target ensemble can be evaluated using Eq. (24), even when \( w \) is complex. However, the expectation values in the numerator and denominator of (24) both involve cancellations that grow exponentially with the volume, and as they are computed by statistical sampling the work needed to make reliable measurements grows exponentially too and the sign problem sets in.

The denominator, denoted as the average reweighting factor \( r \), is independent of the observable and its relative error can be used as a measure of the sign problem. Because of the large fluctuations of the complex weights, which are exactly at the origin of the sign problem, the reweighting factor can not be computed accurately in direct simulations of the auxiliary ensemble \( w_0 \). However, using the identity

\[
r \equiv \left\langle \frac{w}{w_0} \right\rangle_{w_0} = \frac{\int dx w(x)}{\int dx w_0(x)} = \left[ \left\langle \frac{w_0}{w} \right\rangle w_0 \right]^{-1},
\] (25)

it can be computed indirectly to very high accuracy using the subset method as the subset measurements

\[
\left\langle \frac{w_0}{w} \right\rangle_{\Omega} = \frac{1}{\sigma_{\Omega}(\mu, m)} \sum_{n=0}^{N_s-1} w_0(\Psi_u)
\] (26)

are all real and positive. The sign problem is caused by the relative error on the average reweighting factor, which is given by

\[
\varepsilon_r = \sqrt{\frac{2\tau}{N_{MC}}} \frac{\sigma_r}{r},
\] (27)

where \( N_{MC}/2\tau \) is the number of independent measurements and \( \sigma_r \) is the variance of the reweighting factor in the auxiliary ensemble. We computed the reweighting factors and their relative standard deviations \( \sigma_r/r \), which is proportional to the standard error \( \varepsilon_r \), for the following reweighting schemes: quenched (q), phase-quenched (pq), \( \mu \)-quenched (\( \mu \)q) and sign-quenched (sq). A comparison of the results for these schemes is shown in Fig. [9]. The rapid increase of the relative standard deviation of the reweighting factors clearly shows that the sign problem quickly becomes unmanageable, independently of the chosen scheme, as \( N_{MC} \) would have to be increased accordingly to keep the error under control. It is noteworthy that the severity of the sign problem in reweighting methods can be measured accurately with the subset method.
Figure 9. Comparison of the $N_f = 1$ reweighting factors (left) and their relative standard deviations $\sigma_r/r$ (right) as a function of $\mu^2$ for $N = 8$, for different reweighting schemes. These data are genuine predictions as there are no analytic results available for these quantities.

5. Summary
In this talk we presented a subset method that solves the sign problem in dynamical simulations of a two-matrix model. The matrices are gathered into subsets with real and positive weights, which can be simulated using importance sampling methods. In contrast to standard reweighting methods, where the work grows exponentially with $N$ and $\mu$ due to the sign problem, the subset method is free of sign problem: Its results are reliable up to much larger values of $\mu^2$ while the work only shows a mild dependence on $N$. The crucial feature of the subset method is that the cancellations, necessary to get the correct dynamical behavior, no longer happen stochastically through statistical sampling but deterministically inside subsets of size $O(N)$.

To make further progress it will be useful to uncover the mechanism underpinning the subset method in order to extend these ideas to other models or even to QCD itself.

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1 After the conference new results revealed a connection between the subset method and a projection on canonical determinants [20].