Composite reweighting SU(2) QCD at Finite Temperature

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The Glasgow reweighting method is evaluated for SU(2) lattice gauge theory at nonzero \( \mu \) and finite \( T \). We establish that the ‘overlap problem’ of SU(3) measurements, in which the transition points determined from thermodynamic observables have an unphysical dependence on the value of \( \mu \) used to generate ensembles for reweighting, persists for SU(2). By combining the information from different lattice ensembles we alleviate sampling bias in the fugacity expansion, and identify the Lee Yang zeros associated with the transition to a high density phase that can plausibly be associated with diquark condensation. We also confirm the existence of a line of first order transitions above a critical point in the \( T - \mu \) phase plane previously predicted by effective chiral lagrangian calculations.

1. Introduction

Recent speculation over BCS type-instabilities in the Fermi surface at high density \([1][2]\) has led to resurgence of interest in two colour QCD. Lattice models with pseudoreal representations are attractive candidates for simulation at finite density since for such theories the Dirac matrix is positive definite, which permits the use of existing Monte Carlo techniques at \( \mu \neq 0 \). For SU(3) at finite density the lattice action is otherwise complex \([3]\), and so the probabilistic importance sampling step of such methods is therefore undefined. Reweighting methods have proved a useful means of addressing this issue, where the \( \mu \) dependence of the grand canonical partition function \( Z(\mu) \) can be made semi-analytic in a fugacity expansion, as with the Glasgow method \([4]\). The complex action issue is thus avoided, by generating a lattice ensemble in an accessible regime of the parameter space (eg. \( \mu = 0 \) for SU(3)). Naively, one might anticipate that the specific lattice ensemble used in the reweighting has little impact on numerical evaluations of the expansion. In fact quite the reverse is true. For the SU(3) model with dynamical quarks, even at intermediate coupling where one might expect thermal fluctuations to enhance the frequency of sampling physically relevant states, an ensemble generated at \( \mu = 0 \) reproduces a similar phase structure to the quenched model \([5][6]\). This has severe consequences since quenched finite density QCD is understood to be the zero flavor limit \((n \to 0)\) of a theory with equal numbers of quarks and conjugate quarks. The lowest lying baryonic state in the model is thus the unphysical “baryonic pion”, formed from quark-conjugate quark pairs rather than the lightest three quark state \([7][8]\). However, this is of no consequence in two colour QCD \([9]\) as the baryonic pion and baryon propagators are equivalent at \( \mu \neq 0 \).

Pseudoreal models are not entirely free from the effects of the reweighting overlap pathologies, however. Models with quarks in the adjoint representation \((n \text{ odd})\) suffer from the related reweighting pathology: the sign problem. Since \( \det M(\mu) \) is always real for two colour QCD, although reweighting is no longer mandatory it provides a useful opportunity to investigate the overlap issue (where the correct physics may be more easily extracted from lattice measurements by conventional means), and to quantify the signatures of the sampling numerical discrepancies therein.

2. Symmetries of the SU(2) Lattice Action

The \( n \)-flavor symmetry of SU(2) QCD given by quarks in their fundamental representation \([2]\), is \( SU(2n) \) rather than \( U(n)_L \times U(n)_R \) as might be anticipated, as is demonstrated by a change of basis in the free field langrangian.

\[
L = \overline{\psi} \gamma_{\mu} D_{\mu} \psi = i \overline{\psi} \gamma_{\mu} \sigma_{\nu} D_{\nu} \psi
\]  

(1)
\[ \Psi = \begin{pmatrix} \psi_L \\ \sigma_2 \tau_2 \psi_R^* \end{pmatrix} \]  
(2)

where \( \psi \) is a 2 doublet. The inclusion of explicit symmetry breaking terms in \( m \) and \( \mu \) can be shown similarly to lead to the symmetry breaking patterns tabulated above \[8\].

\[ \overline{\psi} \psi = \frac{1}{2} \Psi^T \sigma_2 \tau_2 \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \Psi + h.c. \]  
(3)

\[ -\overline{\psi} \gamma_0 \psi = \overline{\Psi} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \Psi \]  
(4)

Naturally, the lattice model (with Kogut-Susskind fermions), follows a somewhat similar symmetry breaking scheme, having a manifest global \( U(2n) \) symmetry. In the continuum limit, for the choice of \( n = 1 \), this lattice action corresponds to 8 physical flavors through the well-known doubling of fermionic modes \[13\].

At \( m, \mu \neq 0 \) it is argued in \[9\] that since the number of the Goldstone modes differs for nonzero expectations of \( \psi \psi \) and \( \overline{\psi} \psi \), that a phase transition occurs at \( \mu \geq \frac{1}{2} m_\pi \) corresponding to the point at which the number density of quarks becomes nonzero and \( U(n)_V \) is spontaneously broken. It is then further argued with the Landau free energy in \[12\], that since the number of Goldstone modes at high density is odd, that the transition to the free quark phase at finite temperature is necessarily first order.

### 3. Glasgow Method

For the Glasgow reweighting method, the \( \mu \) dependence of the lattice action is made analytic through the formulation of the fugacity expansion, where \( z = \exp(\mu/T) \). This constitutes the characteristic fugacity polynomial which is formed from the propagator matrix \( P \), defined through the fermion matrix \( M \) \[13\]. Where \( P \) is written in terms of the matrices which contain links between lattice sites in the spatial directions \( G \), and forward and backward in the time direction \( V \) and \( V^\dagger \).

\[ 2iM = 2im + G + Ve^\mu + V^\dagger e^{-\mu} \]  
(5)

\[ P = \begin{pmatrix} -(G + 2im) & 1 \\ -1 & 0 \end{pmatrix} V \]  
(6)

\[ \det M = \det(G + 2im + V^\dagger e^{-\mu} + Ve^\mu) \]  
(7)

\[ = e^{n_3 n_\mu} \det(P - e^{-\mu}) \]  
(8)

\[ = e^{n_3 n_\mu} \sum_{n=0}^{2n_3 n_\mu} c_n e^{-n \mu} \]

with \( n_3 n_\mu \) the lattice volume and \( n_\mu \) the number of colours in the expansion. Since \( V \) is an overall factor of \( P \) the order of the expansion is reduced by exploited the unitary symmetry \( Z_{n_\mu} \) defined by multiplying the timelinks in \( V \) by \( e^{2\pi ij/n_\mu} \), where \( j \) is an integer. Since \( n_\mu = 1/T \), the Grand Canonical Partition function \( Z(\mu) \) is thus given defined as an expansion in terms of the fugacity variable and the canonical partition functions \( Z_n \).

\[ Z(\mu) = \int DU \det M(\mu) e^{-S_g} \]  
(9)

\[ = \sum_n Z_n e^{n \mu/T} \]  
(10)

By reweighting this expansion an arbitrary normalisation to \( Z(\mu) \) is introduced, though this leaves the analytic determination of thermodynamic variables unaffected.

\[ \frac{Z(\mu)}{Z(\mu_0)} = \frac{\int DU \det M(\mu) e^{-S_g}}{\int DU \det M(\mu_0) e^{-S_g}} \]  
(11)

\[ \frac{Z_n}{Z(\mu_0)} = \frac{\int DU \frac{c_n}{\det M(\mu_0)} e^{-S_g}}{\int DU \det M(\mu_0) e^{-S_g}} \]  
(12)
Similarly the zeros expansion, centered on the term of order \(n(\mu_o)\).

This effect and the reliability of the averaging can be established for two-colour QCD by measuring the ratio of the ensemble-averaged expansion coefficients between two or more ensembles generated at different values of \(\mu_o\). Having then identified \(n(\mu_o)\) for several ensembles, our composite reweighting method then consists of rescaling the expansion coefficients from different ensembles through these ratios (where the ensemble-averaging is effective). The bias introduced through reweighting the expansion can thus be systematically alleviated, and thermodynamic observables more reliably determined \([14]\).

3.1 Thermodynamic Observables

The eigenvalues \(\lambda_n\) of \(P\) naturally share the symmetries of \(V\), most notably \(\lambda \rightarrow 1/\lambda^*\) relating \(P\) to \(P^{-1}\) up to a unitary transformation. Since SU(2) with quarks in the fundamental representation is pseudoreal it can also be shown that \(\lambda \rightarrow \lambda^*\). By rewriting the expansion in the variable \(y = z + 1/z\) the order can be further reduced by a factor of two to reduce rounding errors in the numerical implementation \([13]\). The quark number density \(n\) and its associated susceptibility \(\chi_n\) for this expansion is then both easily evaluated from the expansion, and in addition is also readily amenable to composite reweighting approach described above.

\[
\langle n \rangle = \frac{T}{n^3} \frac{\partial \ln Z(\mu)}{\partial \mu} \quad (13)
\]

\[
= \frac{\sum_{n=0}^{n^3} n \sinh(-\frac{e_n - n\mu}{T})}{\sum_{n=0}^{n^3} \sinh(-\frac{e_n - n\mu}{T})} \quad (14)
\]

\[
\langle \chi_n(\mu) \rangle = \langle n^2 \rangle - \langle n \rangle^2 \quad (15)
\]

Similarly the zeros \(\alpha_n\) of \(Z(\mu)\) are readily identified from the expansion, which as Lee and Yang showed with an Ising ferromagnetic system, correspond to a phase transition in the thermodynamic limit wherever a zero approaches the real axis in the complex-\(z\) plane \([16]\).

\[
Z(\mu) \propto e^{-n_c^2n^3\mu} \prod_{n=1}^{n^3} (e^{n\mu} - \alpha_n) \quad (16)
\]

4. Results

4.1 Intermediate Coupling

We generated a total of seven ensembles at consecutive values of \(\mu_o\) ranging from \(\mu_o = 0.3 - 1.1\), at \(\beta = 1.5\) both for \(4^3\) and \(6^34\) lattice volumes. From these lattice ensembles we evaluated the Lee-Yang zeros, quark number density susceptibility \(\langle \chi_n \rangle\), and \(\langle \psi\bar{\psi} \rangle\) using a conventional stochastic approach.

For both our measurements at \(\beta = 1.5\) and \(\beta = 2.3\), \(\langle \psi\bar{\psi} \rangle\) decreases gradually to zero over the range of values of \(\mu\) we generated for \(m = 0.05\). However, since \(\langle \psi\bar{\psi} (\mu = 0)\rangle\) is considerably smaller in the latter measurement, plausibly \(U(1)_A\) is spontaneously broken in the chiral limit in the former case for the volumes we used. It then follows that there should be a corresponding transition in the \(m - \mu\) plane at \(\mu_c \sim \frac{1}{T}\) (as we argued in Sec 2), which we were able to identify from our Lee-Yang zeros measurements using composite reweighting. An unphysical \(\mu_o\) dependence dominates our measurements prior to composite reweighting at \(\beta = 1.5\) and is tabulated in Table 2, along with the convergence of our measurements after composite reweighting as we increase the number of included ensembles.

For an ensemble generated at \(\mu_o = \mu_c\) we believe the sampling should be effective enough to circumvent the need for composite reweighting. There is evidence to support this with the ensemble we generated at \(\mu_o = 0.3 \sim \mu_c\) in Fig.1, which shows more evidence of a transition (where the zeros consistently approach the real axis) at \(\mu_c \sim \frac{1}{T}\) than the other ensembles we generated at \(\beta = 1.5\). However, since we are unable to accurately quantify which values of \(\mu_c (\mu_o)\) are the more valid from our jackknife error estimates of the Lee-Yang zeros, and the unphysical \(\mu_o\) dependence of our measurements persists for ensem-
bles generated at values of $\mu_o$ arbitrarily close to $\mu_c$, we found it is more effective to sample the expansion coefficients accurately by generating a covering series of ensembles with our composite reweighting method.

In varying the lattice volume $V$ and $\beta$, we can confirm that this unphysical $\mu_o$ dependence in our measurements behaves as we would expect of a reweighting overlap(sign) problem. The expectation of the sign of the Monte Carlo measure (which is treated as an observable for reweighting in the Potts model), shows a $\beta$ and $V$ dependence of the form,

$$\langle \text{sgn} \rangle = \frac{Z}{Z_{||}} = \exp(-\beta V \Delta f)$$

(17)

where $Z_{||}$ is the partition function of the ensemble modified to exclude the sign problem amenable to a Monte Carlo approach, and $\Delta f$ the difference in free energy densities between ensembles $\mathcal{E}$. This effect is seen Tables 2 and 3 where the imaginary part of the zeros nearest the real axis evaluated from the ensemble at generated at $\mu_o \sim \mu_c$ is comparatively smaller (and therefore more convincing) as $V$ is increased. Similarly, this Lee-Yang zeros effect becomes more pronounced as we increase $\beta$.

We are able to determine the range of values of $\mu_o$ over which to generate ensembles for our effective sampling strategy, from the jacknife error estimates for the ensemble-averaged expansion coefficients, which give us $n(\mu_o)$. The largest of the coefficients $c_{2n_1n_2}$ (related to the canonical partition function for the filled lattice) is of order one for $\mu_o = 1.2$, and the lattice therefore saturated. Our quark number density susceptibility measurements $\langle \chi_n(\mu) \rangle$ become singular at $\mu_c$ as we include more ensembles in the composite reweighting across this range, indicating that the transition at $\mu_c \sim \frac{1}{2}m_\pi$ for $\beta = 1.5$ is first order, Fig 4. We are also able to identify a second smaller peak in these measurements which corresponds to the point at which the expectation of the diquark falls off in existing condensate measurements. As saturation is approached at $\mu = 1.2$ the diquark condensate thus evaporates in a less well determined transition driven by Fermi statistics $\text{[18][19]}$.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{Fig1.png}
\caption{Lee Yang zeros evaluated in the complex $\mu$ plane ($\eta_n = T \ln \alpha_n$) for a 6$^3$4 lattice at $\beta = 1.5$ from an ensemble generated at $\mu_o = 0.3$.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{Fig2.png}
\caption{Lee Yang zeros evaluated in the complex $\mu$ plane for a 6$^3$4 lattice at $\beta = 1.5$ from an ensemble generated at $\mu_o = 0.5$.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{Fig3.png}
\caption{Lee Yang zeros evaluated in the complex $\mu$ plane for a 6$^3$4 lattice at $\beta = 1.5$ from an ensemble generated at $\mu_o = 0.7$.}
\end{figure}
Table 2
Lee Yang zero with the smallest imaginary part evaluated in the complex\(\mu\) plane \((\eta_n = T \ln \alpha_n)\) for two lattice volumes at \(\beta = 1.5\). Dependence on value of \(\mu_0\) used to generate ensembles for the Glasgow reweighting method (upper), and dependence on the number of ensembles included in the new composite reweighting scheme (lower).

\[
\begin{array}{|c|c|c|}
\hline
\mu_0 & \text{Re } \eta_1 & \text{Im } \eta_1 \\
\hline
0.3 & 0.502(0.109) & 0.117(0.171) \\
0.5 & 0.966(0.003) & 0.056(0.024) \\
0.7 & 0.871(0.066) & 0.098(0.103) \\
0.8 & 0.688(0.061) & 0.105(0.114) \\
0.9 & 0.824(0.072) & 0.237(0.077) \\
1.0 & 0.354(0.025) & 0.169(0.081) \\
1.1 & 0.560(0.015) & 0.142(0.069) \\
\hline
\#. Ens. & & \\
1 & 0.688(0.061) & 0.105(0.114) \\
3 & 0.556(0.002) & 0.015(0.025) \\
5 & 0.497(0.001) & 0.024(0.014) \\
7 & 0.480(0.001) & 0.014(0.013) \\
\hline
\end{array}
\]

\[
\begin{array}{|c|c|c|}
\hline
\mu_0 & \text{Re } \eta_1 & \text{Im } \eta_1 \\
\hline
0.3 & 0.411(0.001) & 0.116(0.001) \\
0.5 & 0.830(0.002) & 0.167(0.096) \\
0.7 & 0.523(0.032) & 0.134(0.001) \\
0.8 & 0.822(0.028) & 0.154(0.082) \\
0.9 & 0.546(0.067) & 0.153(0.051) \\
1.0 & 0.434(0.039) & 0.091(0.039) \\
1.1 & 0.461(0.011) & 0.064(0.030) \\
\hline
\#. Ens. & & \\
1 & 0.546(0.067) & 0.153(0.051) \\
3 & 0.467(0.008) & 0.012(0.007) \\
5 & 0.453(0.008) & 0.011(0.007) \\
7 & 0.477(0.001) & 0.006(0.005) \\
\hline
\end{array}
\]

Figure 4. Quark number density susceptibility \(\langle \chi_n(\mu) \rangle\) for a \(4^4\) lattice at \(\beta = 1.5\), with an increasing number of ensembles included in the composite reweighting (upper 1, 3, 5) (lower 7, 9, 11). A prominent peak develops as the number of composite reweighted splines is increased, indicating a first order transition.
4.2. Weak Coupling

There is a marked difference between the unphysical $\mu_o$ dependence of the Lee-Yang zeros associated with $\mu_c$ evaluated before composite reweighting at $\beta = 1.5$ and $\beta = 2.3$ between Tables 2 and 3. In Table 2 there is some indication of competition between the two separate transition points during rootfinding we have identified above as the value of $\mu_o$ is varied, which is now entirely absent in Table 3. From this we can conclude that there is no indication of a second transition point at $\beta = 2.3$, and that a transition can be readily identified at $\mu_c \sim 0.8$. Where the reweighting ensemble is generated at $\mu_o = \mu_c$ there is also good agreement between these zeros measurements and those from composite reweighting. Although again we have not quantified how small the difference between $\mu_o$ and $\mu_c$ must be for the reweighting to be effective, and have relied instead on composite reweighting.

Our composite reweighting Lee-Yang zeros and quark number density susceptibility measurements indicate again (where the zero closest the real $z$-axis goes to zero as the volume is increased and where $\langle \chi_n(\mu) \rangle$ becomes singular) that the transition is first order. The only context in which a first order transition is predicted in the effective chiral lagrangian approach is with a transition from the diquark to the symmetric phase for $\mu_c > \frac{1}{2}m_\pi$, and we therefore confirm the existence of such a transition line in the $T - \mu$ plane.

5. Conclusions

Despite expectations, generating an ensemble for the reweighting method with a value of $\mu_o$ arbitrarily close to $\mu_c$ still leads to an overlap problem in a model with a pseudoreal representation evaluated at $\beta_c$. In fact, for an exploratory study (in which $\mu_c$ is unknown), the fugacity expansion coefficients are more effectively sampled through the combination of terms from a covering series of ensembles. Even with the real Monte Carlo measure of two colour QCD the overlap problem is still pathological for the Glasgow reweighting method. With new multi-parameter ($\beta, \mu$) reweighting approaches to SU(3)\[^{[20]}\] we would therefore expect there to be similar sampling bias.
Lee Yang zero analysis allows the simple identification of a first order transitions in $\mu$ with lattice measurements on comparatively small volumes. To extend the rigor of this approach and determine the critical exponents of the transition at $\mu_c$, however, it will be necessary to increase the lattice size as the zeros scaling at $\beta = 2.3$ is not without finite volume effects. It will also be interesting to repeat this volume scaling analysis for $\beta < \beta_c$ and to compare the measured critical exponents for the diquark phase transition with those predicted with the chiral langragian approach [10], believed to be second order.

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| $\mu_0$ | Re $\eta_1$ | Im $\eta_1$ |
|---------|-------------|-------------|
| 0.3     | 0.816(0.041)| 0.214(0.096)|
| 0.5     | 0.801(0.059)| 0.223(0.106)|
| 0.7     | 0.797(0.042)| 0.099(0.135)|
| 0.9     | 0.747(0.048)| 0.230(0.089)|
| 1.0     | 0.734(0.040)| 0.200(0.094)|
| 1.1     | 0.610(0.003)| 0.167(0.091)|
| # Ens.  |             |             |
| 2       | 0.835(0.029)| 0.113(0.038)|
| 4       | 0.839(0.005)| 0.082(0.036)|
| 6       | 0.830(0.003)| 0.040(0.034)|
| 8       | 0.849(0.005)| 0.031(0.026)|

Table 3
Lee Yang zero with the smallest imaginary part evaluated in the complex $\mu$ plane ($\eta_n = T \ln \alpha_n$) for two lattice volumes at $\beta = 2.3$. Dependence on value of $\mu_0$ used to generate ensembles for the Glasgow reweighting method (upper), and dependence on the number of ensembles included in the new composite reweighting scheme (lower).
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