The Role of the Polyakov loop
in Finite Density QCD

Ph. de Forcrand and V. Laliena
ETH, CH-8092 Zürich, Switzerland

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Abstract

We study the behavior of the fermion determinant at finite temperature and chemical potential, as a function of the Polyakov loop. The phase of the determinant is correlated with the imaginary part of the Polyakov loop. This correlation and its consequences are considered in static QCD, in a toy model of free quarks in a constant $A_0$ background, and in simulations constraining the imaginary part of the Polyakov loop to zero.

1 Introduction

The experimental study of QCD at finite density and temperature, and the possible observation of the quark-gluon plasma are the focus of activity of an increasing fraction of the physics community. A parallel study by computer simulations would be highly desirable. However, after integration over the fermions, the integrand $\rho(U)$ in the finite density partition function is complex. The measure used in Monte Carlo simulations is $\langle \cdots \rangle_{MC} = d[U] |\rho(U)|$, and observables are computed as $\langle O \rangle = \langle O \rho(U)/|\rho(U)| \rangle_{MC}/\langle \rho(U)/|\rho(U)| \rangle_{MC}$. The denominator is exponentially small in the 4-volume of the lattice, and measuring it with a given accuracy requires an exponentially growing amount of statistics. This is the so-called sign problem. Over almost twenty years, progress in controlling the sign problem has been negligible.

For this reason one has turned to approximations to QCD: the strong coupling limit, and more recently the static limit of QCD have attracted a lot of interest [1, 2]. Static QCD is still affected by the sign problem, which limits investigations to small volumes, far from the continuum limit.
It would be very desirable to extend the domain of study of static QCD to more realistic regions of parameters, and to go beyond the static approximation and allow for at least some spatial hopping of the quarks. Our paper proposes and tests a method to do this.

We have analyzed static QCD results of [1] and found a strong correlation between the phase of the determinant \( \phi(\text{det}) \) and the imaginary part \( P_i \) of the Polyakov loop \( P \). We study this correlation in Section I, and show that it is to be expected for heavy quarks.

This provides the motivation for a simple toy model, studied in Section II, where all degrees of freedom are suppressed except the Polyakov loop: free quarks in a gauge field background with constant temporal component \( A_0 \) and vanishing spatial components. This model can be solved easily in Fourier space. It shows several features of QCD. In particular, it exhibits the ordering effect of the chemical potential \( \mu \), similar to that of the temperature \( T \). Under simple assumptions, a phase diagram \( \mu_c(T) \) can be obtained at small \( \mu \). A mechanism for a transition at low temperature is proposed.

Finally, the correlation between the phase of the determinant and the imaginary part of the Polyakov loop can be put to profit by performing constrained simulations, where \( P_i = 0 \). The sign problem is reduced. The validity of imposing such a constraint, and the benefits this constraint provides, are reviewed in Section III.

Figure 1: Correlation between \( \phi(\text{det}) \) and \( P_i \) in static QCD, on a lattice \( L_s^3 \times 2 \) (\( L_s = 6, 8, 10, C = 1/20, \beta = 5.0 \)). On the right, \( P_i \) has been rescaled by \( \sqrt{L_s^3} \) and \( \phi(\text{det}) \) by \( 1/\sqrt{L_s^3} \). The data are from Ref.[1].
2 Correlation between $P_i$ and $\phi(\det)$

We have reanalyzed the static QCD data of [1]. Recall that static QCD is obtained by taking the quark mass $m_q$ and the chemical potential simultaneously to infinity, such that the quark density is finite. This is achieved by keeping constant the parameter $C^{-1} \equiv (e^\mu/2m_q)^{N_t}$, where $N_t$ is the temporal extent of the lattice. The quarks are static, but the fermionic determinant is still sensitive to changes in the gauge field and the quark density. Fig. 1a shows almost perfect correlation between the phase of the determinant and the imaginary part of the Polyakov loop, for 3 spatial volumes $V$. Furthermore, as $V$ is increased, one observes that the fluctuations in $P_i$ vary like $1/\sqrt{V}$, as any extensive variable, and that fluctuations in $\phi(\det)$ increase like $\sqrt{V}$. Under this rescaling, the results for the 3 different volumes become indistinguishable (Fig. 1b).

As the chemical potential (equivalently $C$ in static QCD) increases, or as the temperature decreases, fluctuations in the phase increase, and the correlation becomes harder to unravel because of the compact nature of the phase. Fig. 2 shows the worst case studied by Blum et al. [1]. If one defines $\phi(\det)$ as $\sum_i \phi(\lambda_i)$, with $\phi(\lambda_i) \in [-\pi, +\pi]$, where $\lambda_i$ are the eigenvalues of

![Figure 2: Same as Fig. 1 with $C = 1/0.6$ and $\beta = 5.0$ on a $6^3 \times 4$ lattice.](image)
the Dirac matrix, the correlation remains significant.

This correlation should be expected. In the loop expansion of the fermion determinant, \( \log(\det(1 - \kappa M)) \equiv -S_{\text{eff}} = -\sum_l \kappa^l \ln \Tr M^l \), where \( \kappa \sim 1/m_q \), the first loop affected by the chemical potential \( \mu \) is the (timelike) Polyakov loop. The corresponding contribution to \( S_{\text{eff}} \) is

\[
2(2\kappa)^{N_t} \sum_x (\cosh(N_t \mu) P_r(x) + i \sinh(N_t \mu) P_i(x))
\]

\[
\text{i.e. } \phi(\det) = 2(2\kappa)^{N_t} V \sinh(N_t \mu) P_t,
\]

where the summation \( \sum_x \) is over all spatial coordinates \( x \). Higher-order terms spoil this perfect correlation. They become more important as \( N_t \) increases or \( m_q \) decreases. In static QCD, there is no spatial hopping of the quarks, so that the only additional terms are powers of the Polyakov loop at each site, which are suppressed by powers of \( 2(2\kappa)^{N_t} \sinh(N_t \mu) \).

3 Toy model: free quarks in a constant \( A_0 \) background

We have just seen that static QCD is in fact a Polyakov loop model, where the phase of the determinant is almost equal to the imaginary part of the Polyakov loop. But even in static QCD, calculations are still severely limited by the sign problem. Monte Carlo integration performs an averaging over the gauge fluctuations and the fluctuations of the Polyakov loop \( P(x) \) at each spatial point \( x \). We can simplify this model further by keeping only the zero-mode of such fluctuations and neglecting, for now, the other fluctuations of the gauge field. We end up with a single \( SU(3) \) degree of freedom, the Polyakov loop \( P \). Our model consists of free quarks in a gauge field background with zero spatial components and constant temporal component \( A_0 \). Hence, \( P = \exp(iN_t a A_0) \), where \( a \) is the lattice spacing. Gauge invariance implies that the fermion determinant depends only on \( \Tr P = P_r + i P_i \).

It can be calculated by Fourier transform on the lattice, using staggered quarks. As this work was in progress, the preprint [3] appeared, where the same calculation of the determinant is performed in the continuum. This determinant represents the fermion contribution to the one-loop effective potential of the Polyakov loop. It should become a better approximation as the gauge fluctuations are suppressed, i.e. at high temperature. The behavior of the determinant as a function of \( (P_r, P_i) \) is summarized in Figs.3
to 5 for $m_q = 0$. Increasing the quark mass does not change the qualitative behavior, but only reduces the amount of variation of the determinant.

Figure 3: Isocontour lines for $1/V \log |\det|$ in the toy model.

Fig.3 shows $\frac{1}{V} \log |\det|$, as a function of the Polyakov loop. It is maximum in the free field case $A_0 = 0, P = (3,0)$, in accord with the theorem of E. Seiler [4]. Note that isocontour lines are almost vertical and almost equally spaced, which implies that $\log |\det|$ is almost a linear function of $P_r$ alone: $\frac{1}{V} \log |\det| \sim c(\mu, T, m_q) P_r + c_0$. What is particularly interesting is the variation of the slope $c(\mu, T, m_q)$ with $\mu$ and $T$, since this quantity characterizes the amount by which larger Polyakov loop values $P_r$ are favored, i.e. the ordering effect of the fermion determinant. Fig.4 shows clearly that a similar ordering effect can be achieved by increasing the temperature or the chemical potential.

The oscillatory behavior of the determinant is displayed in Fig.5, which shows the phase $\frac{1}{V} \phi(\det)$, as a function of the Polyakov loop. The isocontour lines correspond to increases of the phase by $2\pi$. They are almost parallel and equally spaced, confirming $\phi(\det) \propto P_i$ in this model. This figure makes it clear how the sign problem occurs: as $V$ increases, the quenched measure $\exp(-S_q)$ allows for fluctuations in $P_i$ of $O(1/\sqrt{V})$, which are sufficient to
Figure 4: Logarithm of the modulus of the determinant for $P_t = 0$ in the toy model: a decrease in temperature (from middle to top curve) can be nicely compensated by an increase in the chemical potential (bottom curve).

Figure 5: Lines where $\phi(\text{det}) = 2k\pi$ in the $(P_r, P_t)$ plane for the toy model, on an $8^3 \times 4$ lattice. The phase is proportional to the lattice volume, so that the lines depicted become denser as the volume increases.
rotate the phase $\phi(\det)$ by $O(\sqrt{V})$, and drive $\langle \cos(\phi(\det)) \rangle$ to zero.

Assume now that the $\mu = 0$ QCD theory admits a deconfinement transition at $T = T_0$, characterized by 2 degenerate minima of the free energy at neighboring (or degenerate) real values $P_1 \leq P_2$ of the Polyakov loop. If the chemical potential $\mu$ is turned on, the fermionic determinant will favor the minimum at $P_2$ because of the ordering effect of $\mu$ (Fig.4). The balance between $P_1$ and $P_2$ can be restored by a compensating decrease in temperature. This is achieved when the derivative $\frac{d}{dP_1} \log(|\det(\mu,T)|)|_{P_1}$ keeps its ($\mu = 0, T = T_0$) value. In this way, a heuristic phase boundary $\mu_c(T)$ can be obtained, as in Fig.6. The phase boundary can be obtained by the same arguments using the continuum expression for the fermion determinant in a gauge field background $A_0$ (Eq. [12] of Ref. [3]). The lines of Fig.6 come out from the continuum expression, and the discrete points from the lattice expression for staggered fermions. The two sets of points correspond to $P_1 = 3$ and $P_1 = 0$, to give some measure of our systematic uncertainties. The phase diagram shows a quadratic dependence of the crit-

![Figure 6: Heuristic phase boundary obtained from the toy model. The lines are derived from the continuum calculation of [3], the data points are obtained from the lattice. The 2 boundaries correspond to different critical values of $P_r$.](image)

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Figure 7: Spectrum of the fermion matrix for \((P_r, P_i) = (0, 0)\) on a \(8^3 \times 4\) lattice, for three values of the chemical potential \(\mu\). Eigenvalues are repelled from the origin as \(\mu\) increases, indicating chiral symmetry restoration.

...ical temperature versus \(\mu\). It even is quantitatively plausible. Nonetheless, several crude approximations have been made: all fluctuations of the gauge field have been ignored except the zero-mode of the Polyakov loop; and the variation of the quenched measure with \(T\) is neglected. The failure of this crude approximation becomes obvious as the temperature is lowered: the critical chemical potential \(\mu_c(T)\) diverges as \(T \rightarrow 0\). Therefore, it is likely that \(\mu_c(T)\) consistently overestimates the true critical \(\mu\).

However, our toy model may still provide some qualitative insight as to what happens at low temperatures. As \(T \rightarrow 0\), the quenched measure for the Polyakov loop becomes Gaussian around the origin: \(\text{Prob}(P) \propto \exp(-cV(P_r^2 + P_i^2))\). On the other hand, note the slight curvature of the contour lines in Fig.3. They indicate that, if \(P_r\) fluctuates little around 0,
log(|det|) increases with |\(P_i|\): the determinant favors large values of \(P_i\), whereas the quenched measure favors small values. The partition function has the form

\[
\int dP_i e^{-cV P_i^2} e^{iV P_i b(\mu) + V d(\mu) P_i^2}
\]

with the first factor coming from the quenched measure, the second one from the fermion determinant. If for some value of \(\mu\), \(d(\mu) = c\), then a phase transition ensues. The major contribution to the partition function, instead of coming from the region \(P_i \sim 0\), will come from the large values of \(P_i\). To support this plausible scenario, Fig. 7 shows the Dirac spectrum in the complex plane for our toy model, at \((P_r, P_i) = (0, 0)\), for increasing values of \(\mu\). As \(\mu\) increases, eigenvalues are repelled from the origin, which would be consistent with \(\langle \bar{\psi} \psi \rangle = 0\) and chiral symmetry restoration at large \(\mu\).

Finally, a remarkable feature of our heuristic phase diagram is that its form remains unchanged for \(SU(2)\). There is no difference at all if one chooses for \(P_1\) its free field value (upper curve in Fig. 6). For any other value the difference between the phase boundary for the \(SU(2)\) and \(SU(3)\) cases is a constant factor. An exact \(SU(2)\) phase diagram should soon be available for comparison, since \(SU(2)\) simulations do not suffer from the sign problem.

### 4 Constrained Monte Carlo

To go beyond our toy model, in \(SU(3)\), one must address the sign problem. We have considered the introduction of a constraint on \(P_i\) in the partition function. Namely we want to study by Monte Carlo the modified partition function

\[
Z' = \int[dU] e^{-S_g(U)} \det^2(U, \mu) \delta(P_i(U))
\]

The benefits are clear: as seen in Section I, the fluctuations in \(\phi(\det)\) will be reduced, especially for heavy quarks. In the same way that the microcanonical and canonical partition functions become equivalent in the thermodynamic limit, the constraint on \(P_i\) becomes irrelevant as \(V \to \infty\), provided \(P_i\) is frozen to its mean value given by the saddle point of its effective potential. However, at finite density, the mean value of \(P_i\) is imaginary, as can be seen from Eq. (3). Therefore, our constraint introduces some systematic error. This can be traced to the following.
The free energy $F_q$ of a single quark at finite $\mu$ is given by the Polyakov loop:

$$e^{-\beta F_q} = \langle \text{Tr} P \rangle = P_r + iP_i$$

(5)

where $P_i$ is pure imaginary. On the other hand, for an antiquark one has

$$e^{-\beta F_{\bar{q}}} = \langle \text{Tr} P^\dagger \rangle = P_r - iP_i$$

(6)

Constraining $P_i = 0$ thus enforces equality of the 2 free energies. This is a good approximation in 2 regimes:
- $|P_r| \ll |P_i|$, i.e. high temperature or small chemical potential;
- $|P_r| = |P_i| = 0$, i.e. zero temperature, for any $\mu < \mu_c$.

This second regime is particularly interesting and difficult to investigate.

To test our ideas, we have implemented a constrained Hybrid Monte Carlo algorithm, and performed quenched $SU(3)$ simulations, measuring the average “sign” $\langle \cos(\phi(\det)) \rangle$ with and without the constraint $P_i = 0$. Fig.8
shows our results as a function of the quark mass, for chemical potential \( \mu = 1.5 \) in lattice units, at \( T \sim 0 \). The relative error on \( \langle \cos(\phi(\text{det})) \rangle \), which propagates to all observables, is reduced by over an order of magnitude as one approaches the phase transition.

5 Conclusion

We have exhibited the strong correlation present in static QCD between the phase of the fermion determinant and the imaginary part of the Polyakov loop. This correlation motivated us to study a toy model which keeps the zero-mode of the Polyakov loop as the only degree of freedom. This toy model clearly shows the ordering effect of the chemical potential and the oscillations of the fermionic measure. A heuristic phase diagram can be obtained, and a mechanism for a \( T = 0 \) phase transition suggests itself. Finally, constrained Monte Carlo simulations where the imaginary part of the Polyakov loop is fixed to zero provide an important reduction of the sign problem, and allow to go beyond static QCD.

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References

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