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On complex Langevin dynamics and zeroes of the measure II: Fermionic determinant

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Lattice QCD at non-vanishing chemical potential is studied using the complex Langevin equation (CLE). One of the conditions for the correctness of the results of the CLE is that the zeroes of the measure coming from the fermionic determinant are outside of the distribution of the configurations, or at least in a region where support for the distribution is very much suppressed. We investigate this issue for Heavy Dense QCD (HDQCD) and full QCD at high temperatures. In HDQCD it is found that the configurations move closest to the zeroes of the measure around the critical chemical potential of the onset transition, where the sign problem is diminished, but results remain largely unaffected. In full QCD at high temperatures the investigation of the spectrum of the Dirac operator yields a similar observation: the results are unaffected by the issue of the poles.

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1. Introduction

At nonzero baryon chemical potential, QCD suffers from the sign problem which invalidates naive importance sampling simulations [1]. The Complex Langevin Equation (CLE) was proposed to circumvent the sign problem by complexifying the field manifold of the theory [2]. In the past few years the method has been the focus of renewed attention [3, 4, 5, 6] (see further references in [1, 7]). In particular with the introduction of gauge cooling [8] it has become possible to simulate gauge theories as well, such as heavy dense QCD (HDQCD) [8, 9] and full QCD using light quark flavors [10, 11].

In fermionic theories the action includes a non-holomorphic term (the logarithm of the fermionic determinant) which might cause problems [5]. Here we investigate this issue for lattice models. The presentation is based on [12] and is accompanied by [13] where the theoretical background is discussed in more detail and toy models are investigated.

2. CLE and poles

Consider a theory with measure $\rho(x)$ where x stands for all the degrees of freedom of the theory. Typically one has $\rho(x) = e^{-S(x)} \det M(x)$ with the action $S(x)$ and the determinant of the Dirac matrix $M(x)$. The Langevin equation is then written as

$$\frac{\partial x}{\partial \tau} = K(x) + \eta(\tau) \qquad\qquad K(x) = \rho'(x)/\rho(x) \tag{2.1}$$

with the Langevin time τ, delta correlated Gaussian noise $\eta(\tau)$, and the drift term $K(z)$. (For curved manifolds such as the $SU(3)$ group space this equation has to be appropriately modified, see e.g. [3].) For complex measures the manifold of x is complexified, for example in QCD SU(3) is extended into SL(3,$\mathbb{C}$).

Note that $K(z)$ has a singularity where the measure vanishes. This in turn invalidates the proof of correctness, which requires fast decay of the distributions of the fields on the complexified manifold as well as holomorphic drift terms (and thus also action) on the whole complex plane [14]. In [12, 13] it is shown that the proof still holds as long as the zeroes of the measure are outside of the support of the distribution of x on the complexified manifold. In the case where the zeroes are inside the distribution one typically observes a 'bottleneck' phenomenon where the zeroes connect two disjoint regions of the configuration space visited during the Langevin process.

3. Heavy Dense QCD

HDQCD is defined as the double limit $\kappa \to 0$ and $\mu \to \infty$ while keeping κe^{μ} fixed [15]. For symmetry we keep terms proportional to $\kappa e^{-\mu}$. The fermionic determinant then simplifies to

$$\det M = \prod_{\mathbf{x}} \det\left(1 + h e^{\mu/T} \mathscr{P}_{\mathbf{x}}\right)^{2N_f} \det\left(1 + h e^{-\mu/T} \mathscr{P}_{\mathbf{x}}^{-1}\right)^{2N_f} \tag{3.1}$$

for N_f fermionic flavors, using the Polyakov loop $\mathscr{P}_{\mathbf{x}}$ and $h = (2\kappa)^{N_\tau}$.

This theory has been studied extensively for the justification of the CLE approach by comparing to reweighting [8], and the phase diagram has been mapped out in [9].

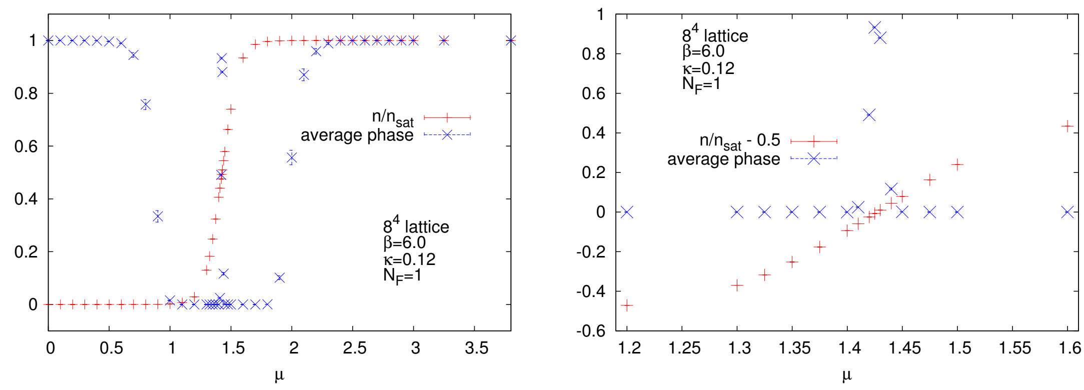

Figure 1: Left: fermionic density in units of the saturation density, n/n_{sat}, and average phase factor, see Eq. (3.3), as a function of the chemical potential. Right: a blow-up around onset.

The quark density in HDQCD at low temperatures shows a Silver-Blaze behavior as expected, with an onset transition at the critical chemical potential

$$\mu_c = -\ln(2\kappa), \tag{3.2}$$

and eventually saturating at the value $n_{\text{sat}} = 6N_f$. At higher temperatures this behavior is somewhat smoothened, with roughly constant critical chemical potential up to moderate temperatures [9]. In Fig. 1 the quark density is shown in units of saturation density, for $\kappa = 0.12, N_f = 1, \beta = 6.0$ on a 8^4 lattice, with $\mu_c = -\ln(2\kappa) \approx 1.427$. Using $[\det M(\mu)]^* = \det M(-\mu^*)$ we also measure the average phase factor in the full theory using the analytic observable

$$\langle e^{2i\varphi} \rangle = \left\langle \frac{\det M(\mu)}{\det M(-\mu)} \right\rangle, \tag{3.3}$$

see also Fig. 1. One notes a severe sign problem except in the initial zero density phase as well as in saturation and a peak in the middle. At the critical chemical potential, the fermions are at 'half-filling', i.e. half of the available fermionic states are filled, and the theory becomes particle-hole symmetric [16]. Exactly at μ_c, the sign problem becomes very mild, as the first factor in Eq. (3.1) becomes real. The sign problem due to the second factor is mild, since $(2\kappa e^{-\mu})^{2N_\tau} \ll 1$.

To investigate the density of configurations around the zeroes of the measure we investigated the spatially local factors in the fermionic determinant, namely

$$\begin{aligned} \det M_{\mathbf{x}} &= \det\left(1 + he^{\mu/T}\mathscr{P}_{\mathbf{x}}\right) \det\left(1 + he^{-\mu/T}\mathscr{P}_{\mathbf{x}}^{-1}\right) \\ &= \left(1 + 3zP_{\mathbf{x}} + 3z^2P_{\mathbf{x}}^{-1} + z^3\right)\left(1 + 3\bar{z}P_{\mathbf{x}}^{-1} + 3\bar{z}^2P_{\mathbf{x}} + \bar{z}^3\right), \end{aligned} \tag{3.4}$$

with $z = he^{\mu/T}, \bar{z} = he^{-\mu/T}$. We find that the determinants largely avoid the zeroes of the measure, except close to the critical chemical potential. In Fig. 2 we show the histogram of the absolute values of the determinants for two different lattice sizes. Far from μ_c one observes that the zero is far from the distribution. Around the critical chemical potential one observes a power law dependence of the histogram on the distance from the origin $P \sim |\det M|^\alpha$ with an exponent $\alpha = 1.5 - 1.6$. It

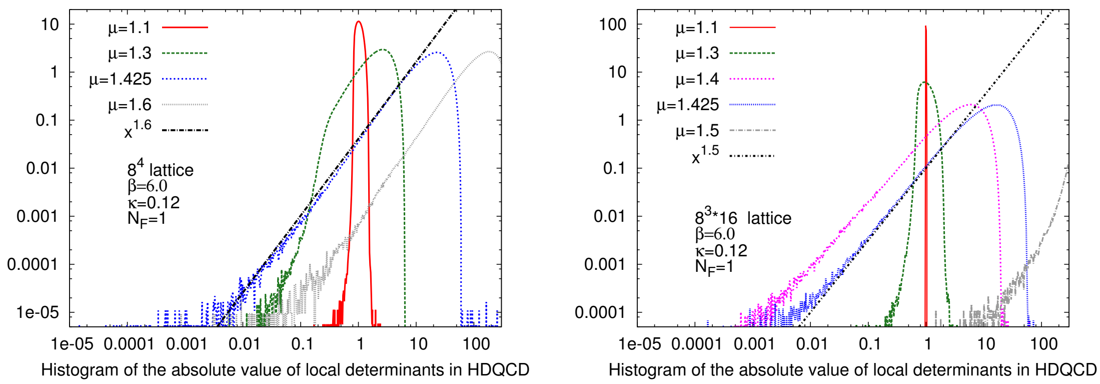

Figure 2: The histogram of the absolute value of the local determinant factors (3.4).

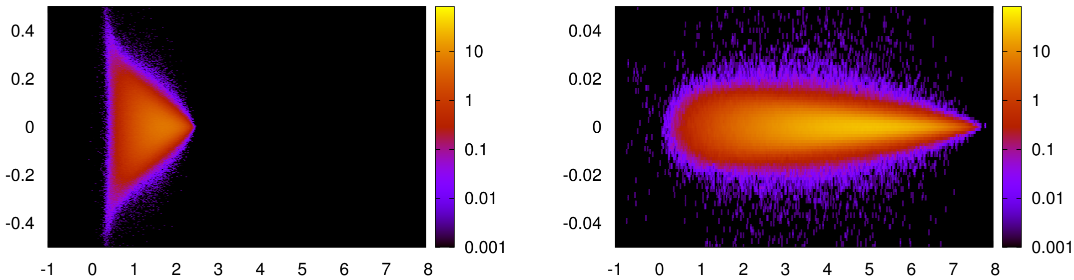

Figure 3: The histogram of the absolute value of the local determinant factors (3.4).

is interesting to note that in the histogram of Φ, the phases of the local determinants also show a power law behavior around μ_c with the dependence $P \sim 1/\Phi^3$. The phase of the total determinant is the sum of $2N_f N_s^3$ phases, and will therefore show large fluctuations as the volume increases. In Fig. 3 we show the distribution of the local determinant factors on the complex plane. Comparing with results of various toy models, we do not observe disconnected regions separated by the singular point which would signal incorrect results. In particular in a one plaquette model with the same determinant factor in the measure, the bad behavior is signaled by 'whiskers' in the histograms [12, 13], which appear here only barely visible, if at all.

To summarize, in HDQCD we see that far from the critical chemical potential, where the sign problem is severe, we see no issue from the poles. Curiously, near μ_c where the sign problem is mild, the distribution of the configurations gets closest to the zeroes, but for the parameters used here we see no sign of problematic disconnected regions in the observables suggesting that the effect of the non-analyticity is very small.

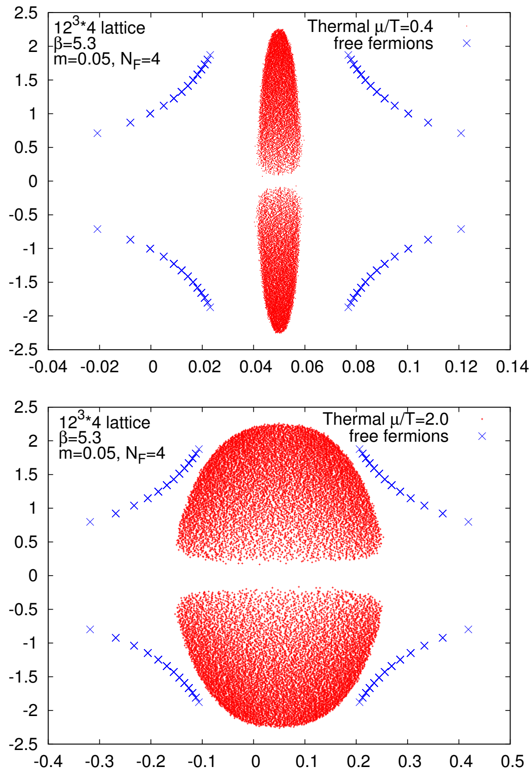

Figure 4: The spectrum of the staggered Dirac operator in full QCD for various chemical potentials. The spectrum of the free staggered Dirac operator is also shown.

4. Full QCD

Finally we investigate the issue of poles for full QCD in the staggered formulation using $N_f = 4$, i.e. not using the rooting procedure to further reduce the number of flavors described by the Dirac operator. Several observations show that at high temperatures (above the deconfinement transition) the CLE is unaffected by the presence of zeroes in the measure: comparisons with systematic hopping expansions using a holomorphic formulation [11], comparisons with reweighting [6], and observations of the spectra of the complexified Dirac operator [7, 12].

In full QCD the determinant can be written as the product of the eigenvalues of the Dirac matrix, and thus the fermionic force is written as $K(U) = \sum_i D\lambda_i(U)/\lambda_i(U)$ with a sum for the eigenvalues $\lambda_i(U)$. Therefore a singularity in the drift term can be traced to a zero eigenvalue of the Dirac matrix. In Fig. 4 we show the spectrum of the complexified Dirac operator on a $12^3 \times 4$ lattice at $\beta = 5.3$ for various chemical potentials for typical configurations taken after sufficient Langevin time has passed to allow for thermalization. One observes that the eigenvalues do not get close to zero. This behavior is also visible on the histogram of the absolute value of the determinants in Fig. 5, where we taken an average of $O(100)$ configurations. Note that this behavior does not mean that the phase of the full determinant remains small. In Fig. 6 we show the histogram of the phase of the determinant for different spatial volumes at quark chemical potentials $\mu/T = 0.4$ and 1.2. Note

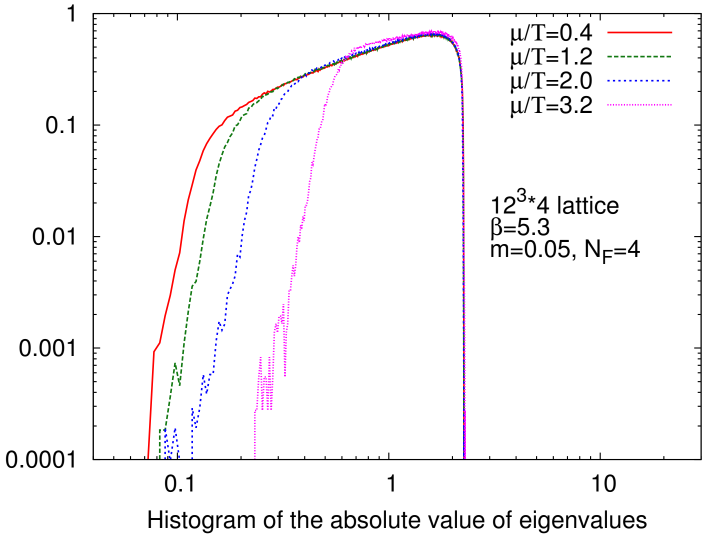

Figure 5: The histogram of the absolute value of the eigenvalues of the staggered Dirac operator in full QCD.

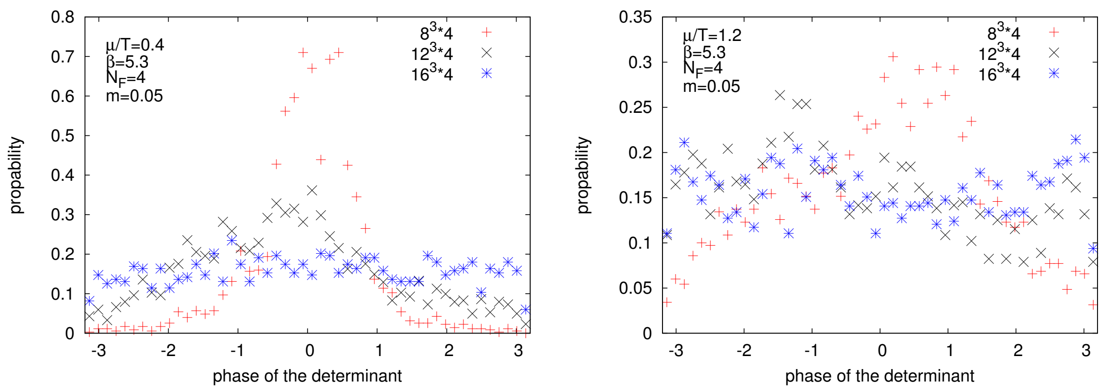

Figure 6: The histogram of the phase of the determinant in full QCD using the staggered formulation.

that even at the smaller μ the phase distribution seems to be flat at $N = 16$, making reweighting very hard. This behavior is expected as the sign average vanishes exponentially fast with the volume.

It is an open question whether at low temperature the zeroes of the measure affect the CLE results, as simulations are more expensive due to the larger lattices required there as the gauge cooling is ineffective on coarse lattices.

5. Summary

We have investigated the issue of the zeroes of the measure in the CLE solution for non-zero density theories HDQCD and full QCD. The proof of correctness still holds as long as the singularity of the drift is outside of the distribution of the configurations. By numerical simulations we have shown that in HDQCD there is potentially a problem around the critical chemical potential of the onset transition but further study shows that the effect seems to be very small. In full QCD at high temperatures we have studied the spectrum of the theory and shown that the eigenvalues of the Dirac matrix remain well separated from the origin for all chemical potentials.

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