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Complex Langevin for Lattice QCD at $T = 0$ and $\mu \geq 0$.

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QCD at finite quark-/baryon-number density, which describes nuclear matter, has a sign problem which prevents direct application of standard simulation methods based on importance sampling. When such finite density is implemented by the introduction of a quark-number chemical potential μ, this manifests itself as a complex fermion determinant. We apply simulations using the Complex Langevin Equation (CLE) which can be applied in such cases. However, this is not guaranteed to give correct results, so that extensive tests are required. In addition, gauge cooling is required to prevent runaway behaviour. We test these methods on 2-flavour lattice QCD at zero temperature on a small (12^4) lattice at an intermediate coupling $\beta = 6/g^2 = 5.6$ and relatively small quark mass $m = 0.025$, over a range of μ values from 0 to saturation. While this appears to show the correct phase structure with a phase transition at $\mu \approx m_N/3$ and a saturation density of 3 at large μ, the observables show departures from known values at small μ. We are now running on a larger lattice (16^4) at weaker coupling $\beta = 5.7$. At $\mu = 0$ this significantly improves agreement between measured observables and known values, and there is some indication that this continues to small μs. This leads one to hope that the CLE might produce correct results in the weak-coupling – continuum – limit.

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1. Introduction

QCD at a non-zero quark-number chemical potential μ has a complex fermion determinant. Hence standard lattice-gauge-theory simulation methods, which are based on importance sampling, cannot be applied directly. However, the Langevin Equation does not rely on importance sampling, and can be adapted to complex actions by replacing real fields by complex fields [1, 2, 3, 4]. For lattice QCD at finite μ, this means promoting the $SU(3)$ gauge fields to $SL(3,C)$.

Early attempts to simulate lattice QCD at finite μ using the Complex Langevin Equation (CLE) were frustrated by runaway solutions which are possible because $SL(3,C)$ is non-compact. Recently it was realized that at least part of the reason why this occurs is that the CLE dynamics has no resistance to the production of unbounded fields which are unbounded gauge transformations of bounded fields. This has led to the concept of 'gauge cooling', gauge transforming configurations to keep them as close as possible to the $SU(3)$ manifold [5]. The CLE with gauge cooling has been applied to QCD at finite μ at large quark mass [6, 7, 8, 9, 10] and with smaller quark masses on small lattices [11] and more recently to QCD at finite temperature and μ [12]. At weak enough couplings these simulations are in agreement with results obtained using other methods.

Even when the CLE converges to a limiting distribution, it is not guaranteed to produce correct values for the observables unless certain conditions are satisfied [13, 14, 15, 16]. The reason one needs to check the validity of the CLE for QCD is to first check the requirement that the gauge fields evolve over a bounded region, which appears to be true. Secondly, the CLE can only be shown to converge to the correct distribution if the 'drift terms' – the derivatives of the (effective) action with respect to the fields – are holomorphic functions of the fields. Because the fermion determinant has zeros, the drift term is only meromorphic in the fields. Hence the CLE will only give correct results if the contribution of the poles in the drift term are negligible. Those of the above mentioned papers, which perform CLE simulations of QCD at finite μ, provide tests of the range of validity of the method.

Recent work reported by Aarts [17] and by Stamatescu [18] presents methods of determining when poles in the drift term of the CLE are likely to produce incorrect results. Studies using random-matrix theory indicate the range of validity of the CLE and suggest modifications of gauge cooling which can extend this range [19, 20]. There is also recent work which suggests other criteria for determining when the CLE will produce correct results and when it will fail [21]. Other studies indicate how the introduction of irrelevant terms to the drift term can direct the CLE to converge to correct limiting distributions [22].

We simulate lattice QCD at zero temperature and finite μ on a 12^4 lattice at $\beta = 6/g^2 = 5.6$ and $m = 0.025$. For these parameters the expected position of the transition from hadronic to nuclear matter at $\mu \approx m_N/3 \approx 0.33$ is well separated from any false transition at $\mu \approx m_\pi/2 \approx 0.21$. We observe that our results are consistent with a transition at $\mu \approx m_N/3$, but not with the expectation that observables will be fixed at their $\mu = 0$ values for $\mu < m_N/3$. At large enough μ the quark number density does saturate at 3 as expected. Very preliminary results of these simulations were reported at Lattice 2015 [23].

We are now simulating on a 16^4 lattice at weaker coupling, $\beta = 5.7$, and $m = 0.025$. At $\mu = 0$ we find that the observables are in far better agreement with known results than for $\beta = 5.6$. We are now moving to $\mu > 0$. We see preliminary indications that for small μ, the observables are still in better agreement with known results than was true at $\beta = 5.6$. This leads us to hope that the CLE will converge to the correct distributions in the continuum – weak coupling – limit.

2. Complex Langevin Equation for finite density Lattice QCD

If $S(U)$ is the gauge action after integrating out the quark fields, the Langevin equation for the evolution of the gauge fields U in Langevin time t is:

$$-i\left(\frac{d}{dt}U_l\right)U_l^{-1} = -i\frac{\delta}{\delta U_l}S(U) + \eta_l \tag{2.1}$$

where l labels the links of the lattice, and $\eta_l = \eta_l^a \lambda^a$. Here λ_a are the Gell-Mann matrices for $SU(3)$. $\eta_l^a(t)$ are Gaussian-distributed random numbers normalized so that:

$$\langle \eta_l^a(t)\eta_{l'}^b(t')\rangle = \delta^{ab}\delta_{ll'}\delta(t-t') \tag{2.2}$$

The complex-Langevin equation has the same form except that the Us are now in $SL(3,C)$. S, now $S(U,\mu)$ is

$$S(U,\mu) = \beta\sum_{\square}\left\{1 - \frac{1}{6}\mathrm{Tr}[UUUU + (UUUU)^{-1}]\right\} - \frac{N_f}{4}\mathrm{Tr}\{\ln[M(U,\mu)]\} \tag{2.3}$$

where $M(U,\mu)$ is the staggered Dirac operator. Note: backward links are represented by U^{-1} not $U^{\dagger}$. Note also that we have chosen to keep the noise-vector η real. η is gauge-covariant under $SU(3)$, but not under $SL(3,C)$. This means that gauge-cooling is non-trivial. Reference [15] indicates why this is not expected to change the physics. After taking $-i\delta S(U,\mu)/\delta U_l$, the cyclic properties of the trace are used to rearrange the fermion term so that it remains real for $\mu = 0$ even after replacing the trace by a stochastic estimator.

To simulate the time evolution of the gauge fields we use the partial second-order formalism of Fukugita, Oyanagi and Ukawa. [24, 25, 26]

After each update, we gauge-fix iteratively to a gauge which minimizes the unitarity norm – gauge cooling [5]:

$$F(U) = \frac{1}{4V}\sum_l \mathrm{Tr}\left[U_l^{\dagger}U_l + (U_l^{\dagger}U_l)^{-1} - 2\right] \geq 0, \tag{2.4}$$

where V is the space-time volume of the lattice.

3. Zero temperature simulations on a 12^4 lattice

We simulate lattice QCD with 2 flavours of staggered quarks at finite μ on a 12^4 lattice with $\beta = 5.6$ and quark mass $m = 0.025$, using the CLE with gauge cooling. μ is in the range $0 \leq \mu \leq 1.5$ which includes the expected phase transition at $\mu \approx m_N/3 \approx 0.33$ and that of the phase-quenched theory at $\mu \approx m_\pi/2 \approx 0.21$. ($m_N$ and m_π are from the HEMCGC collaboration [27, 28, 29]). The upper limit $\mu = 1.5$ lies well within the saturation regime where each lattice site is occupied by one quark of each colour.

We simulate for 1–3 million updates of the gauge fields at each μ value. The input updating increment $dt = 0.01$. Since we use adaptive rescaling of dt to control the size of the drift term, the actual dts used in the updates are considerably smaller than this. The length of the equilibrated part of the run at each β then lies in the range 100–1000 langevin time units. We record the plaquette (action), the chiral condensate and the quark-number density every 100 updates, and the unitarity norm after each update.

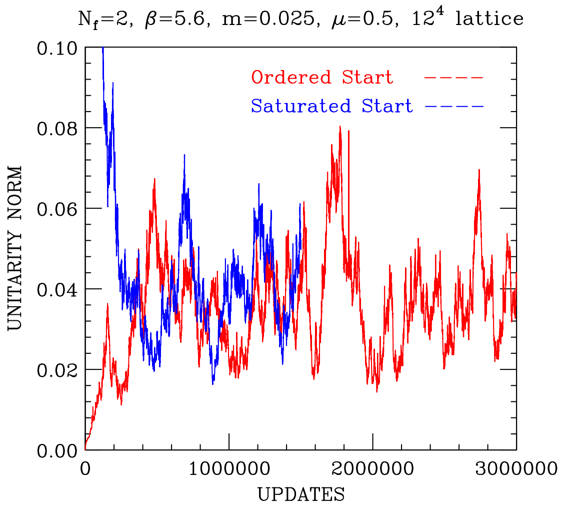

Figure 1: Unitarity norms for $\mu = 0.5$ on a 12^4 lattice. The red curve is for the run starting from an ordered start. The blue curve is for the run starting from a $\mu = 1.5$ configuration.

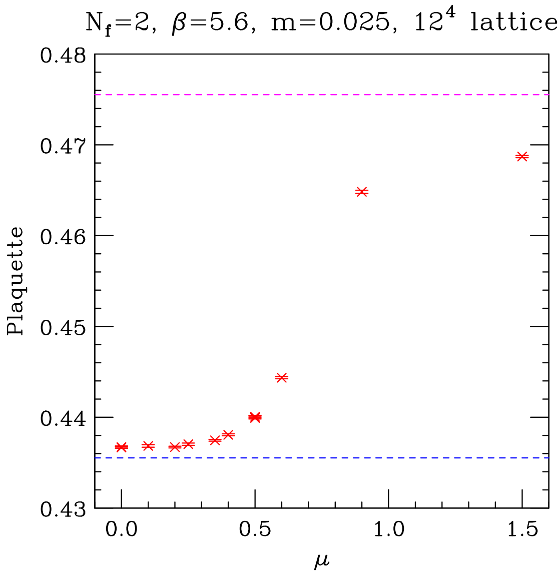

Figure 2: Plaquette as a function of μ. Dashed lines are the correct value at $\mu = 0$ and the quenched value.

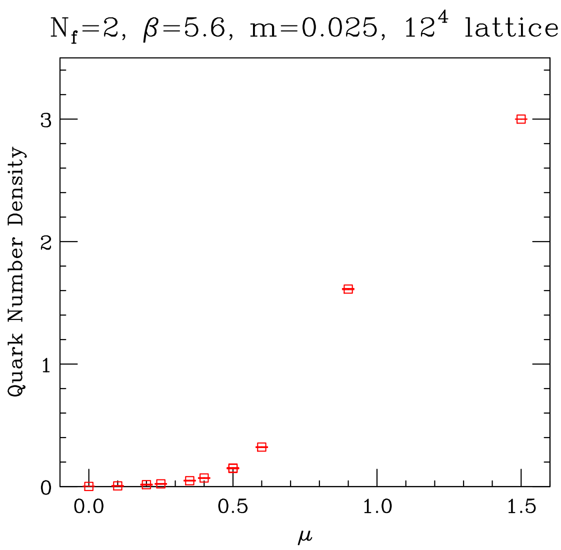

Figure 3: Quark number density, normalized to one staggered quark (4-flavours), as a function of μ.

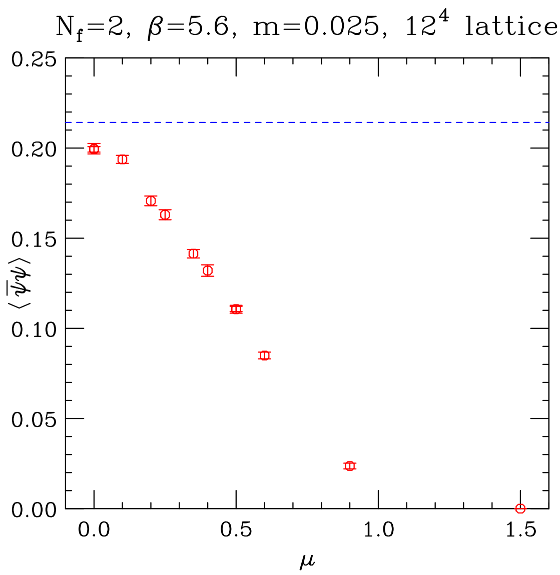

Figure 4: Chiral condensate, normalized to one staggered quark (4-flavours), as a function of μ. Dashed line is the correct value at $\mu = 0$.

At each μ we observe that the unitarity norm appears to evolve over a compact domain, which is one of the requirements for the CLE observables to have a well-defined limit. It is also a necessary but not sufficient condition for it to produce correct results. At $\mu = 0$ and $\mu = 0.5$ we have produced trajectories from both an ordered start and starting from an equilibrated configuration at $\mu = 1.5$. In both cases, it appears that the compact domain is independent of the start, as are the average observables. Figure 1 shows the evolution of the unitary norms at $\mu = 0.5$ from the 2 different starts. It is interesting to note that the unitarity norm has a minimum somewhere in the range $0.35 \leq \mu \leq 0.9$. Does this mean that the CLE produces correct results for μ sufficiently large?

Figure 2 shows the plaquette as a function of μ from these runs. We note that there is a very small but significant difference between the value at $\mu = 0$ and the correct value obtained from an RHMC simulation. The real Langevin equation yields a value significantly closer to the correct value, so this deviation is not due solely to the inexact nature of the Langevin method. For $\mu \leq 0.25$, the plaquette appears to be (almost) independent of μ as expected. For $\mu \geq 0.35$ the plaquette increases with μ up until saturation.

Figure 3 shows the quark-number density as a function of μ. For $\mu \leq 0.25$ this number density is small – it is expected to be zero. For $\mu \geq 0.35$ this number density increases, reaching the saturation value of 3 (3 quarks of different colours at each site), for large μ. We note, however, that this density does not appear to show an abrupt increase at the transition as might be expected for a first-order phase transition.

In figure 4 we plot the chiral condensate ($\langle\bar{\psi}\psi\rangle$) as a function of μ. At $\mu = 0$ it already lies appreciably below the exact value. Instead of remaining constant up to the phase transition to nuclear matter as expected , it starts to fall monotonically once $\mu > 0$, finally reaching the expected value of zero at saturation.

Hence for $\beta = 5.6$, $m = 0.025$ on a 12^4 lattice, the CLE appears to produce the correct phase structure, although the phase transition at $\mu \approx m_N/3$ does not show any evidence for its expected first-order behaviour. The plaquette shows small deviations from the correct values for small μ as does the quark-number density. The chiral condensate shows larger departures from its expected behaviour.

4. Zero temperature simulations on a 16^4 lattice

We are now running CLE simulations on a 16^4 lattice. At $\beta = 5.6$, $m = 0.025$, comparison with our 12^4 runs indicates that finite size effects are small as are finite dt errors.

This larger lattice allows us to run at weaker coupling. We are now running at $\beta = 5.7$, $m = 0.025$. For our $\beta = 5.6$, $m = 0.025$ runs at $\mu = 0$, the CLE measured plaquette value is $0.43690(6)$ compared with the RHMC value $0.43552(2)$, while the chiral condensate is $0.1974(7)$ compared with $0.2142(8)$ for the RHMC. At $\beta = 5.7$, $m = 0.025$, the CLE measured plaquette value is $0.42374(4)$ compared with the RHMC value $0.42305(1)$, so the systematic error has been reduced by roughly a factor of 2. For the chiral condensate the CLE value is $0.1738(11)$ compared with the RHMC value of $0.1754(2)$, almost an order of magnitude improvement. This gives us some hope that the CLE will give correct values for observables in the weak-coupling (continuum) limit. We are now extending these $\beta = 5.7$, $m = 0.025$ simulations to non-zero μ.

5. Discussion, Conclusions and Future Directions

We simulate 2-flavour Lattice QCD at finite μ on a 12^4 lattice at $\beta = 5.6$, and light quark mass $m = 0.025$ using the CLE with gauge cooling. We see indications of the expected phase transition from hadronic to nuclear matter at $\mu \approx m_N/3$, and the passage to saturation at large μ. There are, however, systematic departures from known and expected results. At $\mu = 0$ the plaquette and chiral condensates disagree with known results. For the plaquette the systematic error is very small and for $\mu < m_N/3$ the plaquette is almost independent of μ as expected. At small μ, the chiral condensate decreases with increasing μ rather than remaining constant. These do not appear to be a finite-size effects. The reason for these systematic errors is presumably because zeros of the fermion determinant produce poles in the drift term, which prevent it from being holomorphic in the fields, a requirement for proving the validity of the CLE. These zeros also produce poles in the chiral condensate, which could explain why it shows larger departures from expected values than do other observables.

We are extending our simulations to 16^4 lattices. In addition to showing that finite size (and finite dt) effects are small, these allow us to simulate at smaller coupling, $\beta = 5.7$. Here, simulations at $\mu = 0$ show that systematic errors are significantly reduced. This leads to the hope that, in the weak coupling (continuum) limit, the CLE might yield correct results (after continuing to $dt = 0$). Preliminary results from simulations with $\mu > 0$ look promising.

Modifications to the CLE designed to reduce failures of the method need to be pursued. These include modifications to gauge cooling [19], and modifications to the dynamics by the introduction of irrelevant operators either to the action or to the drift term directly [22].

We plan to extend our zero-temperature simulations to smaller quark masses. Finite temperature simulations are also planned.

Once it is known that the CLE is generating correct results, we will study the high-μ phase for signs of colour superconductivity. This will also require simulations for $N_f = 3$ and $N_f = 2+1$. At finite temperature we will search for the critical endpoint.

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