Exploring Complex-Langevin Methods for Finite-Density QCD

D. K. Sinclair and J. B. Kogut

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Introduction

QCD at a finite chemical potential μ for quark number has a complex action which prevents the direct application of simulation methods based on importance sampling.

The Langevin equation is a stochastic differential equation for the evolution of the classical fields in a fictitious time, which does not rely on importance sampling.

The Langevin equation can be extended to complex actions by complexifying the fields. In the case of QCD this means extending the gauge fields from $SU(3)$ to $SL(3,C)$.

Unfortunately, there is no proof that the long-time evolution of the fields under this Complex Langevin equation (CLE) provides a limiting value for observables. Even when this process does converge, the values it provides for observables are not guaranteed to be correct.

Early attempts at applying the CLE to QCD were stymied by runaway behaviour.

Recently it has been noted that at least some of this undesirable behaviour is due to the production of unbounded gauge transformations of compact gauge fields.

Such behaviour can be controlled by gauge transforming to a gauge which minimizes the magnitudes of the gauge fields – Gauge Cooling.

This has revived interest in the CLE for QCD at finite μ.

We are simulating QCD at zero temperature and finite μ for light quarks using the CLE, to test directly if it converges and produces believable results.

We present very preliminary results of our explorations.

Complex Langevin 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:

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

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:

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

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

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

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 term η real.

To simulate the time evolution of the gauge fields we use the partial second-order formalism of Fukugita, Oyanagi and Ukawa. For an update of the fields by a 'time' increment dt, this gives:

$$U^{(n+1/2)} = e^{X_0} U^{(n)}$$

$$X_0 = dt \frac{\delta}{\delta U} S(U^{(n)}, \mu) + i\sqrt{dt}\eta^{(n)}$$

$$U^{(n+1)} = e^{\gamma(X_0 + X_1)} U^{(n)}$$

$$X_1 = dt \frac{\delta}{\delta U} S(U^{(n+1/2)}, \mu) + i\sqrt{dt}\eta^{(n)}$$

where $\gamma = \frac{1}{2} + \frac{1}{4}dt$ and the Gaussian noise η is normalized such that:

$$\langle \eta_l^{a(m)} \eta_{l'}^{b(n)} \rangle = \left(1 - \frac{3}{2}dt\right) \delta^{ab} \delta_{ll'} \delta^{mn}$$

To proceed, we replace the spacetime trace with a stochastic es-

timator ξ

$$\mathrm{Tr}\{ln[M(U,\mu)]\} \rightarrow \xi^{\dagger}\{ln[M(U,\mu)]\}\xi \ ,$$

where ξ is a vector over space-time and colour of gaussian random numbers, normalized so that:

$$\langle \xi^{*i(m)}(x)\xi^{j(n)}(y)\rangle = \delta^{ij}\delta_{xy}\delta^{mn}$$

which means, in particular, that the ξs in X_0 and X_1 are independent, unlike the ηs. After performing $\frac{\delta}{\delta U}$ of $ln(M)$ it is useful to rearrange the terms proportional to U and U^{-1} so that this term is antihermitian when $\mu = 0$ and U is unitary. That way, in this special case, the complex Langevin equation becomes the real Langevin equation.

We apply adaptive updating, where if the force term becomes too large, dt is decreased to keep it under control.

After each update, we adaptively gauge fix to the gauge which minimizes the unitarity norm:

$$F(U) = \frac{1}{4V}\sum_{x,\mu} Tr\left[U^{\dagger}U + (U^{\dagger}U)^{-1} - 2\right] \geq 0$$

Zero Temperature Simulations

$\mu = 0$

For $\mu = 0$ and infinite precision, Complex Langevin $\longrightarrow$ Real Langevin.

At 64-bit precision, roundoff allows the gauge fields to move (slowly) off the $SU(3)$ manifold.

For $\beta = 5.2$, $m = 0.05$ on an 8^4 lattice we observe runaway solutions, even after Gauge Cooling!

For $\beta = 5.6$, $m = 0.025$ on a 12^4 lattice without gauge cooling we observe runaway solutions.

With gauge cooling, the trajectory moves slowly off the $SU(3)$ manifold. After 100,000 updates ($dt = 0.01$, $dt_{adaptive} \approx 0.00108$), so trajectory ≈ 108 time units, the unitarity norm $\approx 2.5 \times 10^{-8}$.

This we can probably tolerate, especially since we expect it to improve with weaker couplings and larger lattices.

For this run plaquette $= \mathbf{0.4351(1)}$, RHMC $= \mathbf{0.43588(4)}$, and $\langle \bar{\psi}\psi \rangle = \mathbf{0.208(2)}$, RHMC $\mathbf{0.2142(8)}$. Reasonable agreement for a short run with an inexact algorithm.

Figure 1 shows unitarity norms as functions of update number for runs with and without cooling. This is for 10-step cooling. We tried cooling with 5-, 10-, 20- and 100-step cooling. 10 was best.

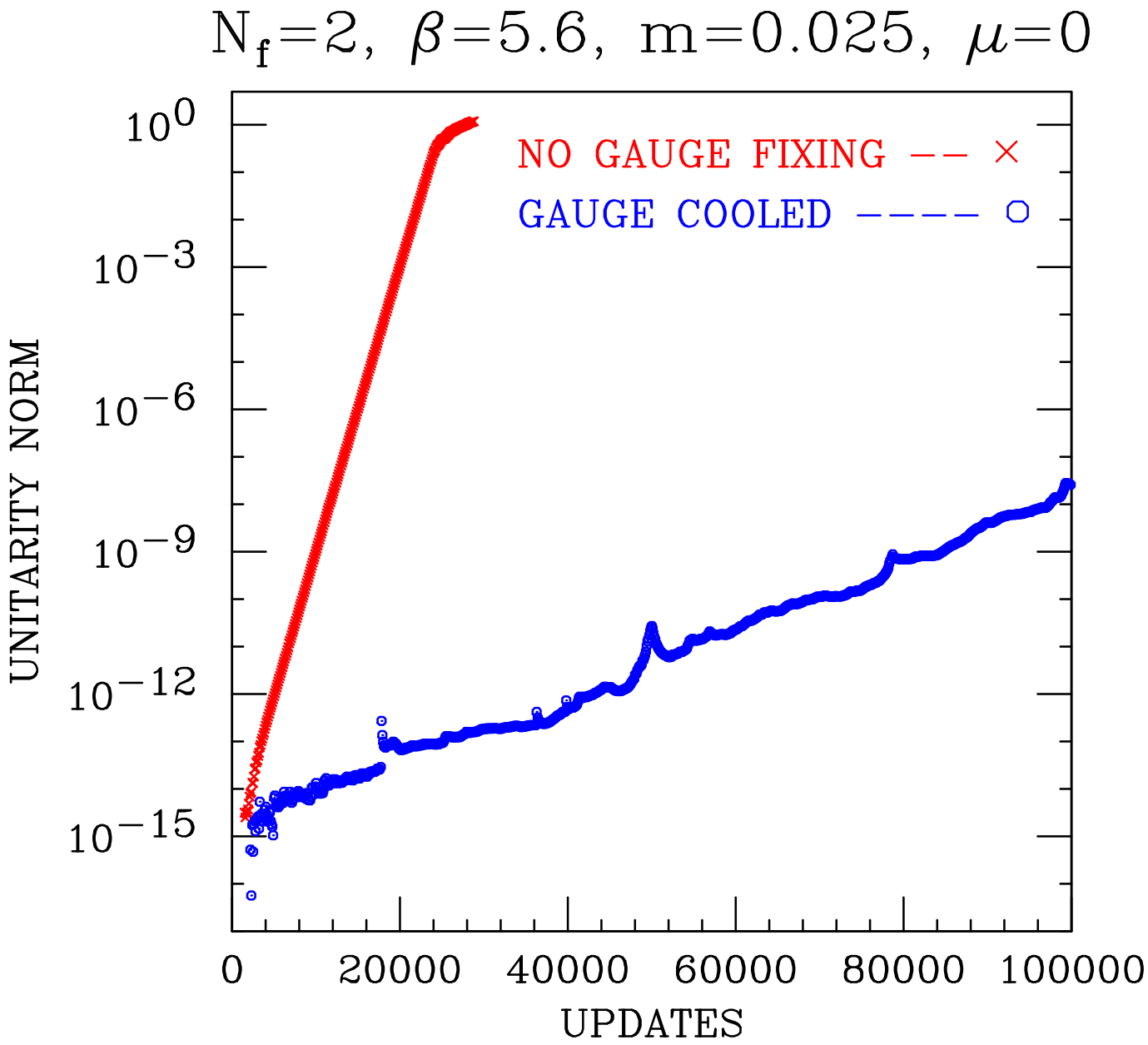

Figure 1: Unitarity norms for runs on a 12^4 lattice. Red curve is for run without gauge cooling. Blue curve is run with 10-step gauge cooling.

$\mu \neq 0$

We simulate on a 12^4 lattice at $\beta = 5.6$, $m = 0.025$ with $\mu > 0$.

Potentially important μ values include $m_\pi/2 \approx 0.21$ and $m_N/3 \approx 0.33$ (masses from HEMCGC collaboration).

We start with a limited number of μ values to probe the various regimes of the zero-temperature phase diagram.

The values we choose are 0.1, 0.2, 0.25, 0.35, 0.5, 0.9 and 1.5. In each case we start the simulation from an ordered start and use a 5-step gauge cool.

The first thing to look for, is evidence that the trajectories for a given set of parameters are restricted to a compact region of the $SL(3, C)$ manifold. Without this it is (almost) impossible for these simulations to produce meaningful results.

If the simulations do converge to a limiting distribution, one must then address the question is whether this is the correct limit.

At $\mu = 1.5$ we have performed sufficient updates for the unitarity norm to level off, indicating that the gauge fields now evolve in a compact domain. The evolution of this norm over the trajectory is shown in figure 2.

The unitarity norm appears to have leveled off, indicating that the system is evolving over a compact domain of $SL(3, C)^{4V}$

The quark number density $j_0 = 2.9999(3)$. Hence the system has reached saturation where $j_0 = 3$, expected for large μ. This is where each site is occupied with 3 quarks in a colour singlet state (nucleon).

The chiral condensate $\langle \bar{\psi}\psi \rangle = 0.2(2) \times 10^{-5}$ – small and consistent with zero as expected.

The plaquette $P = 0.4678(1)$, consistent with the idea that, at saturation, the quarks are frozen out and the system approximates quenched QCD. The quenched plaquette $P = 0.47553(2)$.

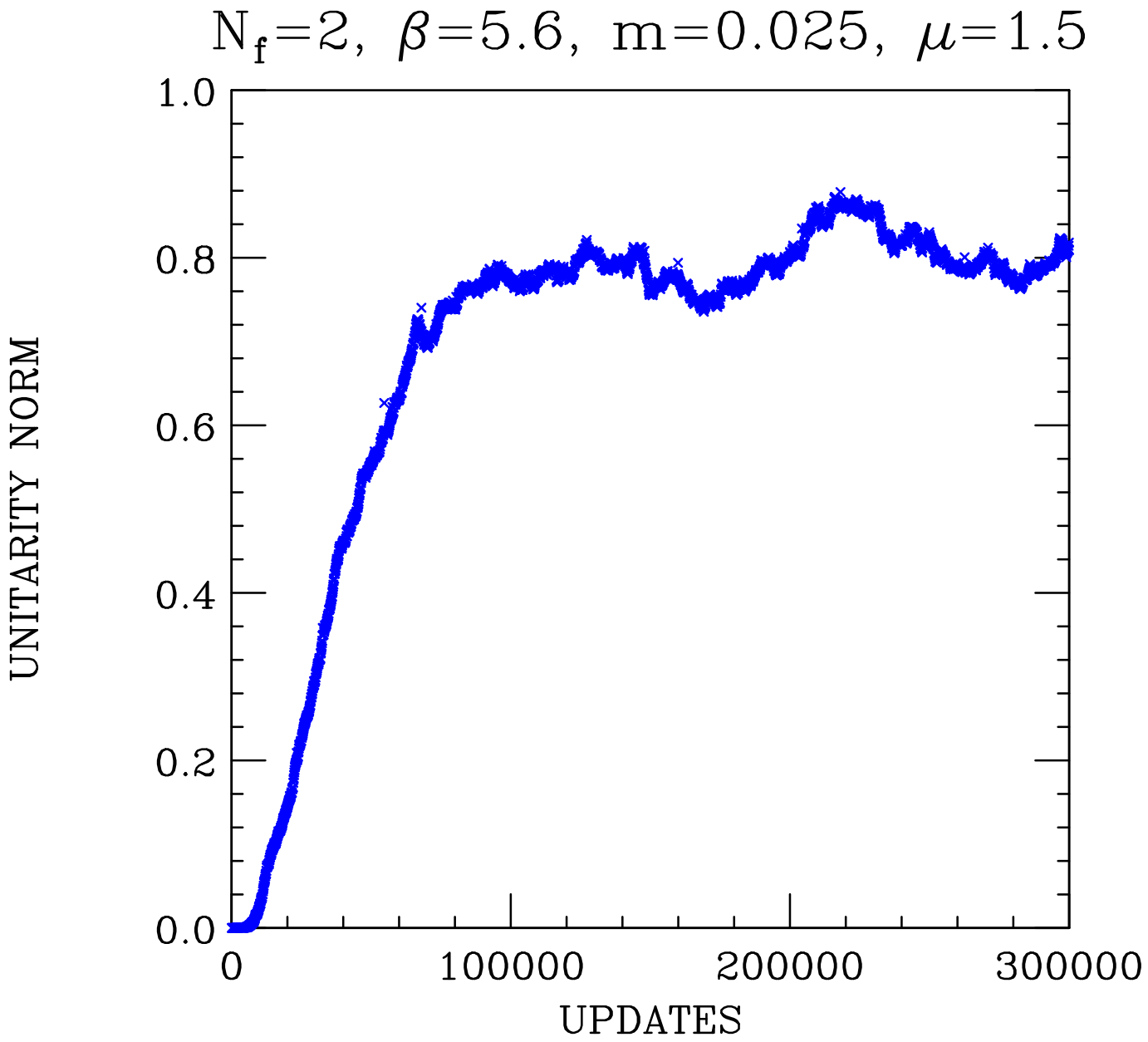

Figure 2: Unitarity norms for run at $\mu = 1.5$ on a 12^4 lattice.

The total trajectory length ≈ 33 time-units. In fact, after equilibration, $dt_{adaptive} \approx 0.000067$.

To date, of the other μ values we are simulating, only $\mu = 0.1$ shows signs of equilibrating. However, we suspect this is because these runs simply need more updates, since their unitarity norms have yet to reach values achieved for the $\mu = 0.1$ simulations.

We present 'data' for the quark-number densities (figure 3), the chiral condensates (figure 4), and the plaquettes (figure 5) as functions of μ with the understanding that these are expected to change to be closer to the values at $\mu = 1.5$ as the system equilibrates (if it does). This is because, as the system equilibrates, the gauge links move away from the $SU(3)$ manifold.

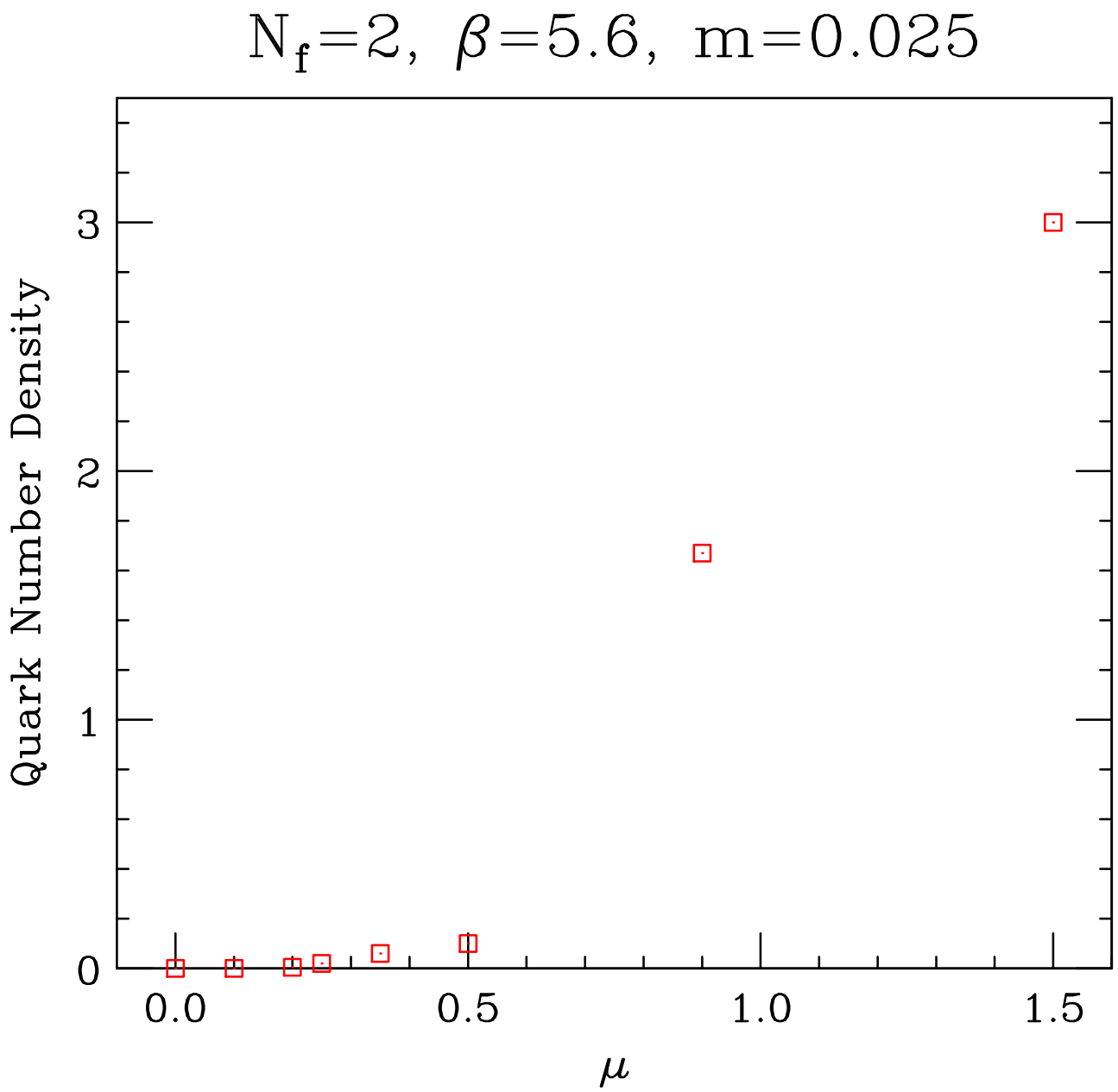

Figure 3: Quark number density as a function of μ. Errors not known.

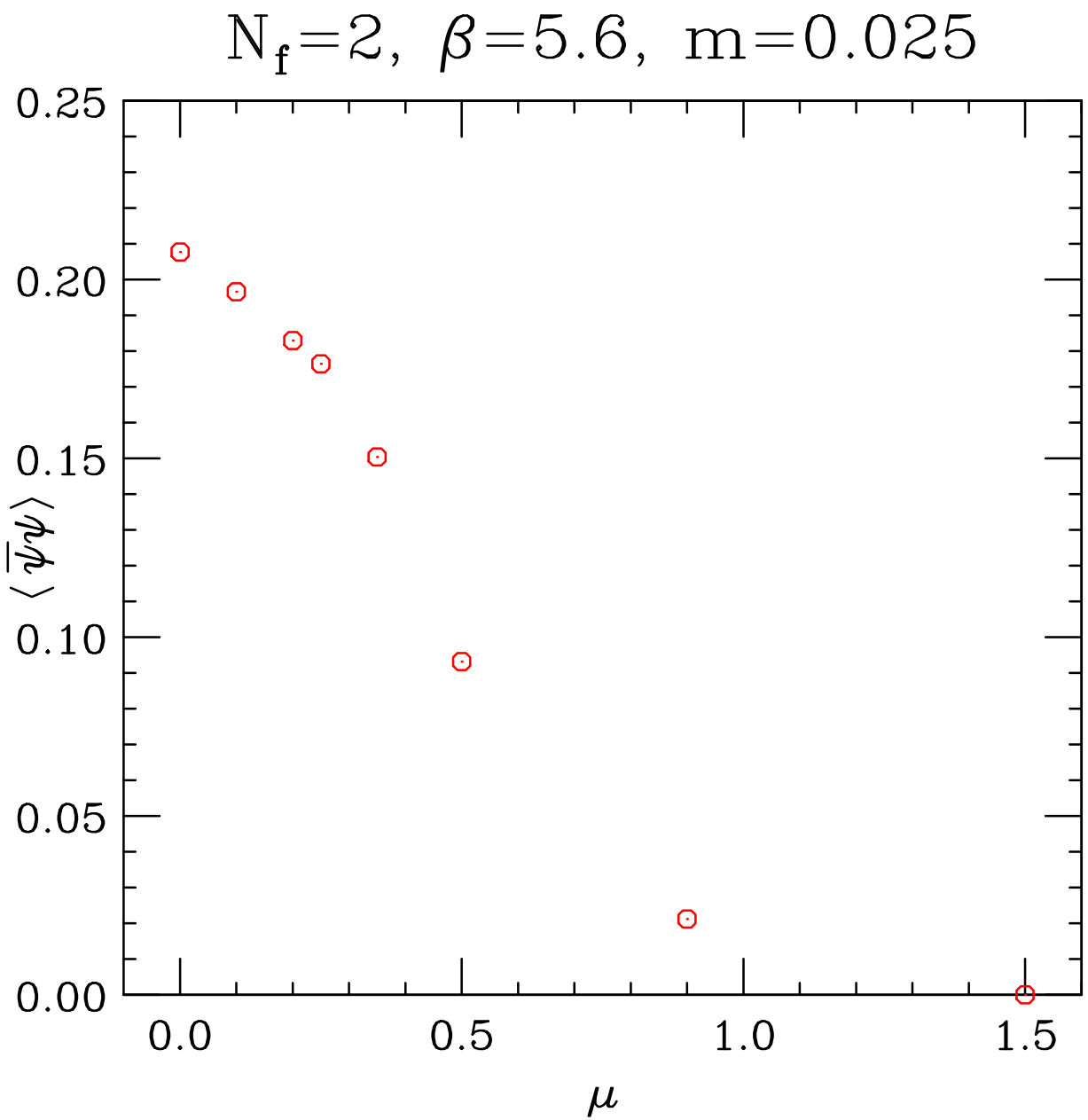

Figure 4: Chiral condensate as a function of μ. Errors not known.

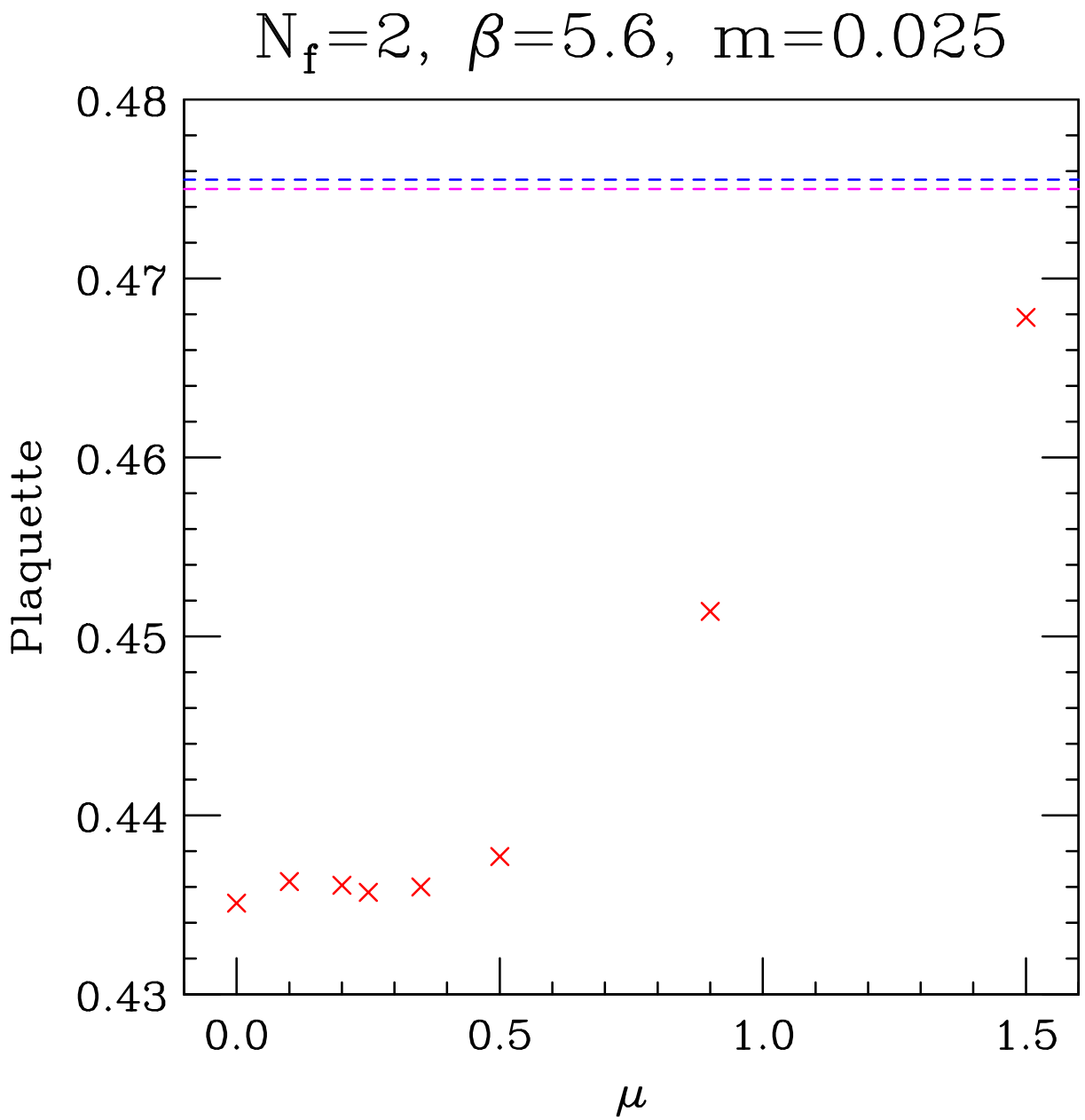

Figure 5: Plaquette as a function of μ. Errors not known. Dashed lines are at quenched value.

These very preliminary results – each point represents 40,000 – 300,000 updates – agree qualitatively with our expectations. We will need to wait until each point has equilibrated to where it is clear that the gauge fields are varying over a compact region in the $SL(3,C)$ manifold, before we can get truly quantitative results. This will probably take longer for $\mu > m_N/3$, since we expect a first-order transition to nuclear matter at $\mu \approx m_N/3$. Since each run is starting from the $SU(3)$ manifold, we expect metastability for $\mu > m_N/3$.

Summary and Future Plans

- We apply Complex-Langevin simulations with gauge cooling to lattice QCD at finite quark-number chemical-potential (μ) at zero temperature.
- Our current simulations are on a 12^4 lattice with $N_f = 2$, $\beta = 5.6$, $m = 0.025$.
- Preliminary results look promising, but more simulations are needed. Adaptive updating with gauge cooling does appear to stabilize the algorithm. Do these simulations converge and converge to the correct limit?
- Do we observe a phase transition to nuclear matter at $\mu \approx m_N/3$?
- Is there a spurious transition at $\mu \approx m_\pi/2$?
- Do these simulations produce the expected 2-flavour colour-superconductor at large μ ($\mu > m_N/3$)?

- Smaller masses needed – $m = 0.01$?. Larger lattices, weaker coupling...
- Current code is inefficient serial code – needs improvement. When we are convinced that the algorithm works we will parallelize our code.
- We will also investigate whether we can make the code fully second-order – the Langevin equivalent of the R algorithm.
- If our 2-flavour simulations are successful, we will also simulate $N_f = 3$ and try to observe the 3-flavour colour-superconductor with its colour-flavour locking.
- We also plan to simulate at high temperature, near the finite-temperature phase transition, and look for the critical endpoint. How good is the resonance-gas model?

I apologize for not listing those people who have contributed to the renewed interest in Complex Langevin methods for QCD at finite μ. You can be certain that their work will be referenced in the writeup.

These simulations are being performed on PCs belonging to Argonne's HEP Division, Edison and Carver at NERSC, and Blues at LCRC Argonne.