Applying Complex Langevin to Lattice QCD at finite μ

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Introduction

QCD at finite chemical potential μ for quark-number density has a complex fermion determinant preventing direct application of standard simulation methods based on importance sampling. A promising method which does not use importance sampling is the complex Langevin equation (CLE).

The CLE can only be shown to converge to the correct results if the drift (force) term is holomorphic in the fields and the domain of its trajectories is bounded. With adaptive updating and gauge-cooling the domain does appear to be bounded for sufficiently weak coupling. However, zeros of the fermion determinant produce poles in the drift term which is therefore meromorphic not holomorphic.

Tests of the CLE for lattice QCD at finite μ indicate that the range of parameters for which it is valid is limited. In particular, at zero temperature, CLE simulations show a transition for $\mu \leq m_\pi/2$ rather than at the expected $\mu \approx m_N/3$.

While it is possible that the correct phase structure might be obtained for sufficiently small coupling, this is possibly beyond the reach of simulations feasible in the near future. People are therefore trying modifications of the action and/or dynamics to avoid these problems.

The fact that the zero-temperature transition occurs below $\mu = m_\pi/2$ suggests that the CLE is not correctly incorporating the effects of confinement and chiral-symmetry breaking.

This suggests adding terms to the action which enhance the effects of confinement and chiral-symmetry breaking in the pion sector.

A simple way of doing this is to add 4-fermion interactions of the Gross-Neveu, Nambu-Jona-Lasinio form to the action. Such terms can produce chiral-symmetry breaking with Goldstone pions, even in the absence of gluon fields. If we choose such interactions with the full $SU(N_f) \times SU(N_f)$ flavour symmetry, we describe QCD, not as a theory of (near-)massless ‘current’ quarks and gluons, but as a theory of pions and massive ‘constituent’ quarks and gluons. (After spontaneous symmetry breaking, the 4-fermion interactions give masses to the quarks.)

Such 4-fermion terms have dimension 6 and are hence irrelevant operators, which do not affect the continuum limit, although they can delay its onset.

Because ‘taste’ breaking for staggered quarks leaves only a $U(1)$ chiral symmetry, we will choose to add only a 4-fermion term which preserves this symmetry. This preserves the symmetries of the staggered action, although it probably worsens ‘taste’ breaking. We refer to Lattice QCD with such 4-fermion interactions as χQCD. (Note, this symmetry becomes $U(1) \times U(1)$ when taste symmetry is restored.)

The inclusion of such 4-fermion interactions has the additional feature in that it allows simulations at zero fermion mass.

We are currently simulating χQCD at $m = 0$. Preliminary results indicate that the zero temperature transition occurs at $\mu > m_\pi/2 = 0$.

Lattice QCD with a chiral 4-fermion interaction at finite μ

For N_f even, the continuum version of the euclidean lagrangian we simulate on the lattice is

$$\mathcal{L} = \frac{1}{4}F_{\mu\nu}F_{\mu\nu} + \bar{\psi}(\not{D} + \gamma_4\mu + m)\psi - \frac{1}{2\gamma N_f}[(\bar{\psi}\psi)^2 - (\bar{\psi}\gamma_5\tau_3\psi)^2].$$

To allow lattice simulations, we introduce auxiliary fields σ and π in terms of which $\mathcal{L}$ becomes

$$\mathcal{L} = \frac{1}{4}F_{\mu\nu}F_{\mu\nu} + \bar{\psi}(\not{D} + \gamma_4\mu + \sigma + i\gamma_5\tau_3\pi + m)\psi + \frac{\gamma N_f}{2}(\sigma^2 + \pi^2).$$

After integrating out the fermion fields, the lattice action for staggered fermions is

$$S = \beta \sum_{\square} \left\{ 1 - \frac{1}{6} Tr[UUUU + (UUUU)^{-1}] \right\} - \frac{N_f}{4} \mathrm{Tr}\{ln[M(U,\mu,\sigma,\pi)]\} + \frac{N_f \gamma}{8} \sum_{\tilde{s}} (\sigma^2 + \pi^2)$$

where $\tilde{s}$ refers to the dual lattice, and the Dirac operator

$$M = D(U,\mu) + \frac{1}{16}\sum{}_i[\sigma_i + i\epsilon(n)\pi_i] + m$$

where $D(U,\mu)$ is the zero mass staggered Dirac operator in the presence of a quark-number chemical potential μ, where backward links are represented by U^{-1} not $U^\dagger$ for use in the CLE; i runs over the 16 sites of the dual lattice adjacent the site under consideration. Note that here τ_3 has been replaced by ξ_5, the analogue of γ_5 in the $SU(4)$ flavour space of the staggered fermion field.

Before continuing the fields to the complex manifold, a chiral transformation to the σ, π fields, is realized as a rotation by an angle ϕ in the complex plane under which

$$\sigma_i + i\pi_i \rightarrow e^{i\phi}[\sigma_i + i\pi_i]$$

and hence

$$\sigma_i + i\epsilon(n)\pi_i \rightarrow e^{i\phi\epsilon(n)}[\sigma_i + i\epsilon(n)\pi_i]$$

while $\sigma^2 + \pi^2$ is invariant. The Dirac operator transforms as

$$M \rightarrow D(U, \mu) + \frac{1}{16}\sum{}_i e^{i\phi\epsilon(n)}[\sigma_i + i\epsilon(n)\pi_i] + m$$

and thus for massless quarks

$$M_{mn} \rightarrow e^{i\frac{1}{2}\phi\epsilon(m)} M_{mn} e^{i\frac{1}{2}\phi\epsilon(n)}.$$

Hence $\mathrm{Det} M$ is chirally invariant, and thus so is the action, as is the Jacobian.

In this massless case at $\mu = 0$, this chiral symmetry breaks spontaneously, σ and $\bar{\psi}\psi$ develop vacuum expectation values related by

$$\langle\bar{\psi}\psi\rangle = \gamma\langle\sigma\rangle$$

and π becomes a massless Goldstone pion. This relation also holds for $\mu \neq 0$. $\langle\sigma\rangle$ gives mass to the quarks. For this reason we are able to simulate at $m = 0$.

The orientation of the condensate in the σ, π plane is arbitrary. On a finite lattice, the orientation of the condensate rotates during the simulations, which avoids having spontaneous symmetry breaking in a finite system.

Complex Langevin

The above action is complex. At $\mu = 0$ this is due to taste breaking and the continuum limit is real and non-negative. This could be remedied by using a quadratic fermion action. However, at $\mu \neq 0$ the action remains complex, even in the continuum limit. We therefore resort to CLE simulations.

The action we use is S, the action after integrating out the fermion fields. The complexified gauge fields are now in $SL(3, C)$ rather than $SU(3)$ and backward links are represented by the inverses of the forward links, *not* their hermitean conjugates. The chiral fields σ and π are now complex.

The Complex-Langevin equations are:

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

for the gauge fields, 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:

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

and:

$$\frac{d\sigma_i}{dt} = -\frac{\delta}{\delta\sigma_i}S(U,\sigma,\pi) + \eta_i^\sigma$$

$$\frac{d\pi_i}{dt} = -\frac{\delta}{\delta\pi_i}S(U,\sigma,\pi) + \eta_i^\pi$$

where i are sites on the dual lattice and η^σ and η^π are independent Gaussian-distributed random numbers, normalized so that:

$$\langle \eta_i^\sigma(t)\eta_{i'}^\sigma(t')\rangle = 2\delta_{ii'}\delta(t-t')$$

$$\langle \eta_i^\pi(t)\eta_{i'}^\pi(t')\rangle = 2\delta_{ii'}\delta(t-t').$$

We choose the noise terms η^a, η^σ and η^π to be real.

To simulate, we discretize the evolution in langevin-time using the partial second order formulation of Fukugita, Oyanagi and Ukawa. The trace over the sites of the lattice and colour indices at each update is replaced by a stochastic estimator. Gauge cooling is applied after each update to minimize the average unitarity norm. This, combined with adaptive rescaling of the updating interval, prevents runaway trajectories.

Complex Langevin simulations and preliminary results.

We are performing CLE simulations of $N_f = 2$ Lattice QCD with chiral 4-fermion interactions (χQCD) at $\beta = 5.6$, $\gamma = 5$, $m = 0$ on a 16^4 lattice. $\beta = 5.6$ is the strongest coupling for which we would trust the CLE to produce reasonable results. We do, however, know that for $\beta = 5.6$, the CLE has non-negligible errors, even in the limit $m \to \infty$, so these runs should be considered exploratory. $\gamma = 5$ represents a stronger 4-fermion coupling than we would like, but exploratory runs with a weaker coupling ($\gamma = 10$ both at $\beta = 5.7$ and $\beta = 5.6$) suggest that it would be difficult to observe a clear signal for spontaneous chiral symmetry breaking on a 16^4 lattice at $\gamma = 10$. Although $\gamma = 5$ is a moderately strong 4-fermion coupling, it is not strong enough for the Gross-Neveu–Nambu-Jona-Lasinio model obtained by switching off the gauge fields to break chiral symmetry on its own. This would require $\gamma < 2$.

Since the orientation of the chiral condensates rotates during the simulations, we define new condensates by the replacements

$$\boldsymbol{\sigma} = \sqrt{[\mathbf{real}(\boldsymbol{\sigma})]^2 + [\mathbf{real}(\boldsymbol{\pi})]^2}$$

and

$$\bar{\psi}\psi = \sqrt{[\mathbf{real}(\bar{\psi}\psi)]^2 + [\mathbf{real}(i\bar{\psi}\gamma_5\xi_5\psi)]^2},$$

where $\boldsymbol{\sigma}$, $\boldsymbol{\pi}$, $\bar{\psi}\psi$, $i\bar{\psi}\gamma_5\xi_5\psi$ are lattice (but not ensemble) averaged quantities. These replacements are justified in the infinite volume limit.

The main problem we observed with the CLE for lattice QCD at finite μ was that instead of the chiral condensate remaining constant up to $\mu \approx m_N/3$ where it should transition to nuclear matter, it started to fall below $\mu = m_\pi/2$, which is where it starts to fall for the phase-quenched theory marking the transition to a superfluid state with a pion-like condensate.

A signal that the CLE for lattice χQCD performs better than that for standard lattice QCD would be that the chiral condensate should fall more slowly with increasing μ than that for the phase-quenched theory indicating a transition to nuclear matter rather than to a superfluid state. At present we do not have any results for the phase-quenched theory. However, our experience with the standard action is that the chiral condensate decreases rapidly with increasing μ once $\mu > m_\pi/2$. If this holds for χQCD, we would expect the phase-quenched chiral condensate for $m = 0$ to decrease rapidly as μ is increased from zero.

We are simulating lattice χQCD with $\beta = 6/g^2 = 5.6$, $\gamma = 5$ and $m = 0$ on a 16^4 lattice, with μ covering the range from 0 to saturation at intervals of 0.1. We have checked that the system does in fact reach saturation for μ sufficiently large in a short run of 250,000 updates at $\mu = 1.5$. This indicated that the quark-number density is consistent with the saturation value of 3, the chiral condensates are very small, and the plaquette is consistent with the value from a CLE simulation of pure $SU(3)$ gauge theory in the absence of quarks. Hence the quarks have decoupled as expected.

So far we have performed runs of 1,000,000 or more updates at each of $\mu = 0$, $\mu = 0.1$, $\mu = 0.2$, $\mu = 0.3$, $\mu = 0.4$ and $\mu = 0.5$.

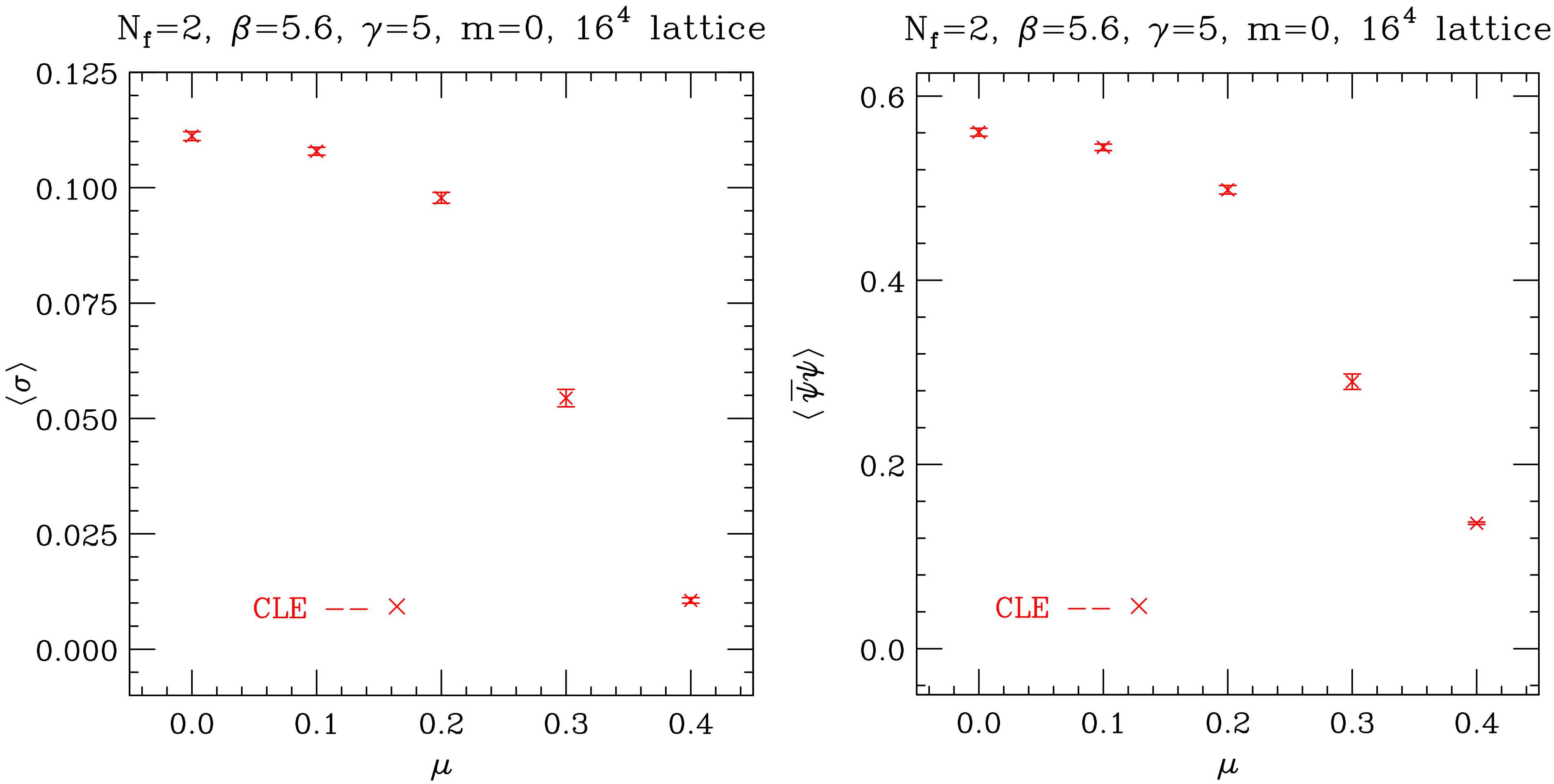

Figure 1: Chiral condensates $\langle\boldsymbol{\sigma}\rangle$ and $\langle\bar\psi\psi\rangle$ as functions of $\boldsymbol{\mu}$.

Figure 1 shows the chiral condensates $\langle\boldsymbol{\sigma}\rangle$ and $\langle\bar{\psi}\psi\rangle$ as functions of $\boldsymbol{\mu}$ from these runs. What we observed during these runs was that, after thermalization, the distributions of the magnitudes of $(\mathbf{real}(\boldsymbol{\sigma}), \mathbf{real}(\boldsymbol{\pi}))$ are clearly separated from zero by a gap over the whole trajectories for $0 \leq \mu \leq 0.3$, indicating chiral symmetry breaking. For $(\mathbf{real}(\bar{\psi}\psi), \mathbf{real}(i\bar{\psi}\gamma_5\xi_5\psi))$ this appears to be true for $0 \leq \mu \leq 0.2$, while for $\mu = 0.3$ the additional noisiness makes this less clear. Note also that the imaginary parts of $\boldsymbol{\sigma}$ and $\boldsymbol{\pi}$ are small relative to the real parts.

What is more, the graphs of the condensates are relatively flat as functions of $\boldsymbol{\mu}$ for $0 \leq \mu \leq 0.2$, falling more rapidly as $\boldsymbol{\mu}$ is increased beyond 0.2. We expect a much steeper falloff as $\boldsymbol{\mu}$ is increased from zero for the phase-quenched theory. If this is indeed the case CLE simulations of lattice χQCD show more physical behaviour than those of standard lattice QCD. We note that, for $0 \leq \mu \leq 0.3$, the relation $\langle\boldsymbol{\sigma}\rangle = \gamma\langle\bar{\psi}\psi\rangle$ is obeyed as well as expected.

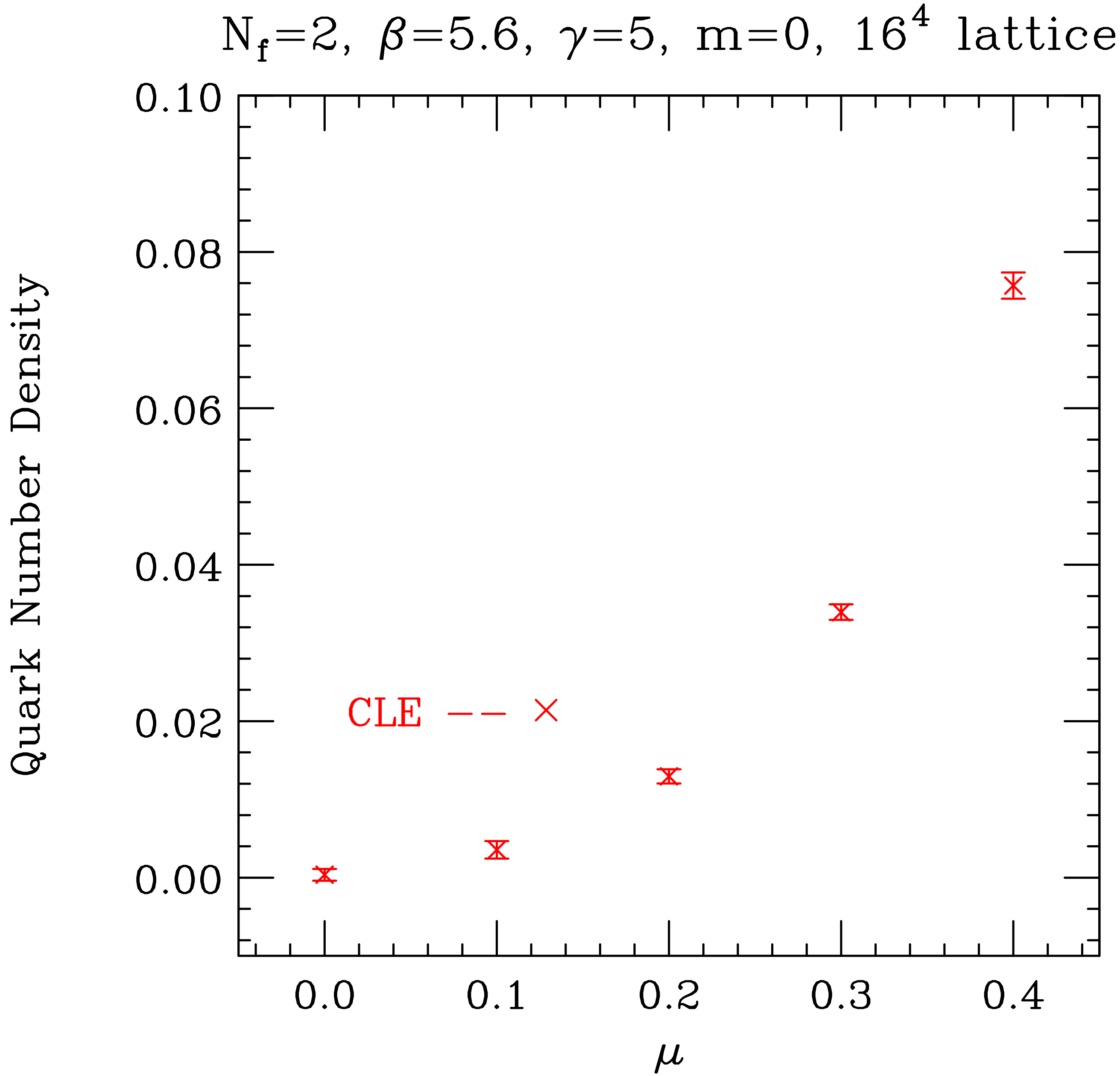

Figure 2: Quark-number density as a function of μ

Figure 2 shows the quark-number density as a function of μ. This quantity rises smoothly from zero as μ is increased. Although not shown on this graph, it reaches its saturation value of 3 for μ sufficiently large – somewhere below $\mu = 1.5$.

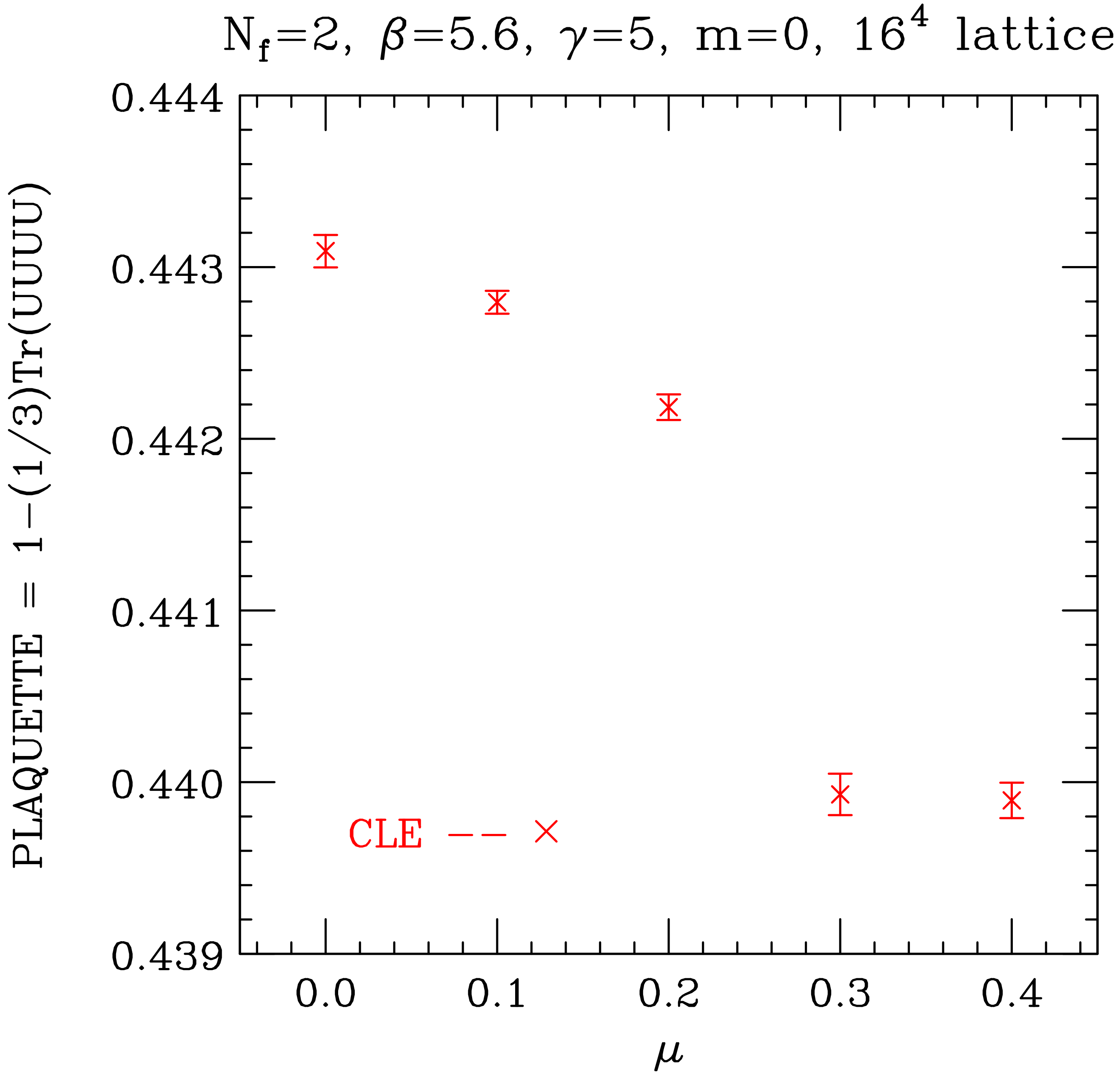

Figure 3: Plaquette as a function of μ

Figure 3 shows the plaquette as a function of μ. So far we have observed it decrease by a small amount as μ is increased from zero. For larger μ it is expected to rise, reaching the value determined by a CLE simulation of pure $SU(3)$ gauge theory with no quarks, i.e ~ 0.469, at saturation.

One interesting aspect of these CLE simulations is that the fluctuations of observables defined in terms of gauge fields, σ and/or π but not fermions are well behaved over the trajectories. This contrasts with fermionic observables. These are well behaved near the beginning of each trajectory (starting from a real ordered start). At some point, the fluctuations abruptly become significantly larger and remain so for the remainder of the trajectory. This is presumably because these quantities have poles at zeros of the fermion determinant and hence become significantly noisier once the trajectory gets close to these poles.

Discussions and Conclusions

- We simulate lattice QCD with an irrelevant dimension-6 chiral 4-fermion interaction (χQCD), which preserves the $m = 0$ chiral symmetry of the staggered fermion action at finite μ, using the CLE. Such an irrelevant term should not affect the continuum limit. It has the additional advantage that it allows simulations with massless quarks.
- Our CLE simulations are performed on a 16^4 lattice with $N_f = 2$, $\beta = 6/g^2 = 5.6$, $\gamma = 5$, and $m = 0$, over a range of μs ranging from zero to saturation. Our preliminary results are for small μs.
- Our previous CLE simulations using the standard lattice-QCD action showed an unphysical transition at $\mu < m_\pi/2$ instead of $\mu \approx m_N/3$. The χQCD simulations show no such spurious transition.

- The slow decrease in the condensates from $\mu = 0$ to $\mu = 0.3$ could be due to the same mechanism that causes the falloff of the condensate for the standard action for $\mu < m_\pi/2$.
- It is important to simulate phase-quenched χQCD using the exact RHMC algorithm for comparison.
- We need to simulate χQCD at weaker gauge and 4-fermion couplings, even if it requires larger lattices, to observe spontaneous chiral-symmetry breaking.
- Eventually we will need to use actions with 4-fermion interactions which have full $SU(N_f) \times SU(N_f)$ chiral symmetry in the continuum limit.
- It remains to be seen if CLE simulations of the standard action will produce correct results for weak enough gauge couplings. We have seen that modifying the standard action by the addition of carefully selected higher dimensional operators can improve the behaviour of the CLE. It remains to be determined as to whether these improvements can survive to the continuum limit.

These simulations were performed using an allocation on the Bebop cluster belonging to the Laboratory Computing Resource Center at Argonne National Laboratory.