Complex Langevin for Lattice QCD

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Introduction

QCD at finite baryon/quark-number density has a sign problem which prevents direct application of standard lattice simulations that are based on importance sampling.

When finite density is implemented introducing a quark-number chemical potential μ, the sign problem manifests itself by making the fermion determinant complex.

Since Langevin simulations are not based on importance sampling, they can be extended to the case of complex actions. For lattice QCD this requires analytically continuing the gauge fields from $SU(3)$ to $SL(3,C)$.

Complex Langevin simulations cannot be guaranteed to produce correct results unless the trajectories are restricted to a compact domain and the drift term is holomorphic in the fields. The solutions should also be ergodic. Thus disconnected regions of complex field space could be problematic.

For lattice QCD the domain is kept compact and close to the

$SU(3)$ manifold by adaptively adjusting the updating increment and using gauge cooling (at least at weak coupling).

- However, zeroes of the fermion determinant produce poles in the drift term making it meromorphic not holomorphic in the fields. Thus convergence to the correct limits cannot be guaranteed.

  A good discussion of what is known about the behaviour of the CLE for lattice QCD at finite μ and related models, as well as a guide to the literature, is given in Aarts-Seiler-Sexty-Stamatescu, JHEP05, 044 (2017).

- We have simulated lattice QCD at zero temperature and μs ranging from zero to saturation, at $\beta = 6/g^2 = 5.6$ and $\beta = 5.7$. The weaker coupling shows good agreement with expectations at small and large μs, but fails for couplings in the transition region. The results are compared with those of the phase-quenched approximation.

- Since it appears that good results might be obtained if the trajectories remain close to the $SU(3)$ manifold, we are studying how the unitarity norm, which measures this closeness, depends on quark mass (m) and β.

Complex Langevin for Lattice QCD at finite μ

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

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

where $M(U,\mu)$ is the staggered Dirac operator. Backward links are represented by U^{-1} not $U^{\dagger}$. We choose to keep the noise term η real. We simulate the time evolution of the gauge fields using a partial second-order formalism.

We apply adaptive updating: if the force term becomes too large, dt is decreased to keep it under control. After each update, we gauge cool, gauge fixing to the gauge which minimizes the unitarity norm:

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

We use unimproved staggered quarks.

Zero Temperature Simulations at $\beta = 5.6$ and $\beta = 5.7$

We perform CLE simulations of 2-flavour lattice QCD at zero temperature at $\beta = 5.6$, $m = 0.025$ on a 12^4 lattice and at $\beta = 5.7$, $m = 0.025$ on a 16^4 lattice from $\mu = 0$ up to saturation. For comparison, we perform RHMC simulations of the phase-quenched approximation over the same parameter range, since random matrix theory suggests that when the CLE simulations fail they produce the phase-quenched results.

The phase-quenched approximation is known to undergo a phase transition to a superfluid phase with a quark-anti-conjugate-quark condensate at $\mu \approx m_\pi/2$. The chiral condensate is constant up to this transition and decreases beyond it, vanishing at saturation. The quark-number density is zero up to the transition beyond which it rises up to saturation, where all states are filled (density=3 in our normalization). At saturation the quarks decouple and we have a pure gauge theory.

For the full theory one expects the observables to remain at their $\mu = 0$ values up to $\mu \approx m_N/3$ above which they evolve towards saturation.

For $\beta = 5.6$, $m = 0.025$, $m_\pi/2 \approx 0.21$, $m_N/3 \approx 0.33$, while for $\beta = 5.7$, $m = 0.025$, $m_\pi/2 \approx 0.194$, $m_N/3 \approx 0.28$.

We typically run for 2-3 million updates at each β and μ.

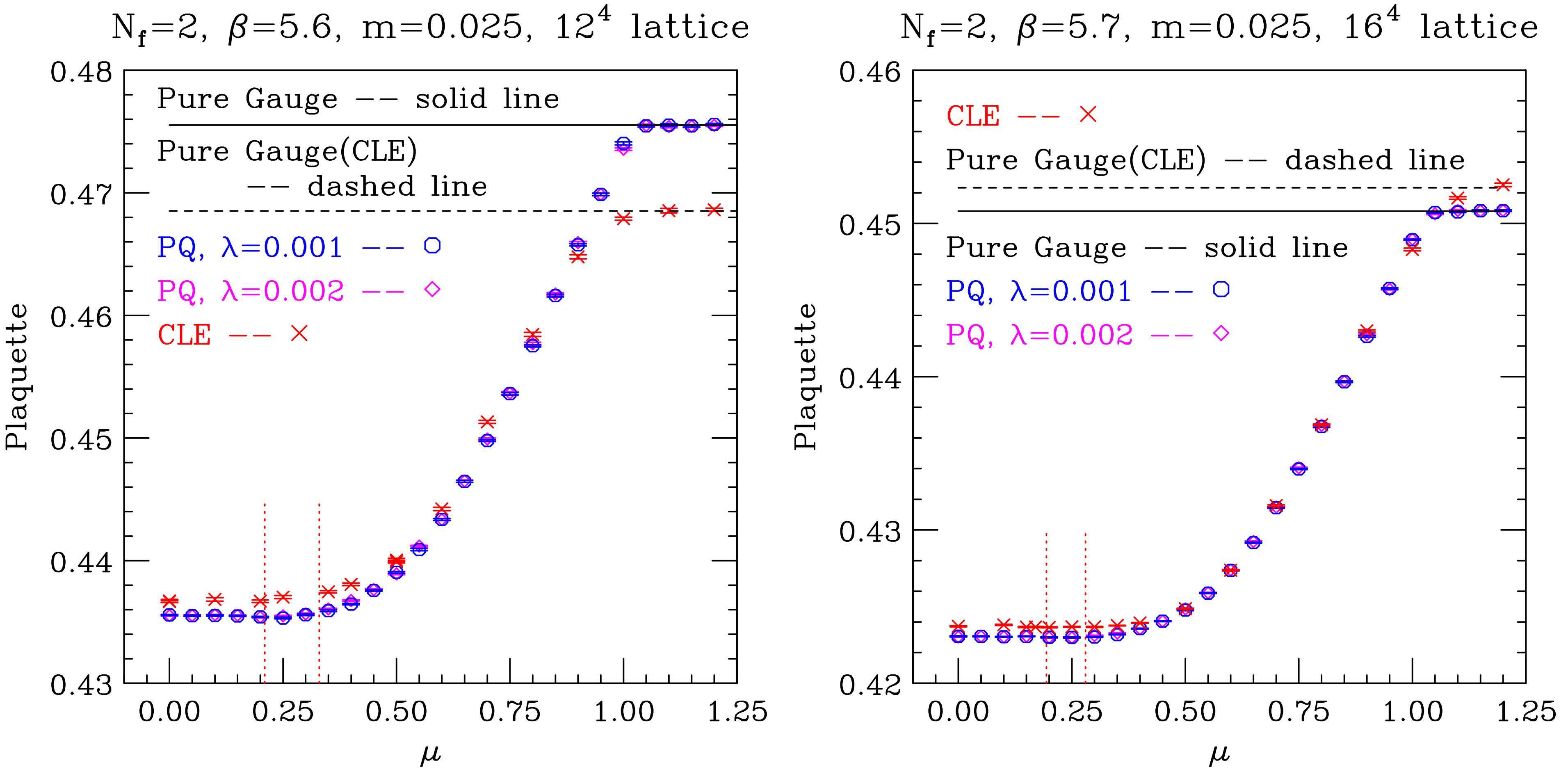

Figure 1: Plaquettes as functions of μ for $\beta = 5.6$, $m = 0.025$ on a 12^4 lattice and for $\beta = 5.7$, $m = 0.025$ on a 16^4 lattice.

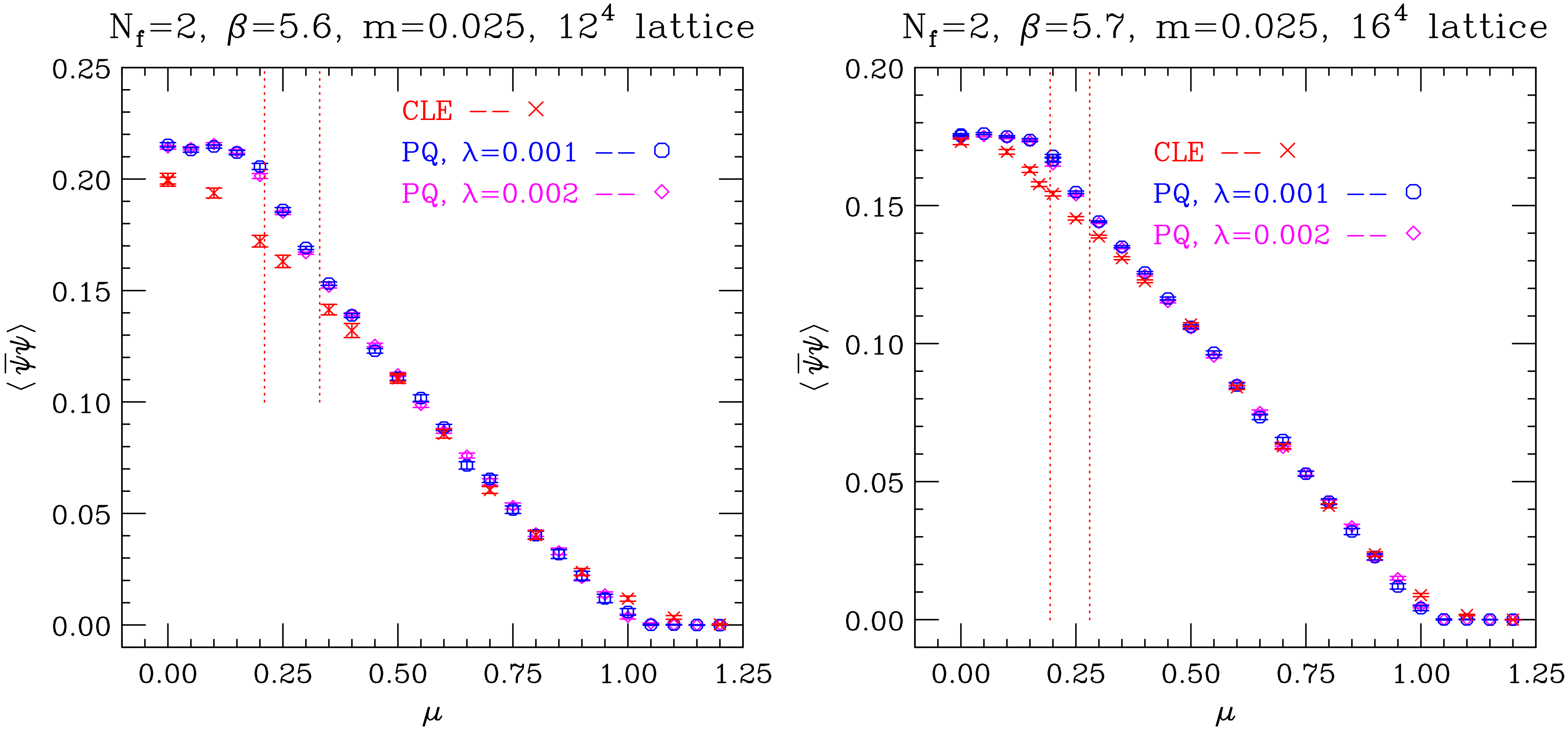

Figure 2: Chiral condensates as functions of μ for $\beta = 5.6$, $m = 0.025$ on a 12^4 lattice and for $\beta = 5.7$, $m = 0.025$ on a 16^4 lattice.

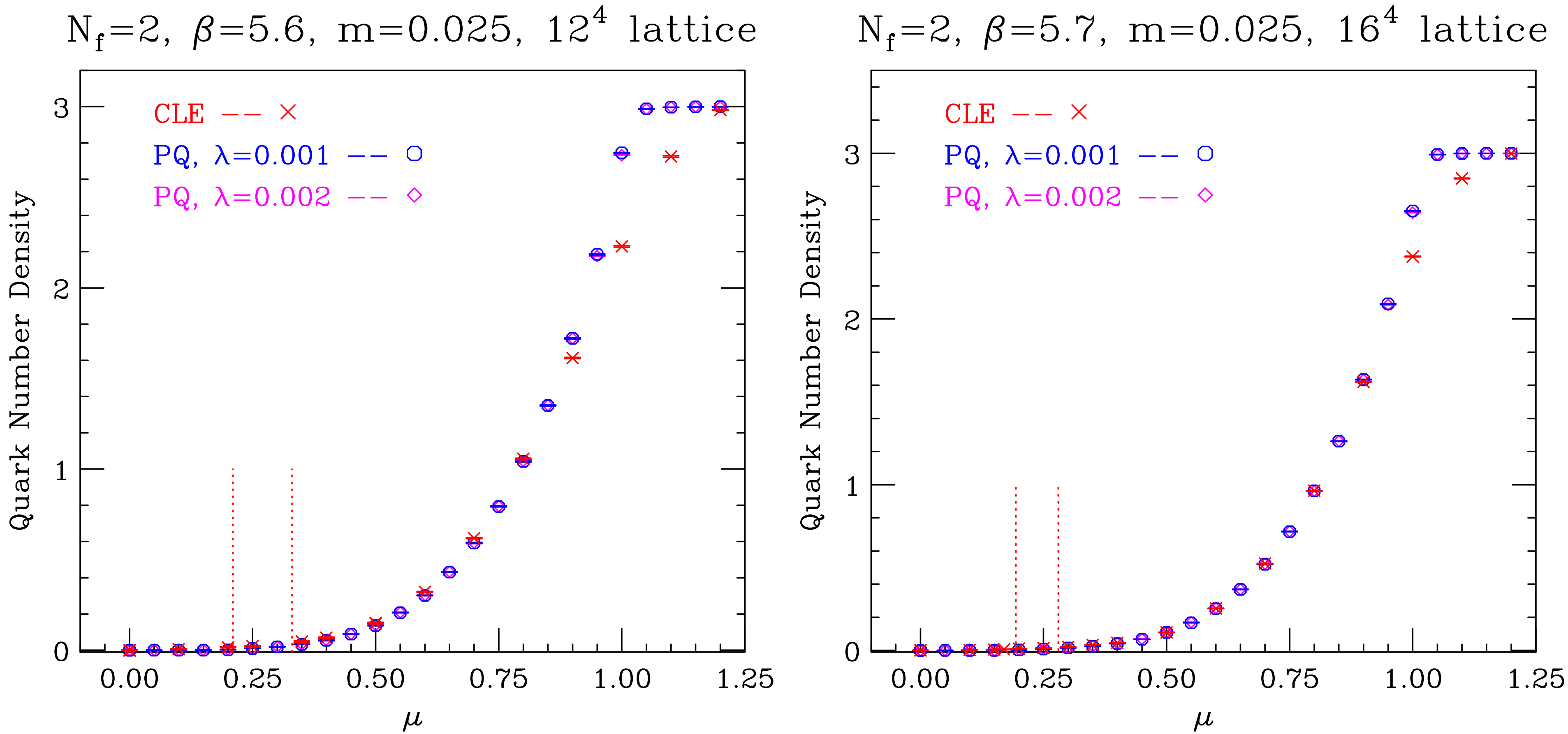

Figure 3: Quark-number densities as functions of μ for $\beta = 5.6$, $m = 0.025$ on a 12^4 lattice and for $\beta = 5.7$, $m = 0.025$ on a 16^4 lattice.

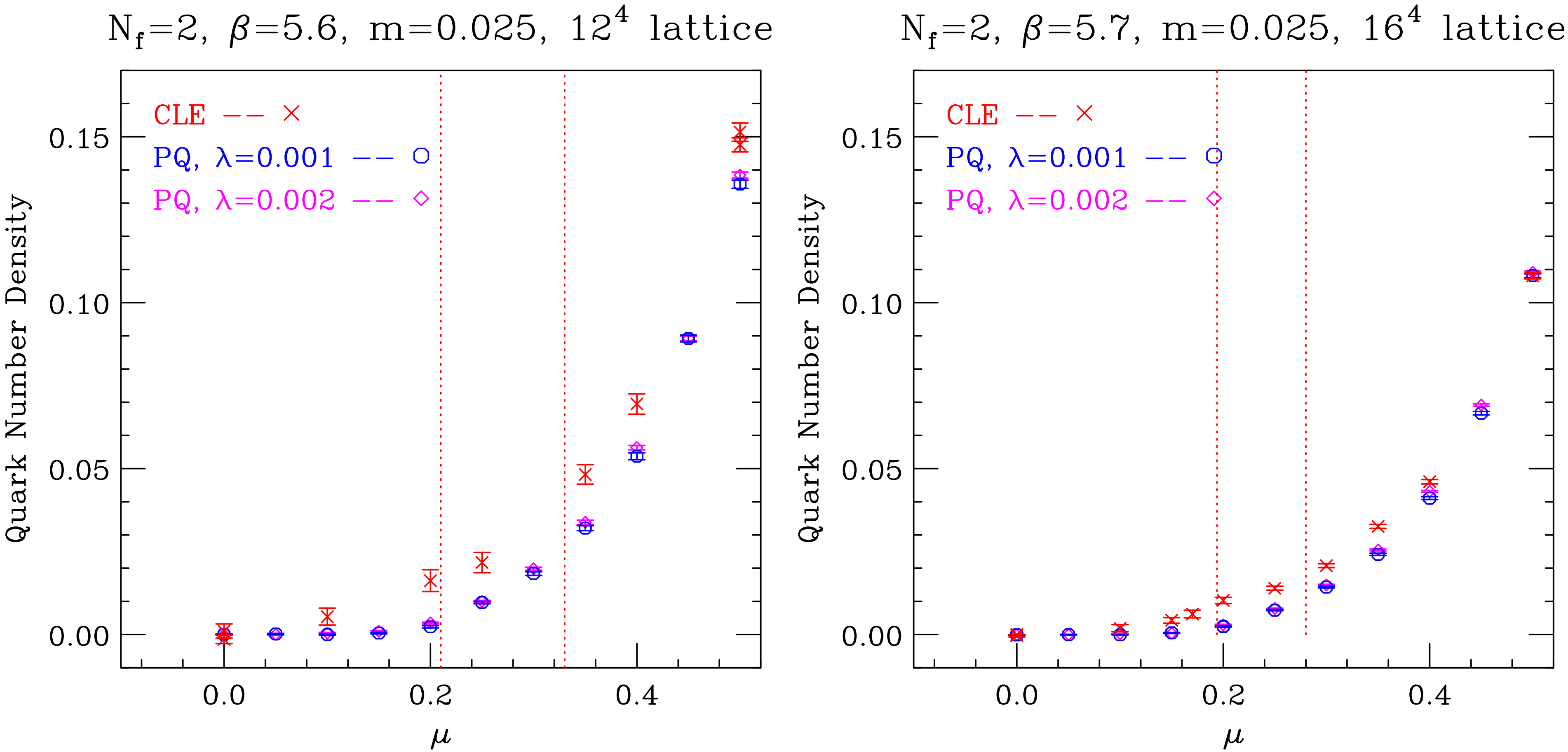

Figure 4: Quark-number densities as functions of μ for $\beta = 5.6$, $m = 0.025$ on a 12^4 lattice and for $\beta = 5.7$, $m = 0.025$ on a 16^4 lattice.

$\beta = 5.7$ shows significant improvement over $\beta = 5.6$ for μ at or near zero, and near saturation. $\beta = 5.7$ observables show good agreement with known results for small and large μ.

At saturation, the quarks effectively decouple from the gluons, and the gauge fields exhibit pure gauge dynamics. This agrees with expectations.

In the transition region for these parameters, the CLE results are even worse than the phase-quenched approximation.

The unitarity norm is significantly greater than zero throughout the transition region for both β values. It becomes small around $\mu = 0.5$. At $\beta = 5.7$, it remains small, at least through $\mu = 0.8$, increasing towards its pure-gauge value at saturation. However, in this high μ region the quarks are starting to decouple. We conjecture that this means that for $\beta = 5.7$, we can probably trust the CLE for $\mu \geq 0.5$.

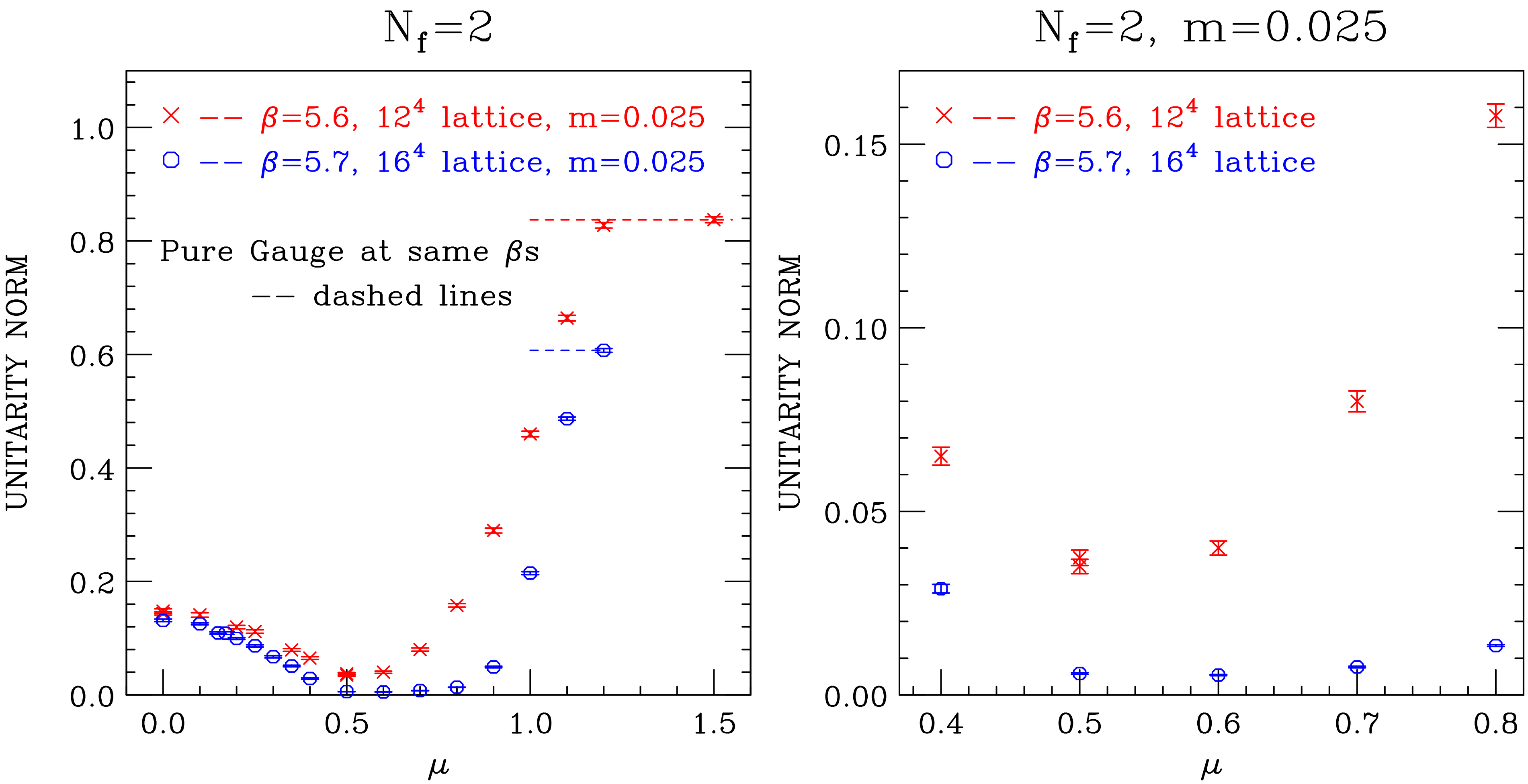

Figure 5: Average unitarity norm as a function of μ for $\beta = 5.6$, $m = 0.025$ on a 12^4 lattice – red. Same, but for $\beta = 5.7$ on a 16^4 lattice – blue.

Dependence of the Unitarity Norm on quark mass m

The behaviour of the CLE seems to improve if the gauge fields remain close to the $SU(3)$ manifold, i.e. if the unitarity norm remains small. It is thus useful to study how the average unitarity norm depends on the simulation parameters.

With β fixed at 5.6, we determine the dependence of the unitarity norm on the quark mass m at $\mu = 0$.

We have varied m from infinity (pure gauge) down to $m = 0.01$. What we find is that the unitarity norm decreases as m is decreased. This is important, since small m is the region of most interest.

In addition, running with a small mass increases the gap between $m_\pi/2$ and $m_N/3$.

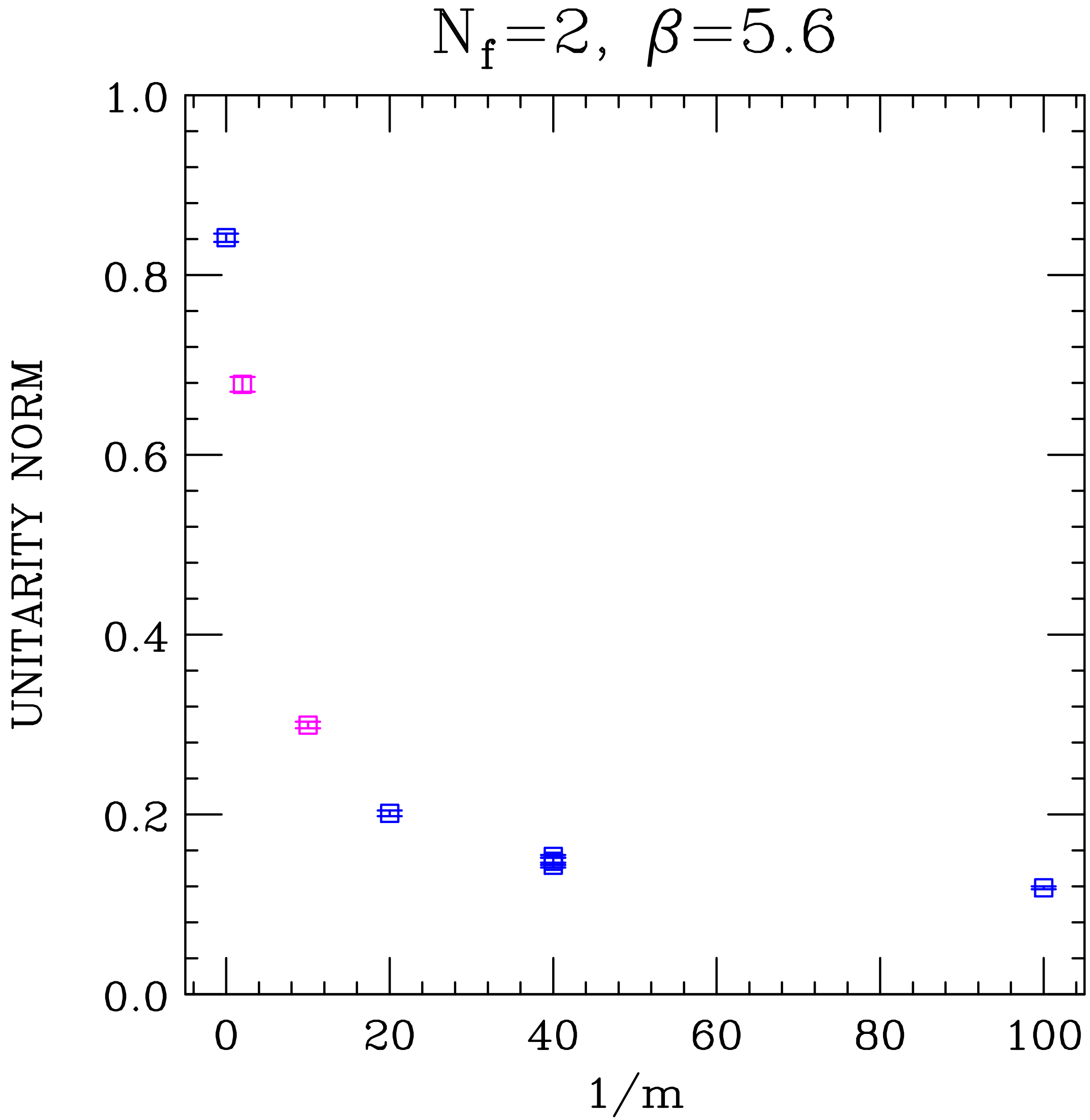

Figure 6: Unitarity norm as a function of inverse quark mass at $\boldsymbol{\beta = 5.6}$

Dependence of the Unitarity Norm on $\beta = 6/g^2$

We have already noted that going from $\beta = 5.6$ to $\beta = 5.7$ with quark mass fixed at $m = 0.025$ results in a decrease in the unitarity norm, and improved behaviour of the CLE.

One could argue that one should change β and m along a line of constant physics and compare the unitarity norms at identical physical values of μ.

To avoid such complications we choose to work with the pure gauge (quenched) theory, i.e. that at infinite quark mass, where there is no μ dependence. The unitarity norms we measure are upper bounds on the finite mass values at $\mu = 0$.

Using the quenched theory allows us to run on smaller lattices for a given β. Also with no dynamical quarks the CLE runs much faster.

For pure gauge theories on the lattice, the CLE has solutions where the gauge fields remain in $SU(3)$ and the unitarity norm is zero. These are the solutions of the real Langevin equation.

However these ‘real’ solutions are unstable to (small) perturbations away from the $SU(3)$ manifold into $SL(3, C)$, which lead to stable solutions with non-zero unitarity norms, and appear to evolve over a compact manifold. It is these solutions that we are studying.

The pure-gauge drift is holomorphic in the fields, so we expect that the CLE simulations will produce the correct values of observables (up to $\mathcal{O}(dt^2)$ corrections). In fact this appears to be true for $\beta \geq 5.7$. This agreement with Monte Carlo simulations improves as we go to weaker coupling (larger β).

We find that the unitarity norms decrease as β increases, showing that going to weak-coupling can produce the desired effect.

In addition to completing our simulations at $\beta = 7.0$, we plan simulations at lower β values to better understand why the CLE breaks down at strong couplings despite the fact that the drift is holomorphic in the fields.

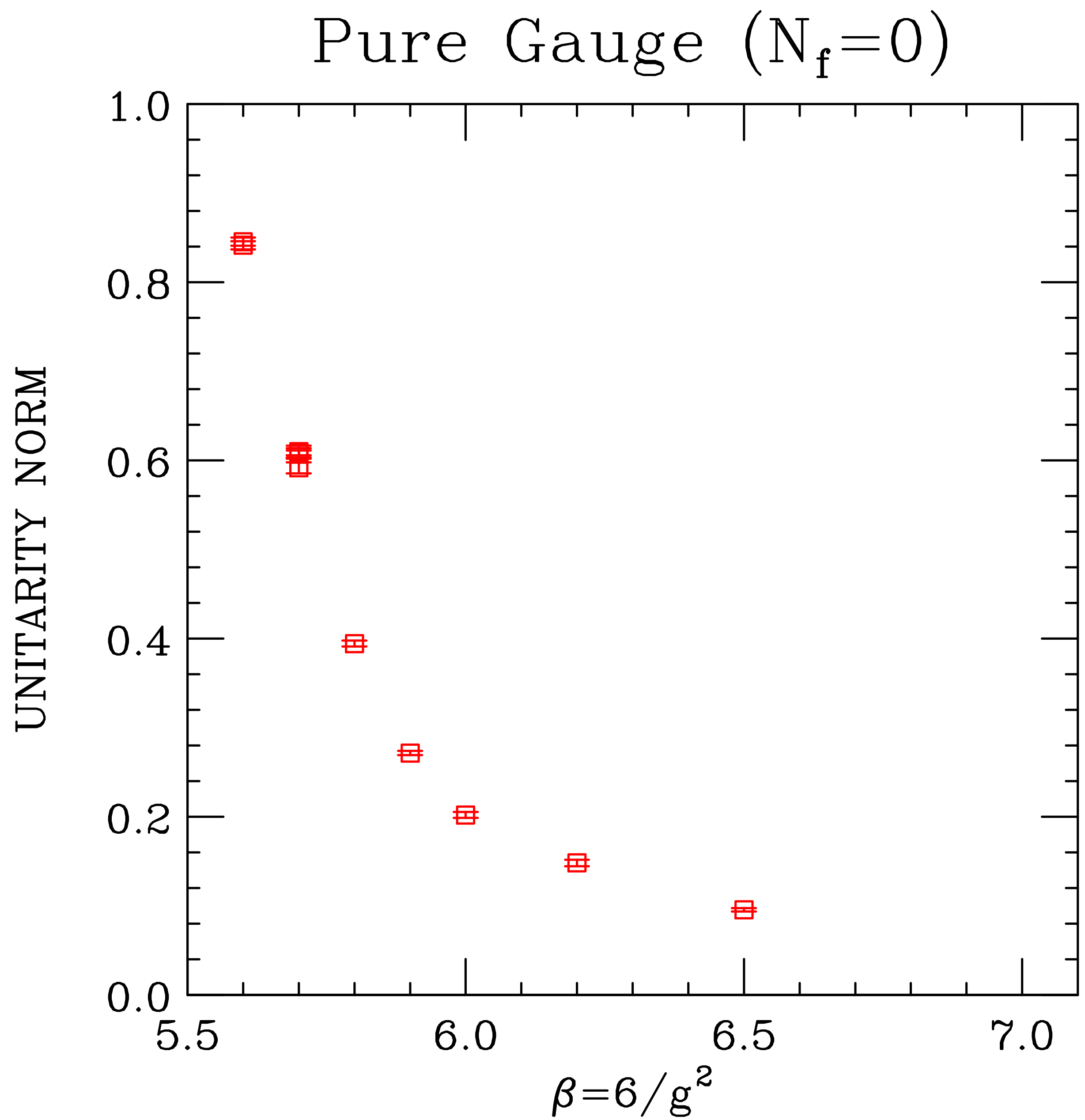

Figure 7: Unitarity norm as a function of $\beta = 6/g^2$ for pure $SU(3)$ gauge theory.

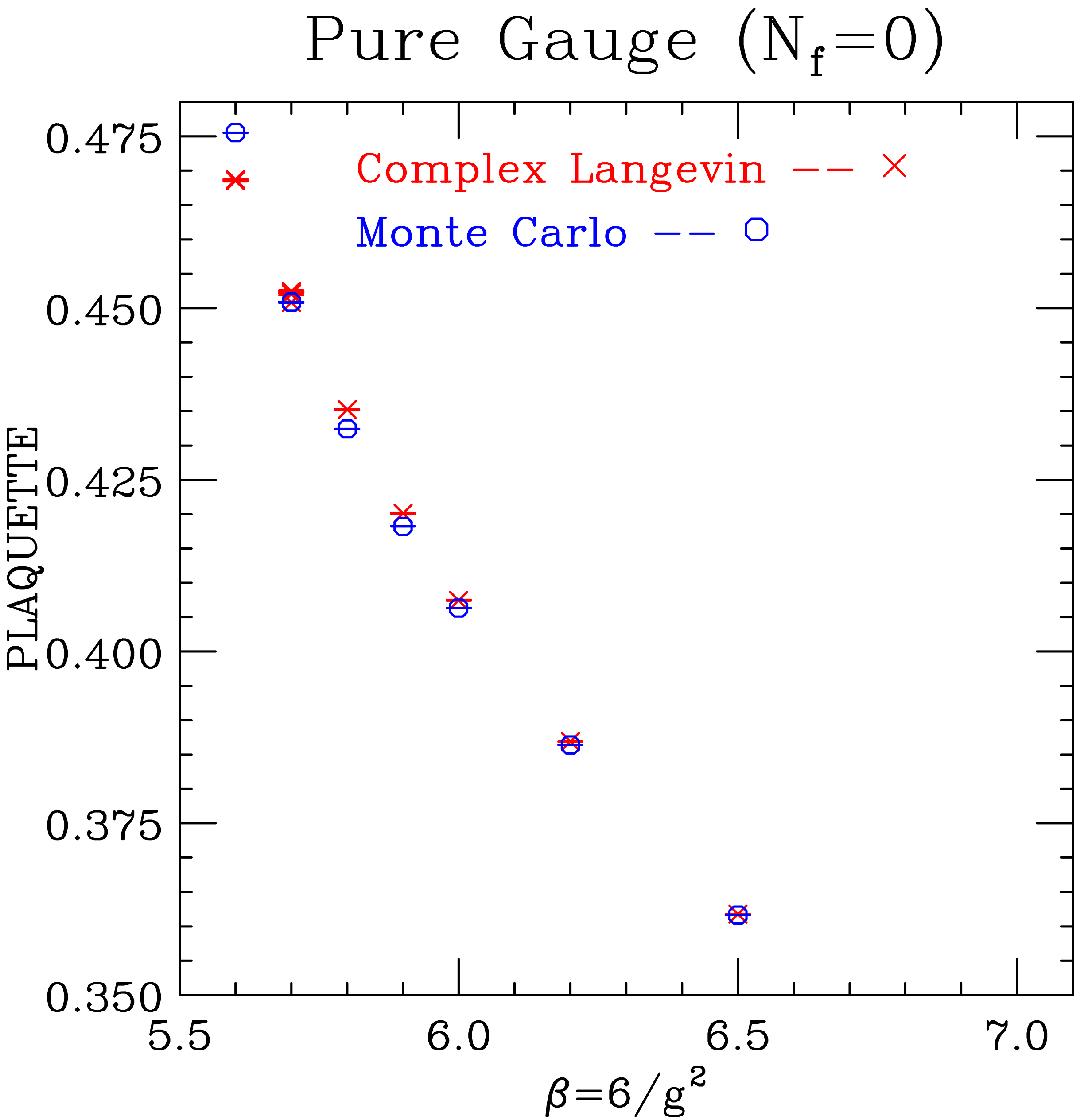

Figure 8: Plaquette as a function of $\beta = 6/g^2$ for pure $SU(3)$ gauge theory. Monte Carlo values are shown for comparison.

Finite temperature and density

We have performed some exploratory CLE simulations of 2-flavour QCD at finite temperature on a $12^3 \times 6$ lattice on the interval $5.3 \leq \beta \leq 5.6$ at $m = 0.025$, which includes the finite-temperature transition.

Even at $\mu = 0$ we were unable to produce results which were in even qualitative agreement with known (RHMC) values of the chiral condensate and Polyakov loop.

We believe that, in order to perform CLE simulations with any hope of producing reasonable results, we will need to run on lattices with N_t large enough that $\beta = 5.6$ lies in the low-temperature phase. This requires $N_t \geq 12$.

This contrasts with 4-flavour QCD where Fodor *et al.* found at least qualitatively reasonable results for $N_t = 6$ and quantitatively reasonable results for $N_t = 8$. This can be understood, because the larger number of flavours reduces the unitarity norms so that they take reasonable values (~ 0.1) in the low-temperature phase, whereas for the 2-flavour case the unitarity norm at $\beta = 5.3$ (in the low-temperature phase for $N_t = 6$) is ~ 0.7.

Summary and Discussions

- We simulate lattice QCD with 2 flavours of light quarks ($m = 0.025$) at $\beta = 5.6$ and $\beta = 5.7$ at a range of μ from zero to saturation, using CLE. We compare these results with those of the phase-quenched approximation.
- Decreasing the coupling from $\beta = 5.6$ to $\beta = 5.7$ results in significant improvement at small and large μ where the full and phase-quenched theories should agree. At large μ (saturation) we observe that the fermions decouple and we obtain the pure gauge (quenched) results.
- At intermediate μs (the transition region) we still obtain results which disagree with expectations and with the phase-quenched theory.
- Since it is expected that improved results will obtain if one can reduce the unitarity norm, i.e. keep the system closer to the $SU(3)$, we are studying the dependence of the unitarity norm on m and β.

- At fixed β and $\mu = 0$ we observe that the unitarity norm decreases as we decrease the quark mass.
- At $m = \infty$ (pure gauge/quenched QCD) the unitarity norm decreases as β is increased (weaker coupling), becoming quite small by $\beta = 7.0$.
- We are starting simulations at $\beta = 5.8$, $m = 0.02$ and $\beta = 5.9$, $m = 0.015$ on 32^4 lattices, where the unitarity norms at $\mu = 0$ are ~ 0.106 and ~ 0.091 respectively.
- Because simulations at βs large enough to make the unitarity norms small requires very large lattices for $N_f = 2$, it might be reasonable to run at the physically less interesting $N_f = 4$ (following Fodor *et al.*), where smaller lattices could be used, to test the CLE.
- It remains an open question as to whether, in the weak coupling limit at small quark masses, the CLE produces the results of full QCD at finite μ or its phase-quenched approximation as does the RMT.

Our simulations are performed on the Bebop cluster at Argonne's LCRC, Crays Cori and Edison at NERSC, the Stampede 2 cluster at TACC, the Bridges cluster at PSC, the Comet cluster at SDSC and Linux PCs belonging to the HEP division at Argonne.