3-flavour lattice QCD at finite density and temperature

(QCD at finite isospin density and temperature revisited)

D. K. Sinclair
J. B. Kogut

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Introduction

We are interested in QCD at small quark-number chemical potential μ and temperature. In particular, we are looking for the critical end-point.

QCD at finite isospin chemical potential μ_I has some similarities to QCD at finite μ, but lacks the sign problem. In particular, T_c for the finite-temperature transition at small μ_I appears to be the same as for small μ provided $\mu_I = 2\mu$. We conjecture that the critical endpoints might be coincident.

De Forcrand, Kim and Takaishi have noted that QCD at small μ_I is a better candidate for reweighting approaches to QCD at small μ, than QCD at $\mu = 0$. This is a further indication that the physics at (β, μ) and at $(\beta, \mu_I = 2\mu)$ is similar. When the phase of the fermion determinant is under control, this is perhaps not so surprising.

We are simulating 3-flavour lattice QCD (staggered fermions) at small μ_I and at T close to T_c on $8^3 \times 4$ and $12^3 \times 4$ lattices. Binder cumulants (B_4) for $\bar{\psi}\psi$ are used to study the nature of the transition.

We are studying the dependence of B_4 on dt in hybrid molecular-dynamics simulations. B_4 and $\chi_{\bar{\psi}\psi}$ show considerable dt dependence.

Lattice QCD at finite isospin density

The staggered quark action for lattice QCD at finite μ_I is

$$S_f = \sum_{sites} \left\{ \bar{\chi}[\not{D}(\frac{1}{2}\tau_3\mu_I) + m]\chi + i\lambda\epsilon\bar{\chi}\tau_2\chi \right\}.$$

The explicit symmetry breaking term proportional to λ is only needed for $\mu_I \geq m_\pi$ where, in the low temperature phase, I_3 is broken spontaneously by a charged pion condensate. The fermion determinant is

$$\det \left\{ [\not{D}(\frac{1}{2}\mu_I) + m]^\dagger [\not{D}(\frac{1}{2}\mu_I) + m] + \lambda^2 \right\},$$

which is positive.

3-flavour QCD at finite isospin density and temperature — finite dt effects

For $N_t = 4$ the finite temperature transition for 3 flavours of staggered quarks changes from first order to a crossover at $m_c \approx 0.033$ (Karsch, Laermann and Schmidt) for $\mu, \mu_I = 0$.

It is believed that for $\mu > 0$ or $\mu_I > 0$, m_c increases and becomes the critical end point.

We are simulating 3-flavour lattice QCD at $0 \leq \mu_I < m_\pi$ for $0.25 \leq m \leq 0.4$ on $8^3 \times 4$ and $12^3 \times 4$ lattices, using Binder cumulants (B_4) for $\bar{\psi}\psi$ to determine the position and nature of the transition. 5 stochastic estimates of $\bar{\psi}\psi$ (and j_0^3) are made at the end of each trajectory. This gives us unbiased estimators for $B_4(\bar{\psi}\psi)$ and $\chi_{\bar{\psi}\psi}$.

$$B_4(\bar{\psi}\psi) = \frac{\langle(\overline{\bar{\psi}\psi} - \langle\overline{\bar{\psi}\psi}\rangle)^4\rangle}{\langle(\overline{\bar{\psi}\psi} - \langle\overline{\bar{\psi}\psi}\rangle)^2\rangle^2}$$

and

$$\chi_{\bar{\psi}\psi} = V\langle(\overline{\bar{\psi}\psi} - \langle\overline{\bar{\psi}\psi}\rangle)^2\rangle.$$

where the overline is the space-time average and V is the space-time volume.

The graphs of B_4 at the transition versus m or μ_I for different spatial volumes should cross at a critical point. For the critical end-point this should occur at $B_4 = 1.604(1)$ (Ising). We graph B_4 as a function of m at $\mu_I = 0$ and as a function of μ_I for fixed m for $0.02 \leq dt \leq 0.0625$. The expectation values which contribute to B_4 at fixed m and μ_I are calculated at each of 4

βs close to the transition and extrapolated to the transition using Ferrenberg-Swendsen reweighting. The position β_c of the transition is determined from the minimum of B_4 which is consistent with that obtained from the maximum of χ. The length of the runs at each (m, μ_I, β) is (will be) 160,000 $\Delta t = 1$ trajectories.

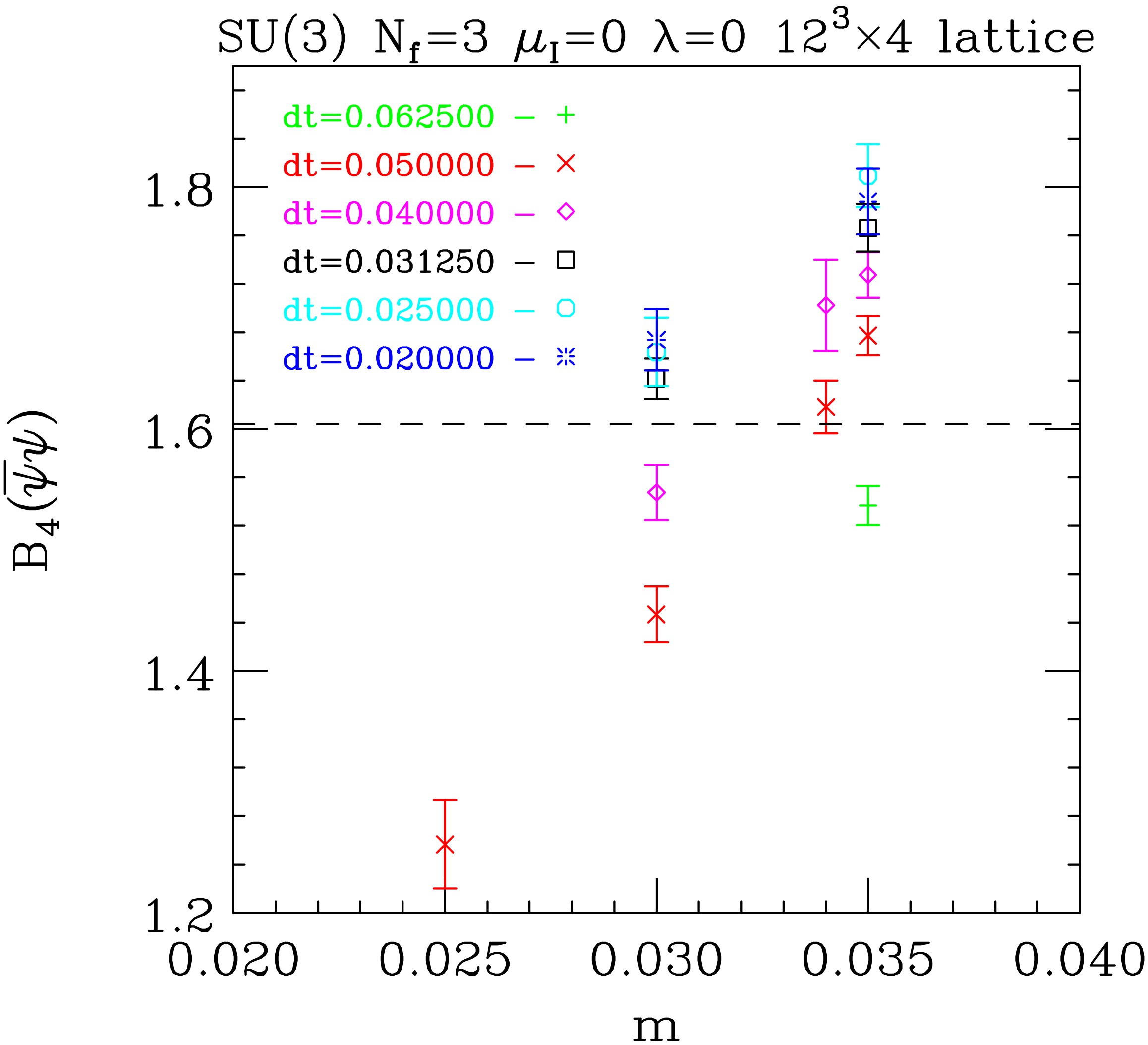

Figure 1: Mass dependence of $B_4(\bar{\psi}\psi)$ for various values of the updating increment dt.

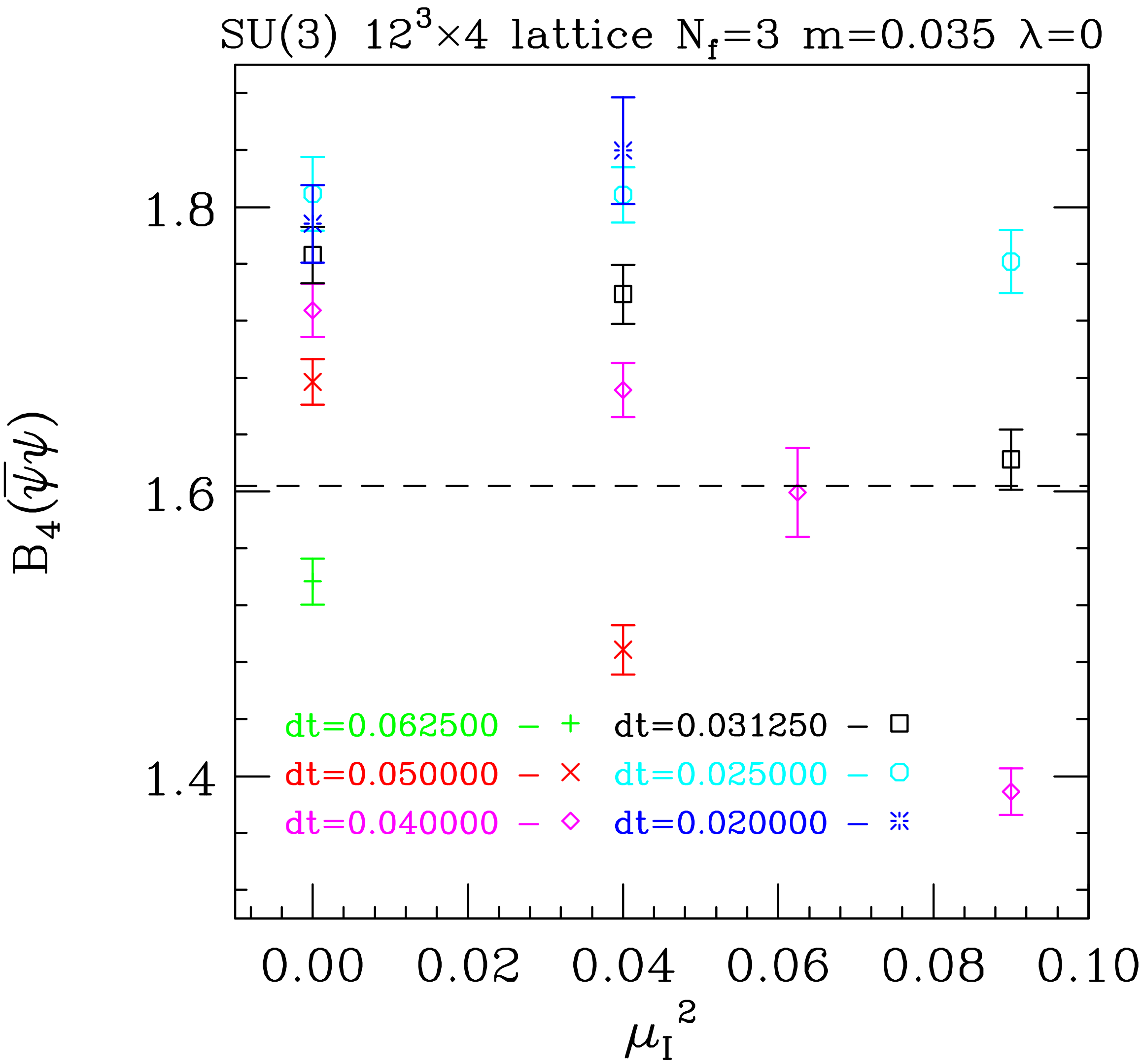

Figure 2: μ_I dependence of $B_4(\bar{\psi}\psi)$ for various values of the updating increment dt at $m = 0.035$.

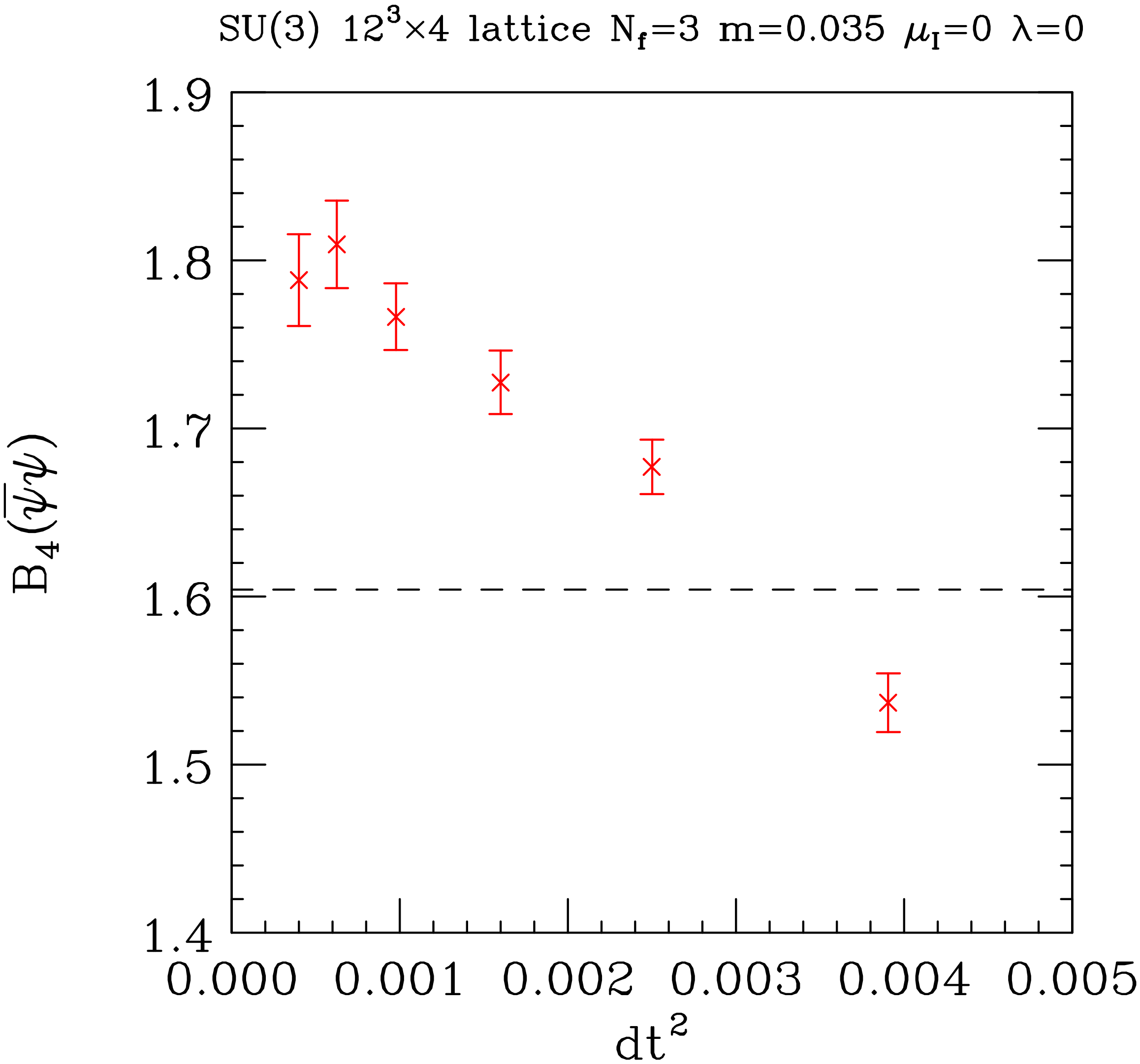

Figure 3: dt dependence of $B_4(\bar{\psi}\psi)$ at $m = 0.035$ and $\mu_I = 0$

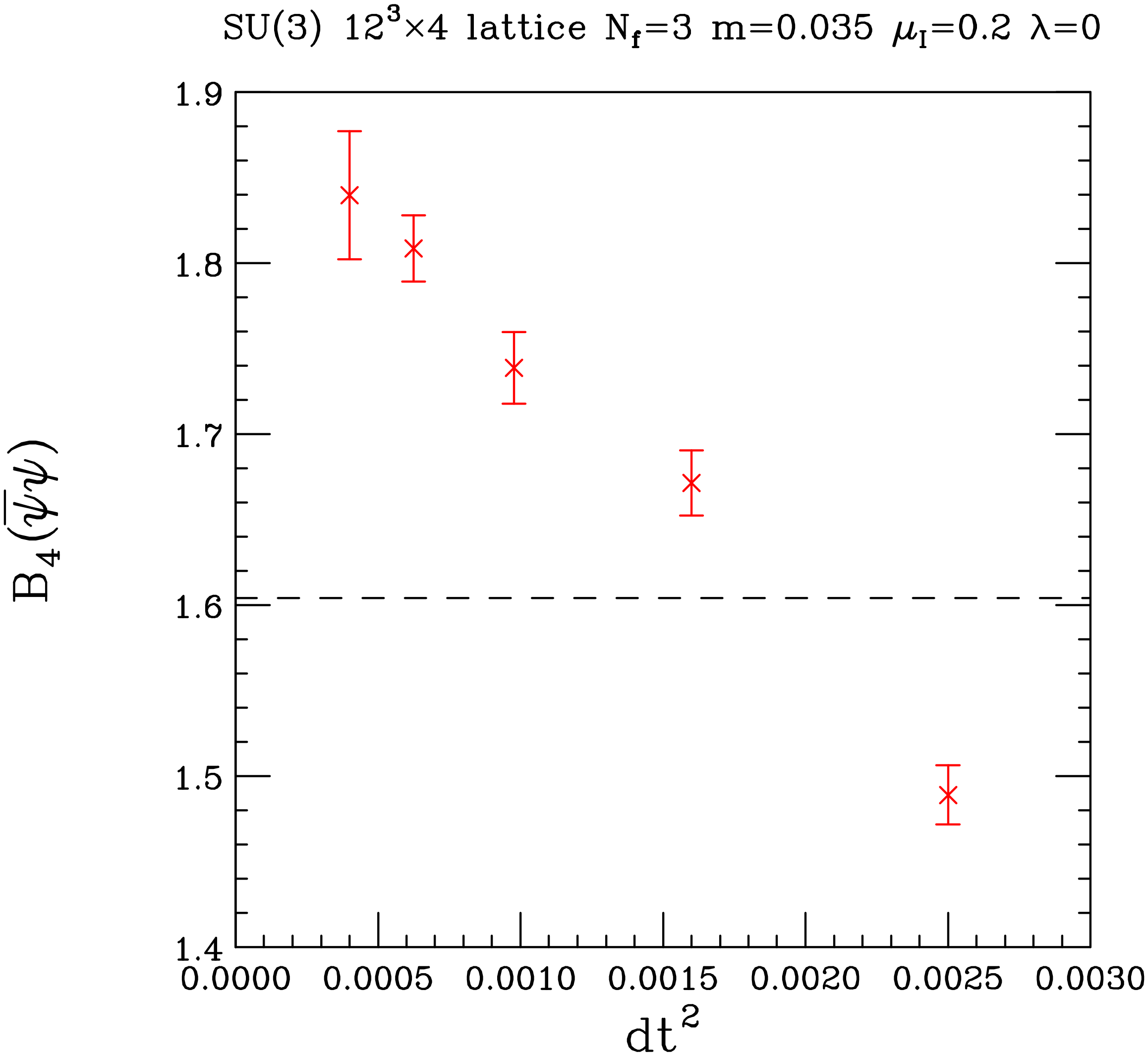

Figure 4: dt dependence of $B_4(\bar{\psi}\psi)$ at $m = 0.035$ and $\mu_I = 0.2$

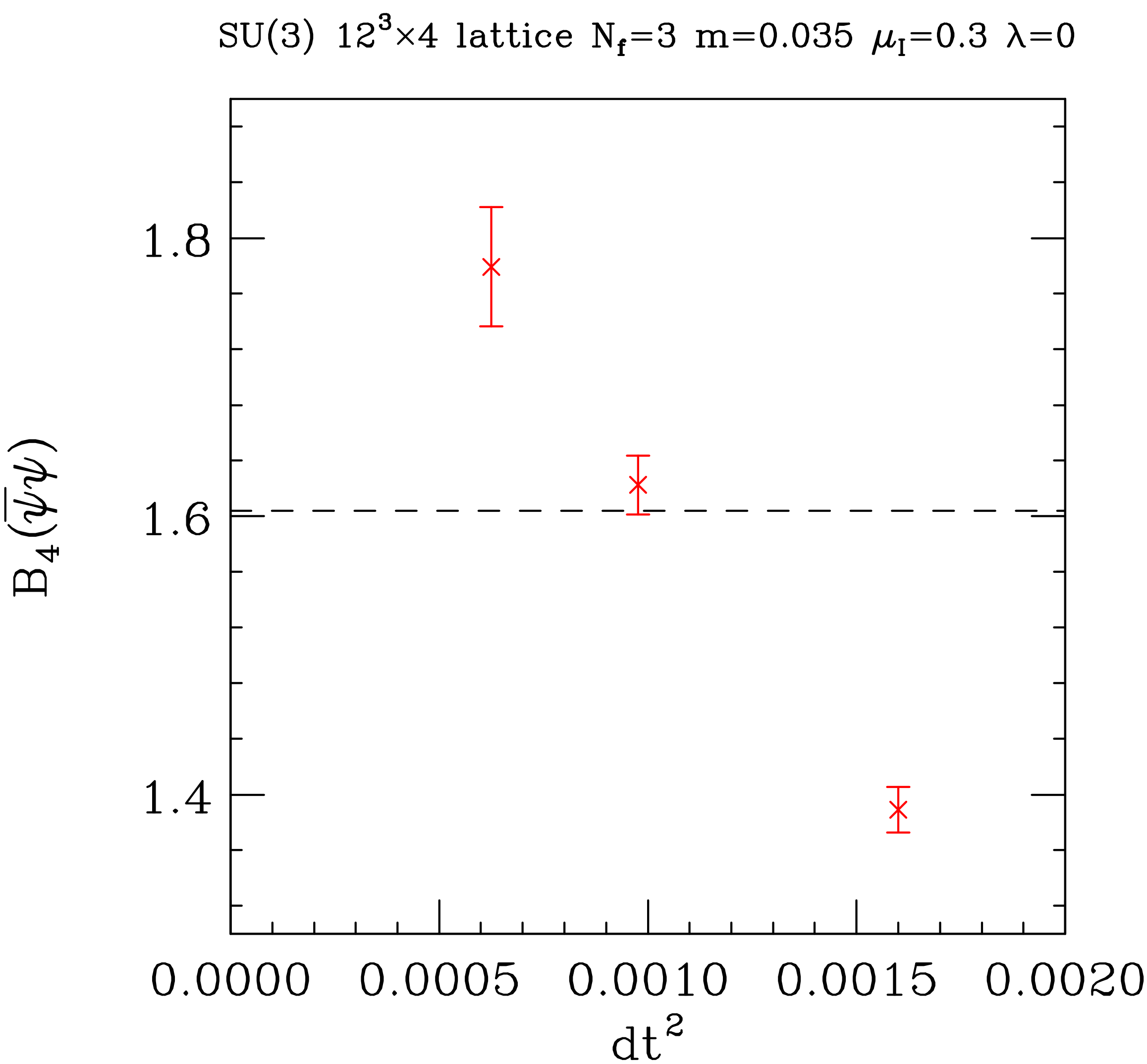

Figure 5: dt dependence of $B_4(\bar{\psi}\psi)$ at $m = 0.035$ and $\mu_I = 0.3$

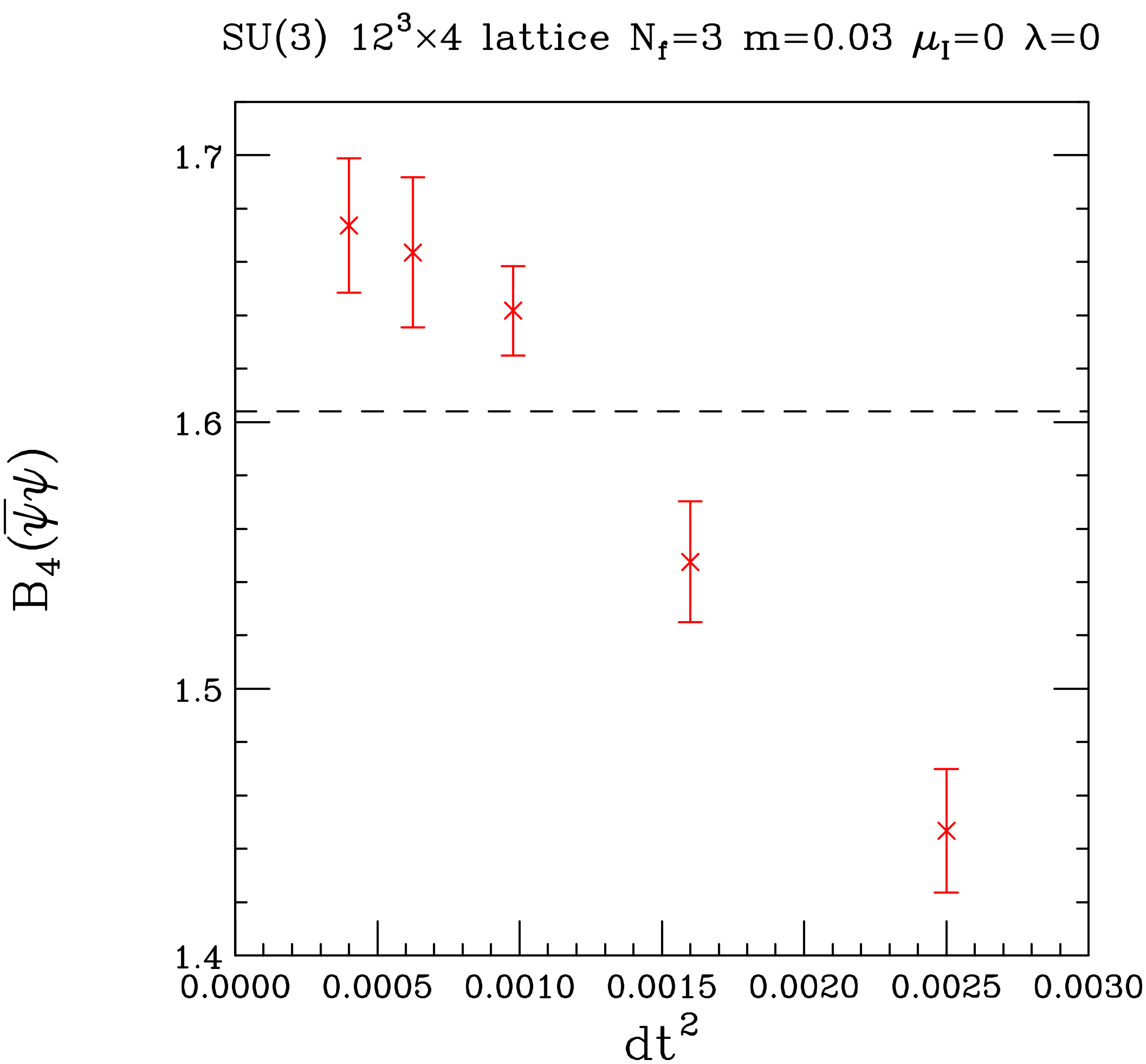

Figure 6: dt dependence of $B_4(\bar{\psi}\psi)$ at $m = 0.03$ and $\mu_I = 0$

The $dt = 0.05$ 'data' predicts $m_c \approx 0.0335$. By $dt = 0.02$ this has dropped to $m_c \approx 0.027$, i.e. by $\approx 20\%$. B_4 increases with decreasing dt – does this continue to lower dt ?

For $m = 0.035$, the μ_I dependence diminishes as $dt \to 0$. Is there a critical endpoint?

One can understand why B_4 increases with decreasing dt, since

$$\Delta\beta = \beta - \beta_{effective}$$

is much larger below the transition than above, and $\Delta\beta \to 0$ as $dt \to 0$. This reduces tunneling and makes the transition appear more first order.

This effect is also seen in the susceptibilities as seen in the figure after next.

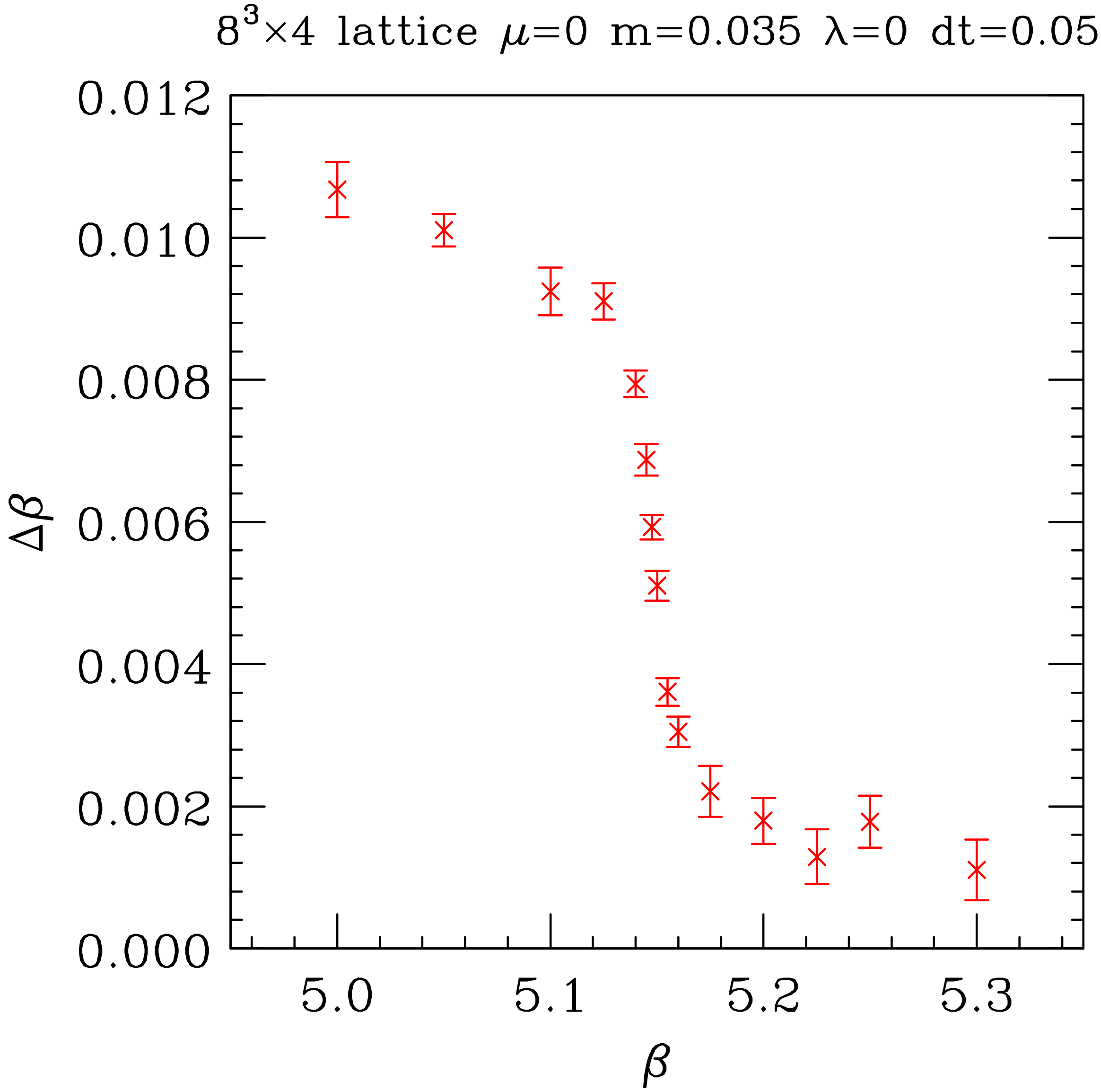

Figure 7: $\Delta\beta$ as a function of β close to the transition on an $8^3 \times 4$ lattice with $m = 0.035$ and $dt = 0.05$.

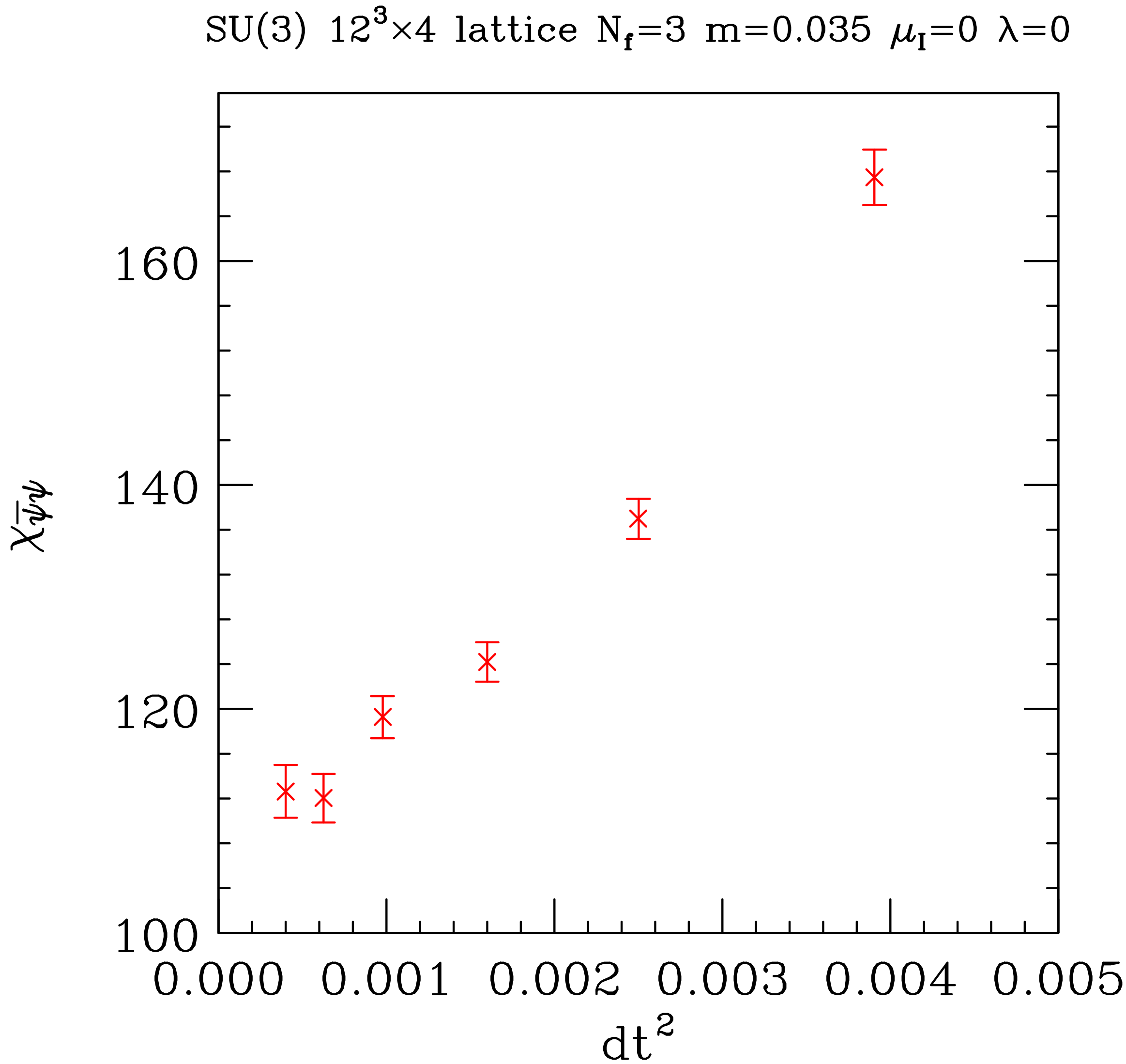

Figure 8: dt dependence of $\chi_{\bar{\psi}\psi}$ at $m = 0.035$ and $\mu_I = 0$.

The transition moves to lower β as μ_I is increased as can be seen in the following plot of the Wilson Lines as functions of β for different values of μ_I. The μ_I dependence of β_c for the lowest dt values is shown in the next graph. This dependence is reasonably close to that predicted by de Forcrand and Philipsen for finite μ if we take $\mu_I = 2\mu$. The straight line is:

$$\beta_c = 5.15195 - 0.1781\mu_I^2$$

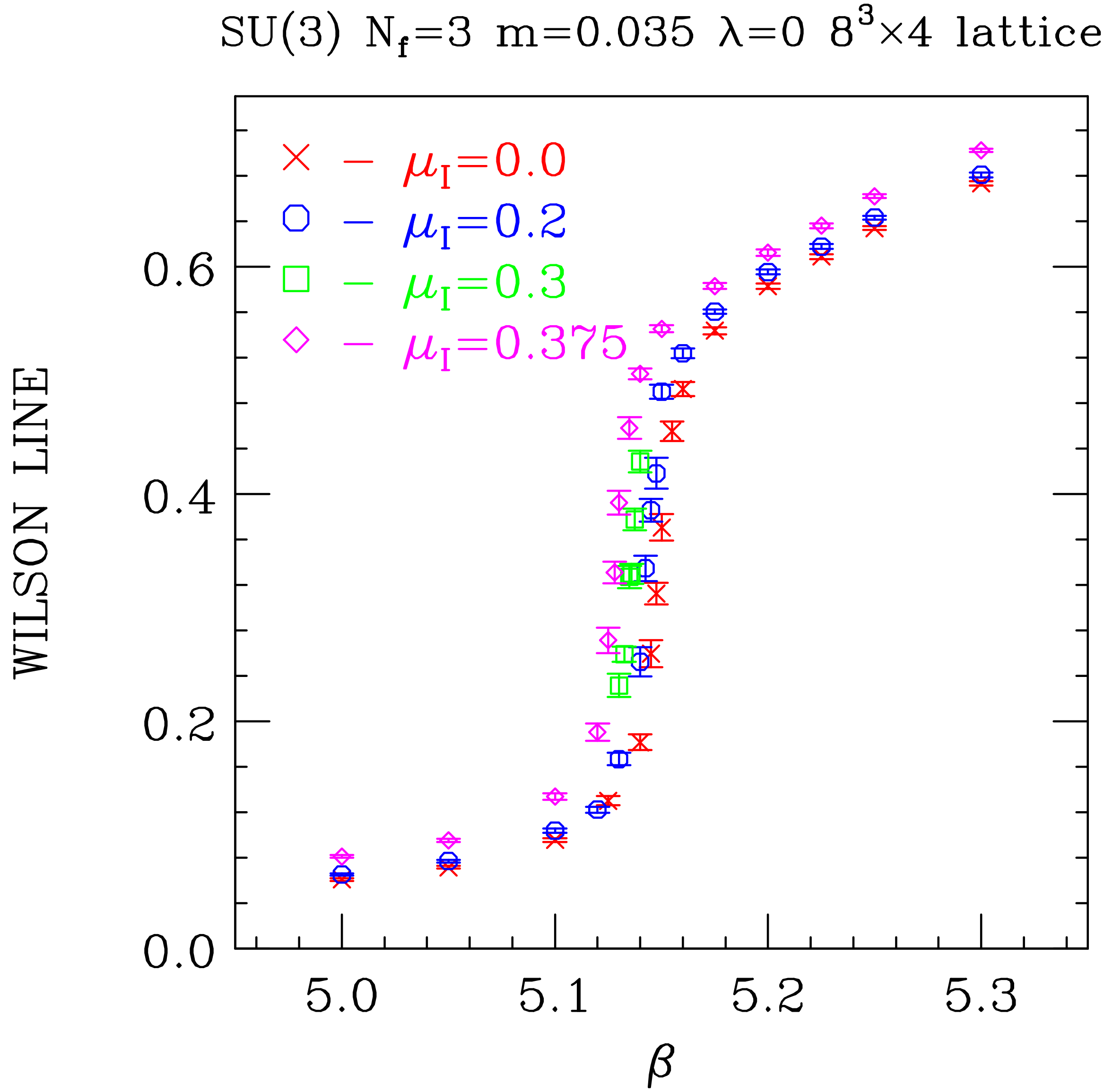

Figure 9: The Wilson Lines as a functions of β for values of μ_I in the range $0 \leq \mu_I \leq 0.375$ on an $8^3 \times 4$ lattice.

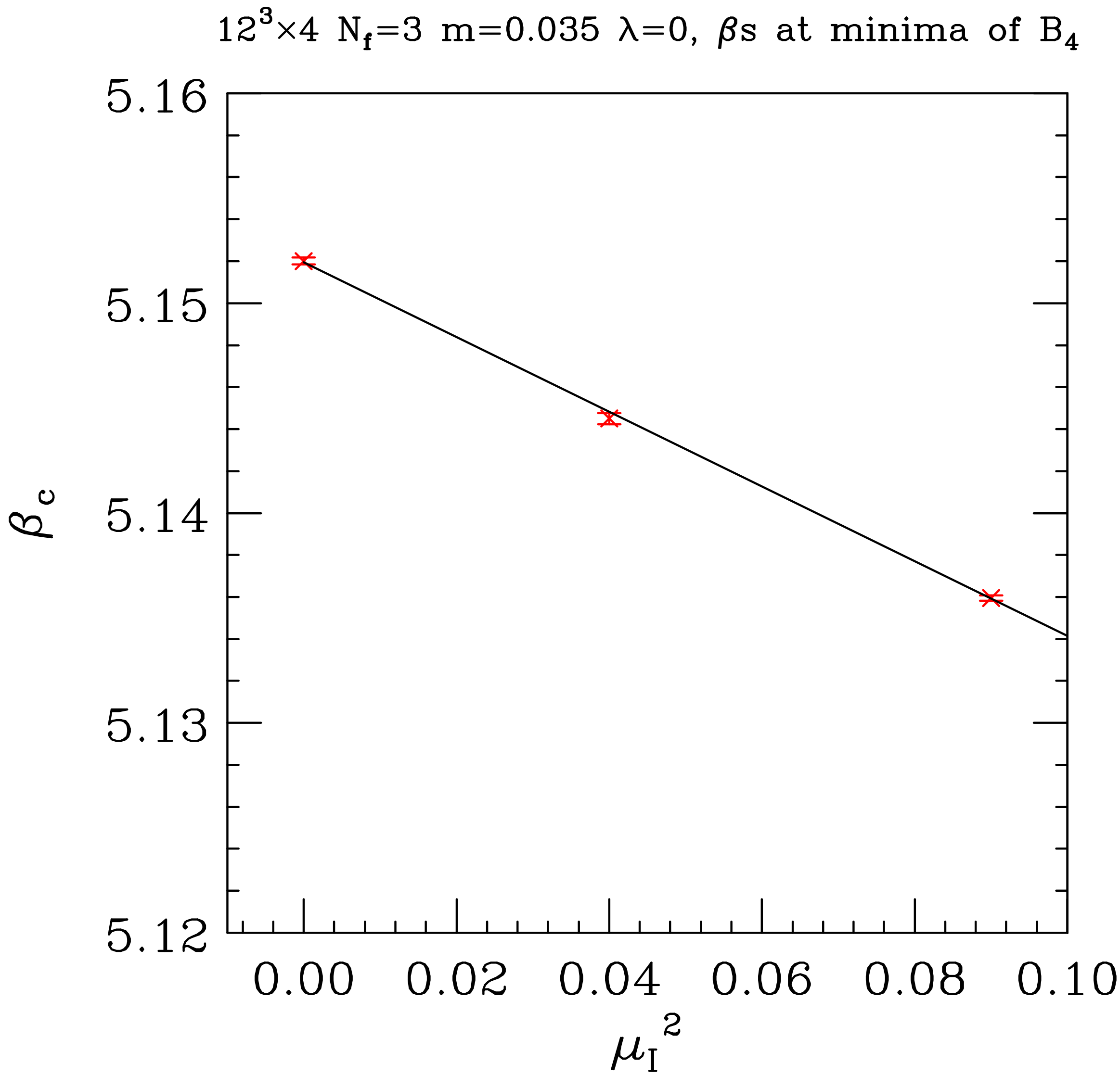

Figure 10: Graph of the μ_I dependence of β_c for $m = 0.035$ on a $12^3 \times 4$ lattice.

From finite μ_I to finite μ ?

Speculation.

The strong dependence of B_4 on dt suggests that we should replace the hybrid molecular-dynamics algorithm with one of the newer exact methods. Our choice should be governed by the fact that we wish to use the simulations at small μ_I and finite T as a basis for reweighting to finite μ. This suggests that we should use methods which use polynomial approximations to the inverse Dirac operator — multiboson or PHMC, where we can write formal expressions for a stochastic estimator for the fermion determinant, which suggests we might be able to get closed expressions for an estimator for the fermion phase.

These multiboson methods have the important property of locality. This gives the possibility of performing independent and simultaneous multiple updates of appropriately separated parts of the lattice, providing (some of) the exponential statistics needed to overcome the sign problem. Here 2 methods are worthy of consideration. The first is to expand around the finite μ_I theory. Here we need to contend with the fact that the quadratic Dirac operator in the action is not as local as one might like, so we would probably need to divide the lattice into relatively large domains. Thus this is probably only of use for relatively large lattices with a fine mesh.

The second is to include the whole fermion contribution in the measurements, allowing us to use the more local Dirac operator itself. This means using the exponential statistics to estimate the determinant of the Dirac operator, even at $\mu = 0$. Such a method could be tested by applying it to this case.

Discussion and conclusions

- QCD at small isospin chemical potential and QCD at small quark-number chemical potential appear to behave similarly close to the finite temperature transition.
- The Binder cumulant which is used to determine the nature of the finite temperature transititon shows large dt dependence, as does the chiral susceptibility.
- At zero μ_I and μ, the critical mass m_c is $\sim 20\%$ lower than previously thought.
- We have yet to see evidence for a critical endpoint. More simulations are in progress.

- Exact algorithms should be implemented to avoid dt errors.
- QCD at finite μ_I shows promise for reweighting to finite μ.
- Polynomial methods (Multiboson, PHMC, etc.) show promise for avoiding exact determinant calculations.
- Locality of polynomial methods might provide ways of reducing QCD at finite μ from an exponential- to a polynomial-time problem.

These simulations are being run on the Jazz cluster at Argonne's LCRC, the Tungsten and Cobalt clusters at NCSA, and the Jacquard cluster at NERSC. Some of the small lattice runs were done on Linux PCs in the HEP division at Argonne.