Lattice QCD at finite T and small μ ignoring the fermion phase.

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Introduction

Simulating lattice QCD directly at finite baryon/quark-number density or equivalently at finite chemical potential μ for quark number, suffers from a sign problem. This makes the use of standard simulation methods difficult if not impossible.

We have been studying lattice QCD at finite chemical potential μ_I for isospin (I_3). This theory has a positive fermion determinant so standard simulation methods work. We use hybrid molecular dynamics simulations with "noisy" fermions (quarks).

Although the phase structures of QCD at finite μ and QCD at finite μ_I are very different, we shall argue that at small

μ/μ_I their behaviour close to the finite temperature (deconfinement/chiral) transition from hadronic matter to a quark-gluon plasma is (almost) identical. Small means $\mu_I < m_\pi$ ($\mu < m_\pi/2$). To the extent that this is correct, it offers an alternative to other methods – series expansion, analytic continuation, reweighting... – for determining the phase structure of QCD at small μ and finite T.

The expected phase structure of the 2 theories for $N_f = 2$ is shown below:

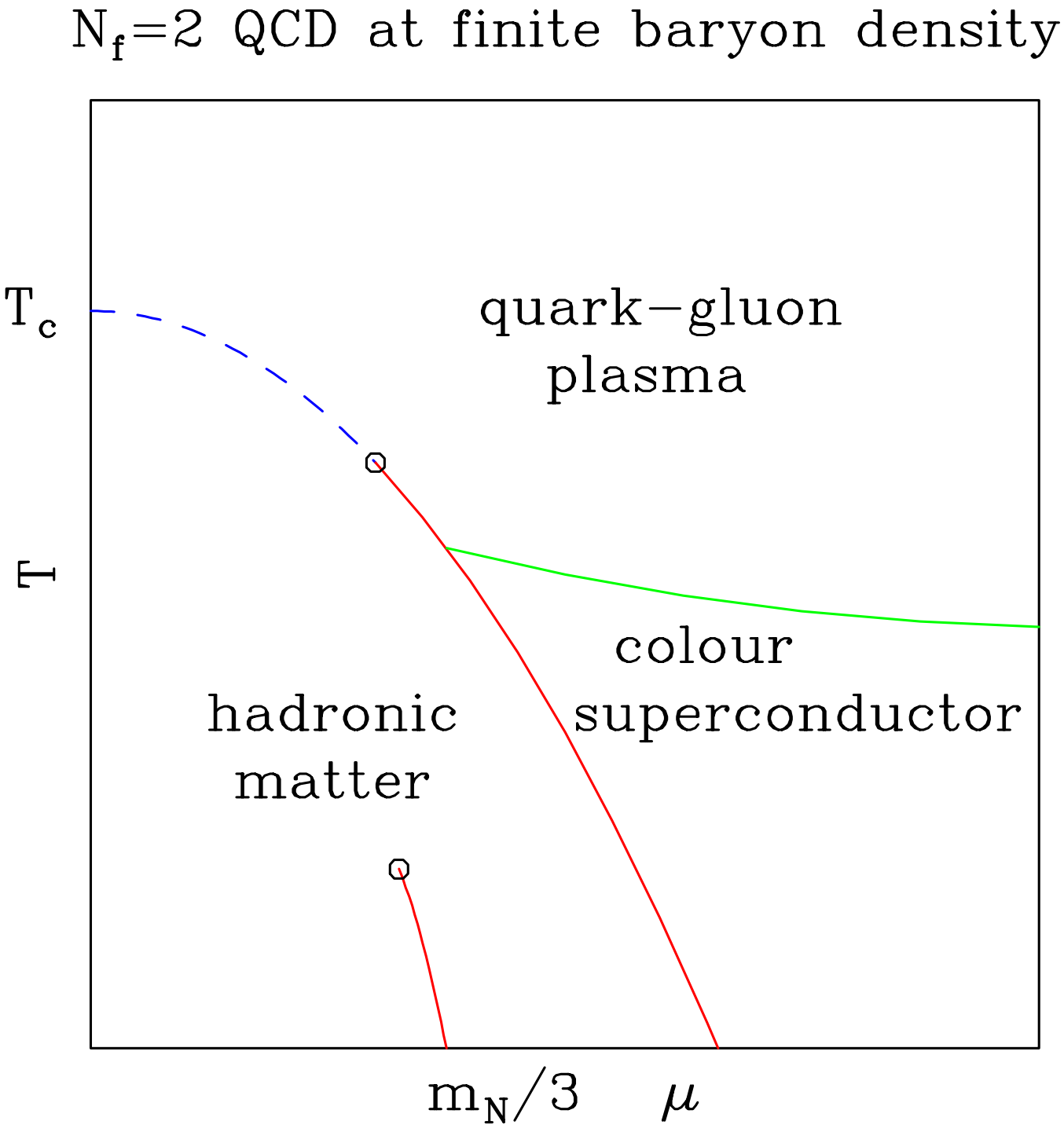

Figure 1: Proposed phase diagram for 2-flavour QCD at finite quark-number chemical potential μ and temperature T.

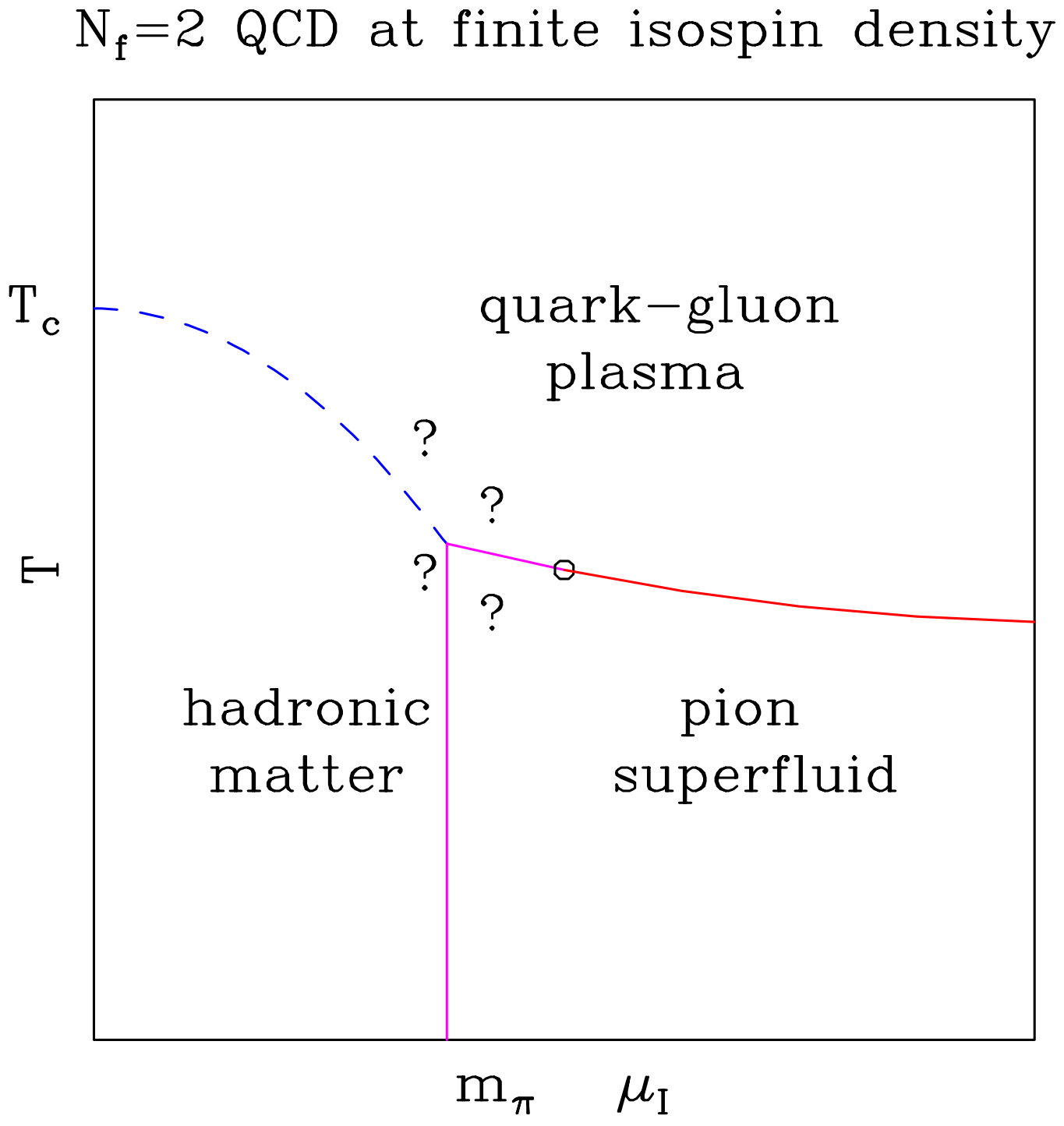

Figure 2: Proposed phase diagram for 2-flavour QCD at finite isospin chemical potential μ_I and temperature T.

As indicated in the second figure, we have been unable to find the expected critical endpoint in 2-flavour QCD.

In 3-flavour QCD there exists a critical quark mass m_c below which the transition is first order at $\mu/\mu_I = 0$, so the critical endpoint is at $\mu/\mu_I = 0$. For $m > m_c$, the critical endpoint is expected to move to finite μ/μ_I which can be kept as small as desired, in particular to where the μ/μ_I behaviours are identical.

Lattice QCD at finite μ_I

The staggered quark action for lattice QCD at finite μ_I is

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

where $\not{D}(\frac{1}{2}\tau_3\mu_I)$ is the standard staggered quark $\not{D}$ with the links in the $+t$ direction multiplied by $\exp(\frac{1}{2}\tau_3\mu_I)$ and those in the $-t$ direction multiplied by $\exp(-\frac{1}{2}\tau_3\mu_I)$. The λ term is an explicit I_3 symmetry breaking term required to see spontaneous symmetry breaking on a finite lattice. The determinant

$$\det[\not{D}(\frac{1}{2}\tau_3\mu_I)+m+i\lambda\epsilon\tau_2] = \det[\mathcal{A}^\dagger\mathcal{A}+\lambda^2], \quad (2)$$

where

$$\mathcal{A} \equiv \not{D}(\frac{1}{2}\mu_I) + m, \tag{3}$$

is positive allowing us to use standard hybrid molecular dynamics simulations.

For $\lambda = 0$ this determinant is just the magnitude of the determinant for 8-flavour lattice QCD with quark-number chemical potential

$$\mu = \frac{1}{2}\mu_I \tag{4}$$

We use hybrid molecular-dynamics simulations and tune the number of flavours to 2 (or 3).

At zero temperature, this theory undergoes a second order phase transition with mean-field critical exponents to a superfluid phase in which the third component of isospin I_3 is broken sponta-

neously by a charged pion condensate, at $\mu_I = m_\pi$. The orthogonal charged pion state is the associated Goldstone boson.

2-flavour lattice QCD at small μ_I and finite T

We simulate the above theory using the hybrid molecular-dynamics method with the number of flavours set to 2. Finite temperature is achieved using a lattice with temporal extent $aN_t = 1/T$ and spatial size $aN_s >> aN_t$. From here on we set $a = 1$. Small μ_I means $\mu_I < m_\pi$.

We have used an $8^3 \times 4$ lattice, and have performed simulations for quark masses $m = 0.05, 0.1, 0.2$. $\beta = 6/g^2$ and hence [since $a = a(g^2)$] $T = 1/(aN_t)$, are varied across the transition (crossover) from hadronic matter to a quark-gluon plasma. Since $\mu_I < m_\pi$ we were able to run with $\lambda = 0$.

I will now show the variation of the

chiral condensate, thermal Wilson line (Polyakov loop) and isospin (I_3) density. In addition I show the corresponding susceptibilities and that for the plaquette. For the chiral condensates and number density susceptibilities, we use 5 noise vectors for each measurement and discard the noise diagonal contributions, thus obtaining an unbiased estimate for these susceptibilities.

$$\chi_{\mathcal{O}} = V\langle \mathcal{O}^2 - \langle \mathcal{O} \rangle^2 \rangle \qquad (5)$$

with $V = N_t N_s^3$. (Note that for the Wilson line this is really χ_{Wilson}/T.)

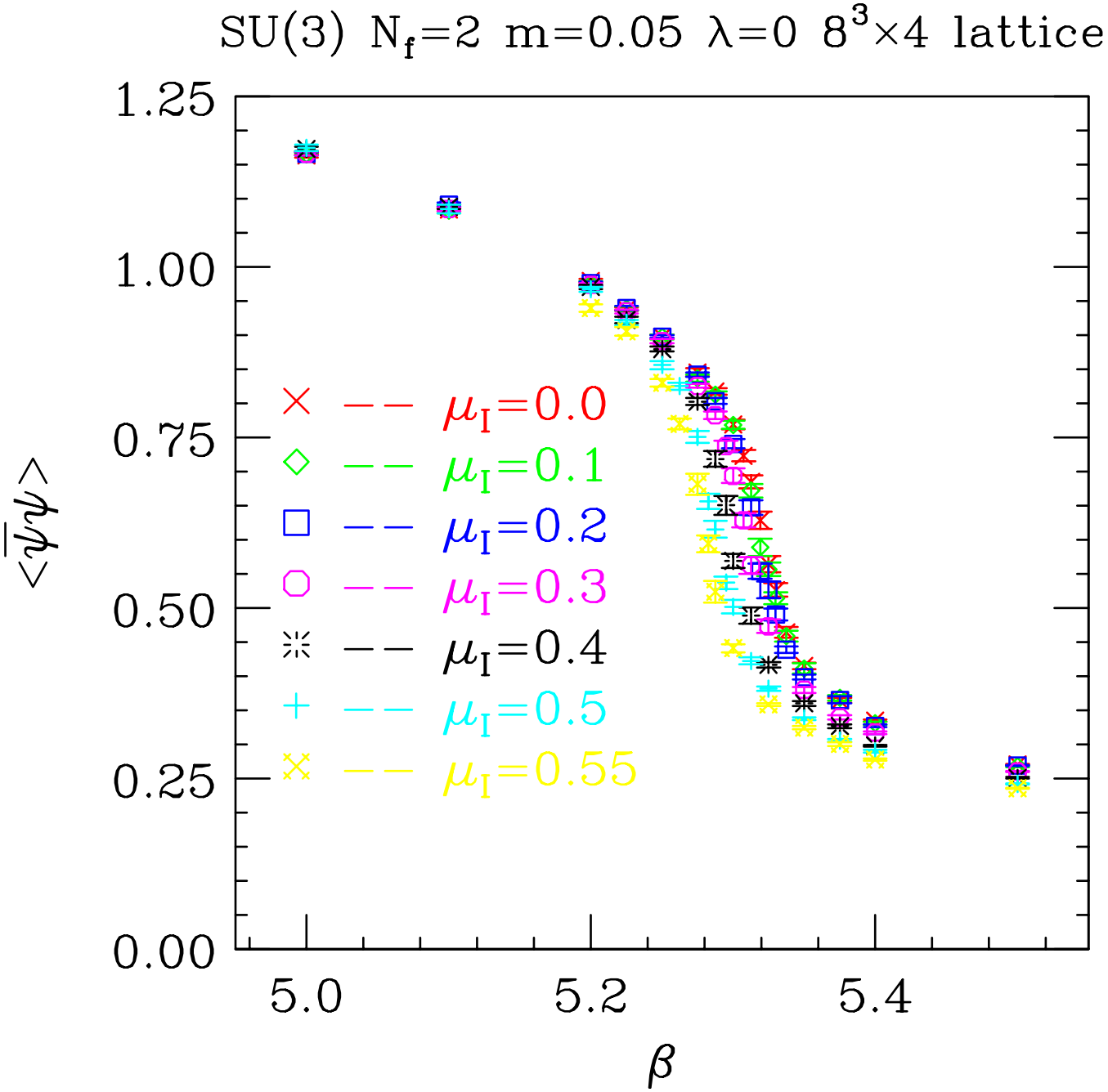

Figure 3: Chiral condensate as a function of $\beta = 6/g^2$ for μ_I values ≤ 0.55.

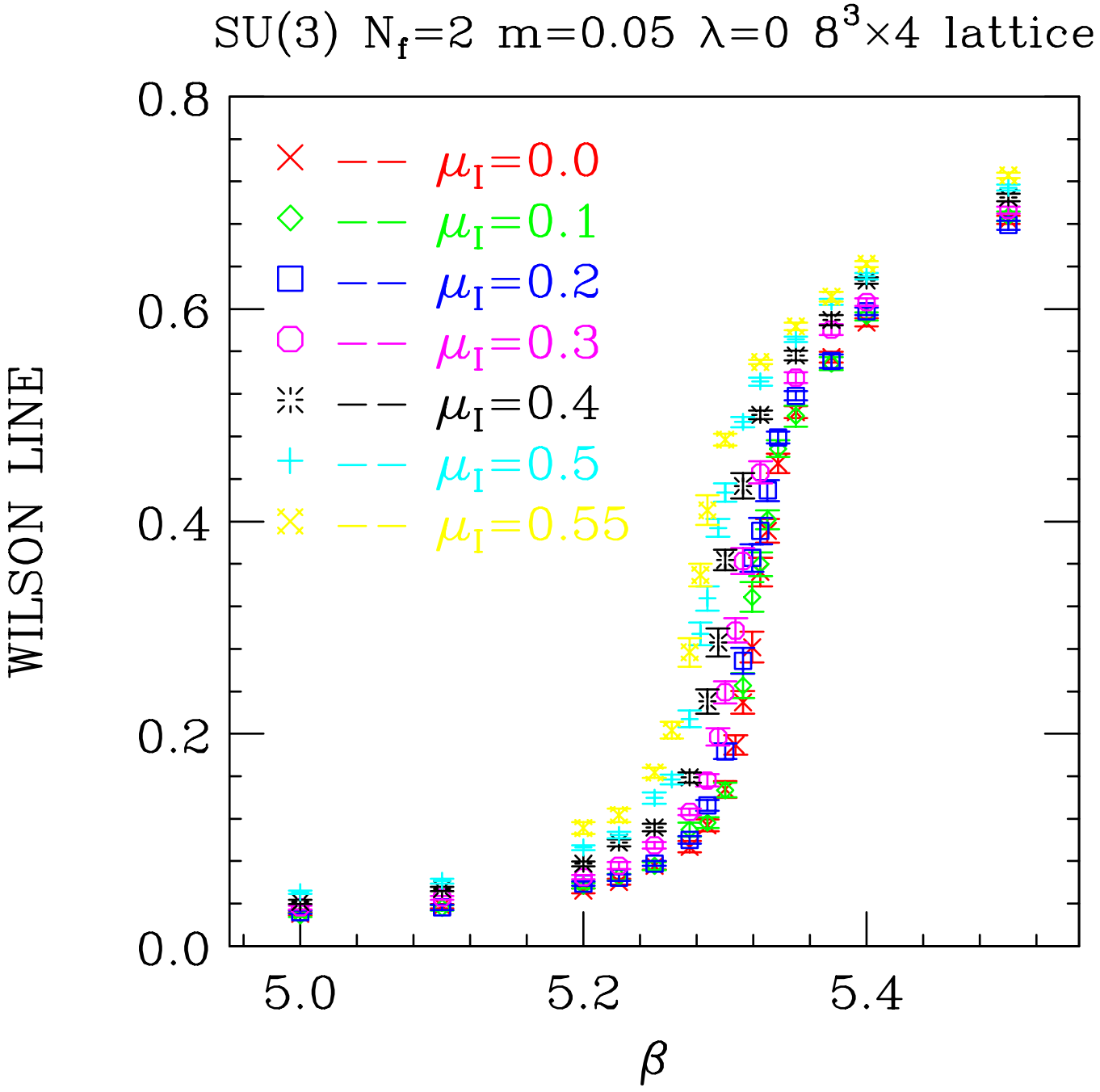

Figure 4: Wilson Line as a function of $\beta = 6/g^2$ for μ_I values ≤ 0.55.

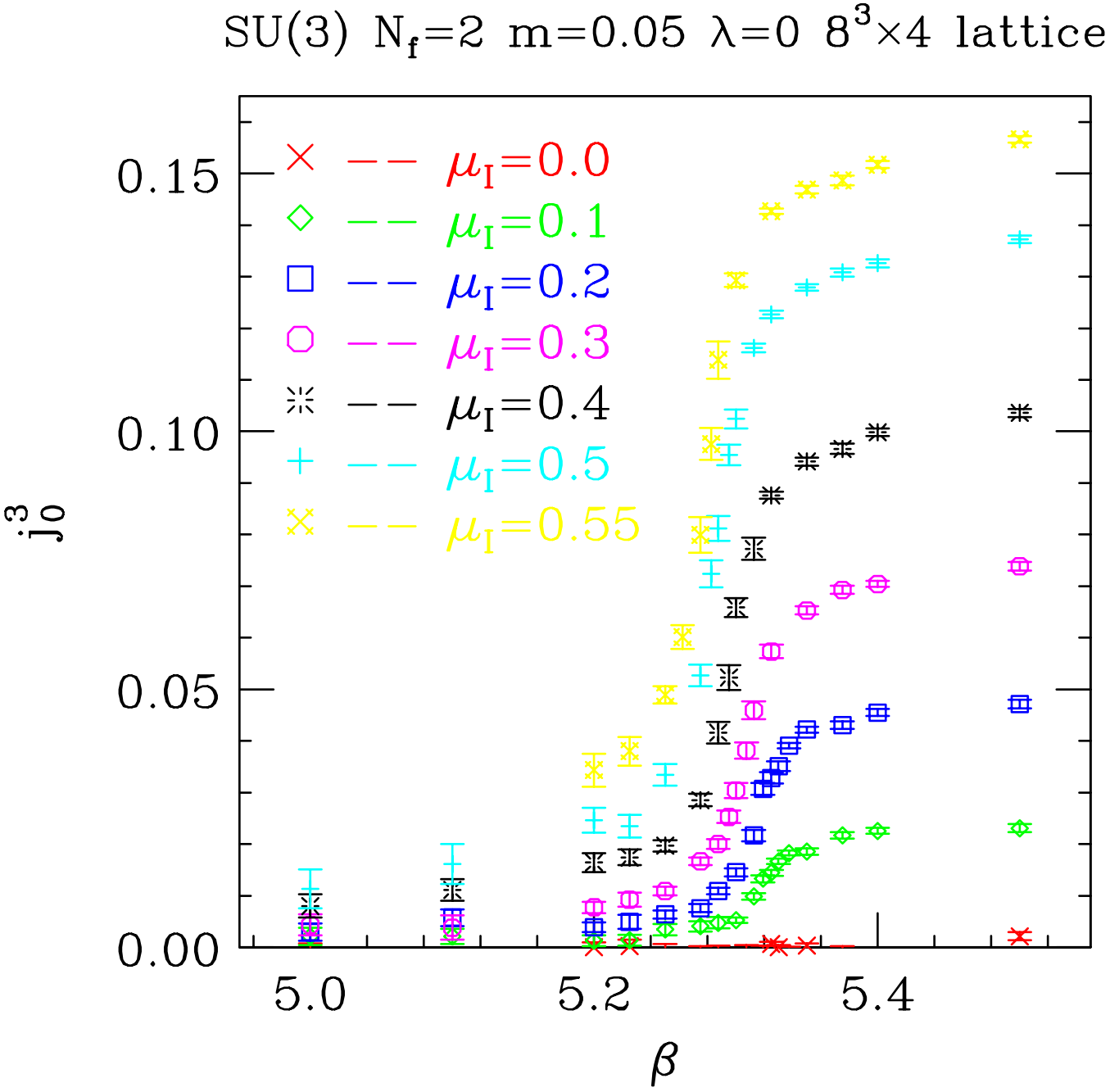

Figure 5: Isospin density as a function of $\beta = 6/g^2$ for μ_I values ≤ 0.55.

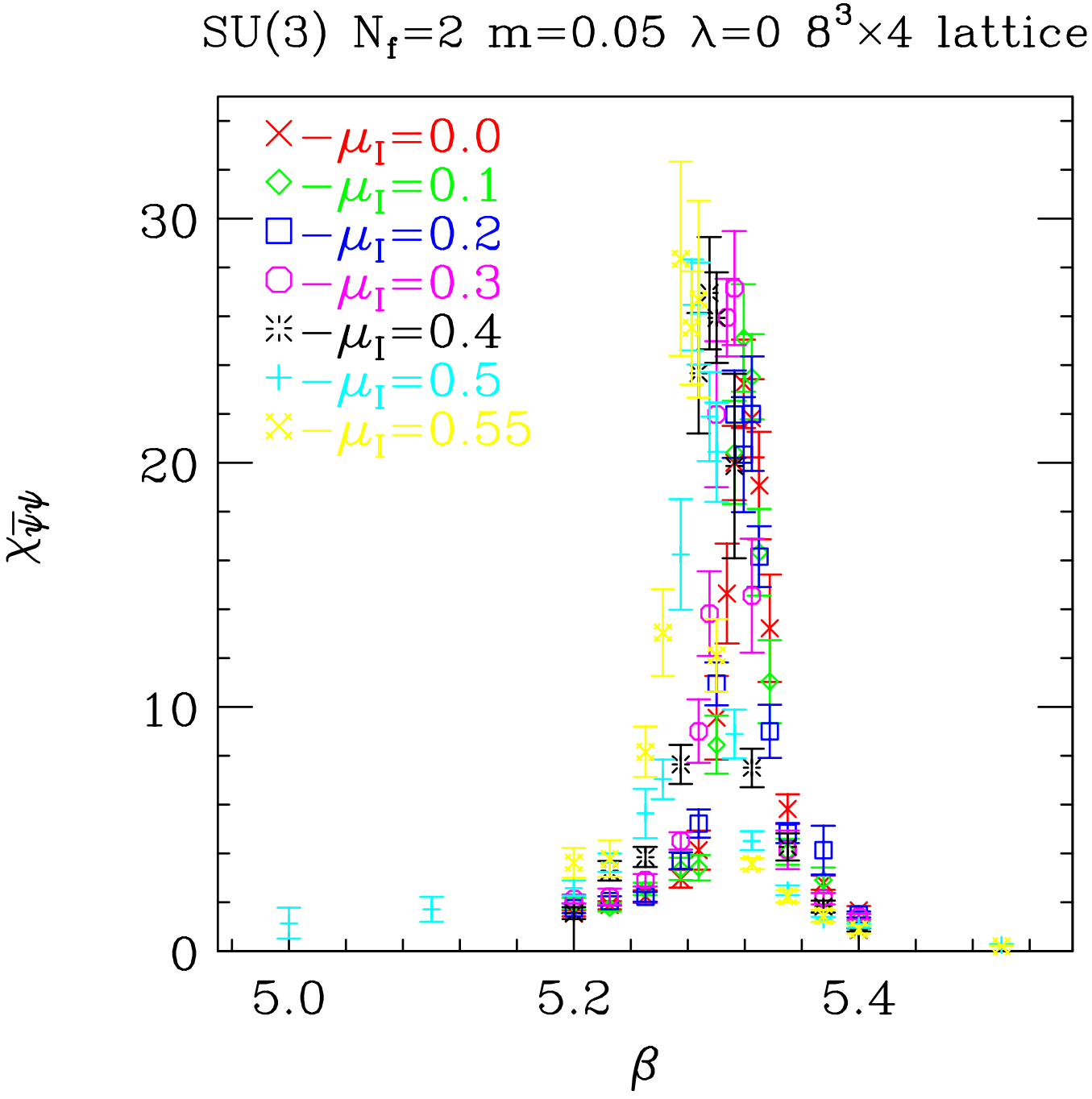

Figure 6: Chiral susceptibility as a function of $\beta = 6/g^2$ for μ_I values ≤ 0.55.

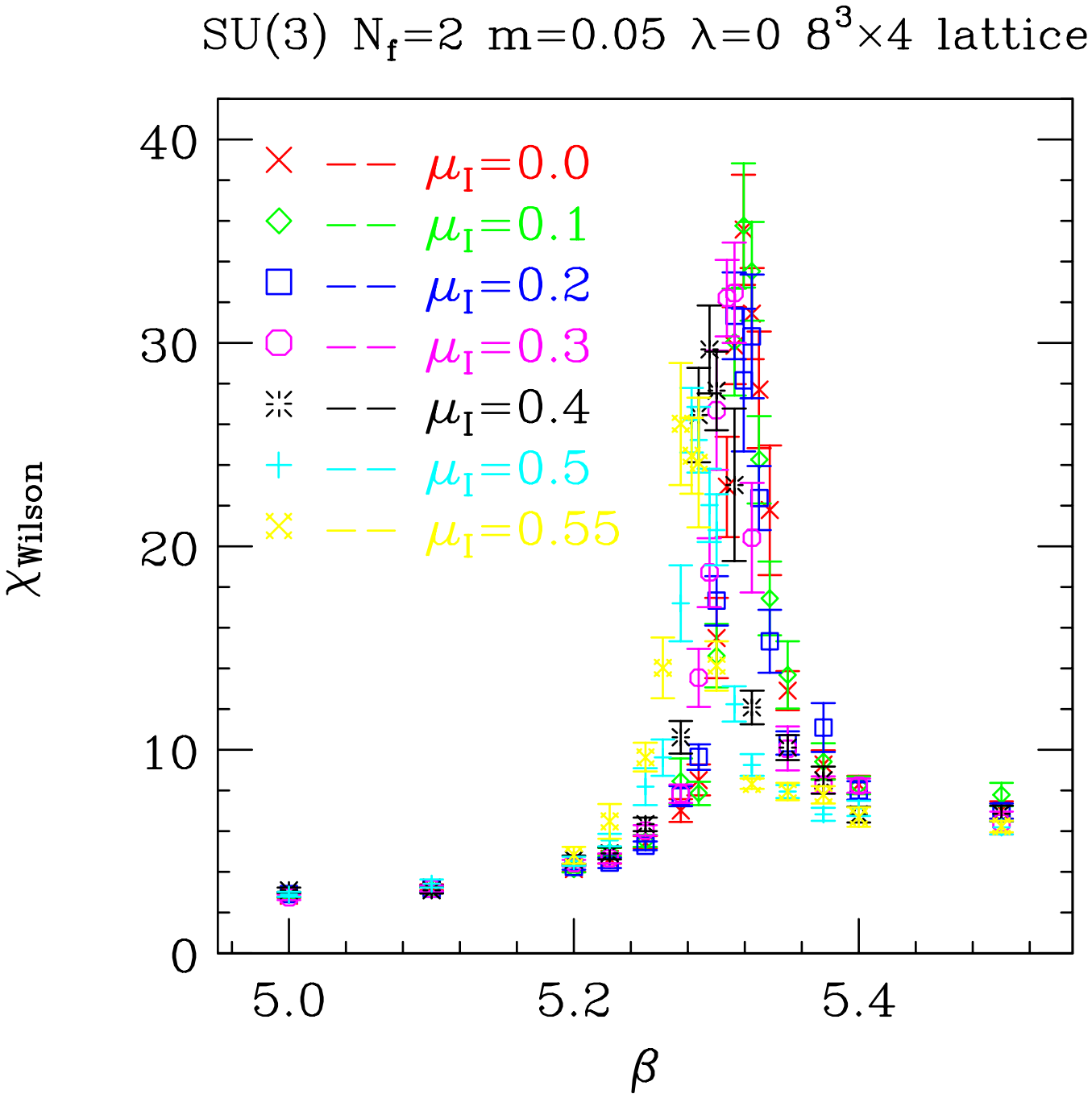

Figure 7: Wilson Line susceptibility as a function of $\beta = 6/g^2$ for μ_I values ≤ 0.55.

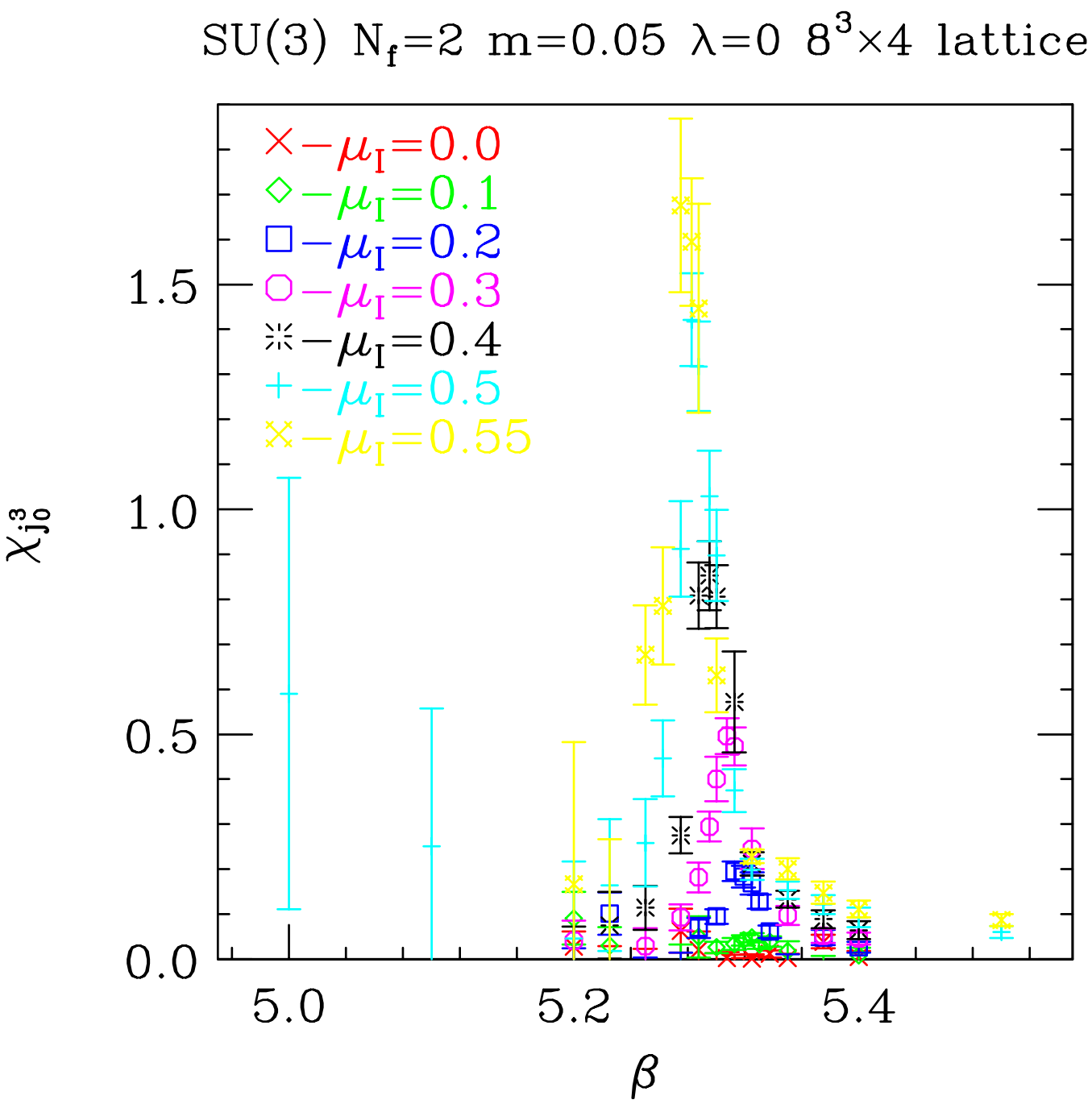

Figure 8: Isospin susceptibility as a function of $\beta = 6/g^2$ for μ_I values ≤ 0.55.

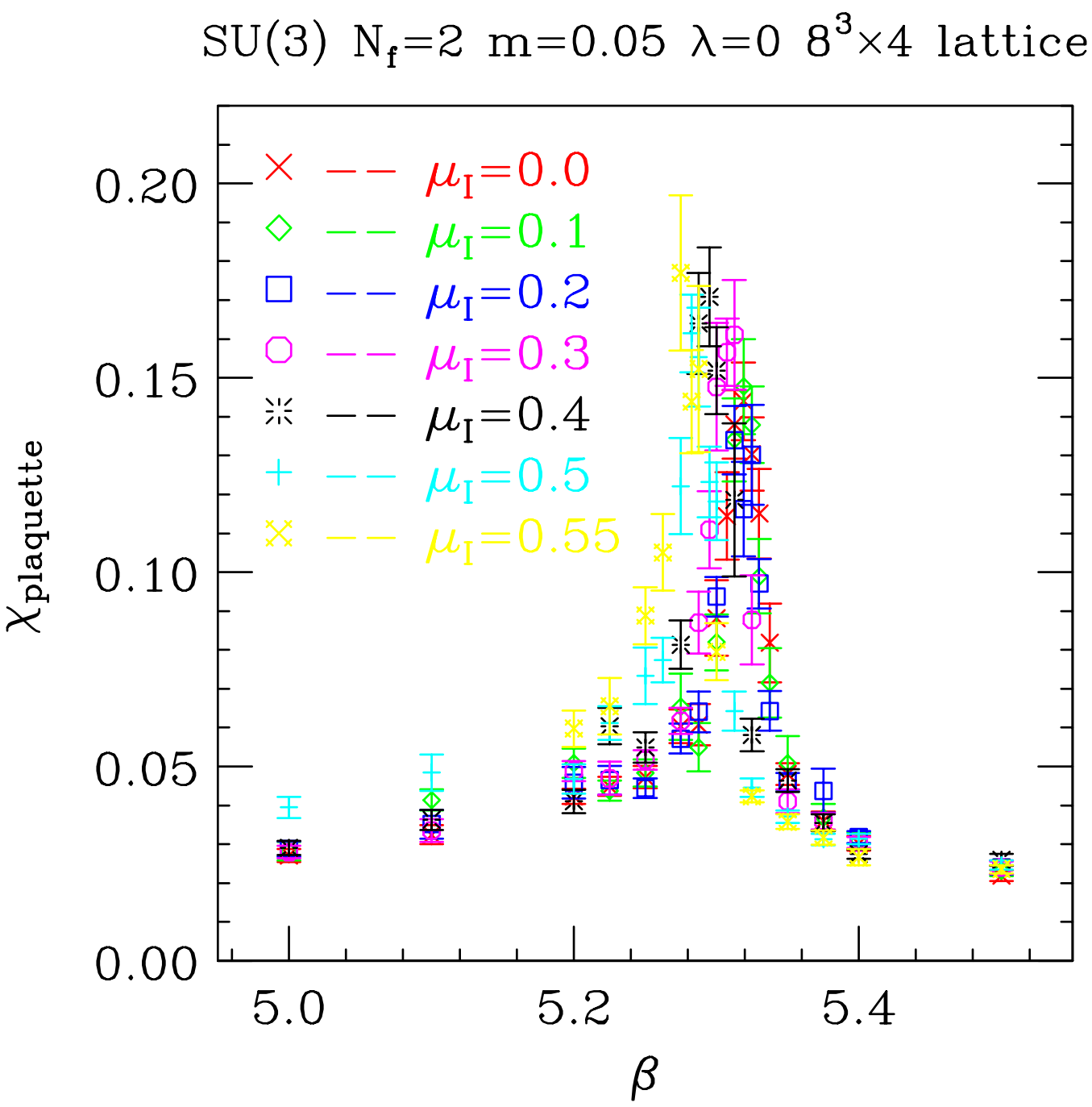

Figure 9: Plaquette susceptibility as a function of $\beta = 6/g^2$ for μ_I values $\leq$ 0.55.

The graphs for $m = 0.1$ and $m = 0.2$ are similar. No sign that this transition is anything but a crossover is seen for any of the m and μ_I values used.

Ferrenberg-Swendsen reweighting is then used to find the peaks (β_c) of the susceptibility curves. In each case we have several βs which are close enough to the maximum to be used. We note that the estimates from these several βs are consistent. What is also reassuring is that the estimates from the 4 different susceptibilities are close, indicating that they provide a reasonable definition of the position of the crossover. The next graph shows the positions (β_c) of these susceptibility peaks as functions of μ_I for the 3 mass values. We note a slow

decrease of β_c with increasing μ_I. For $m = 0.05$, taking $T_c \approx 173$ MeV at $\mu_I = 0$, then by $\mu_I \approx 381\,\mathrm{MeV}, T_c(\mu_I) \approx 164$ MeV.

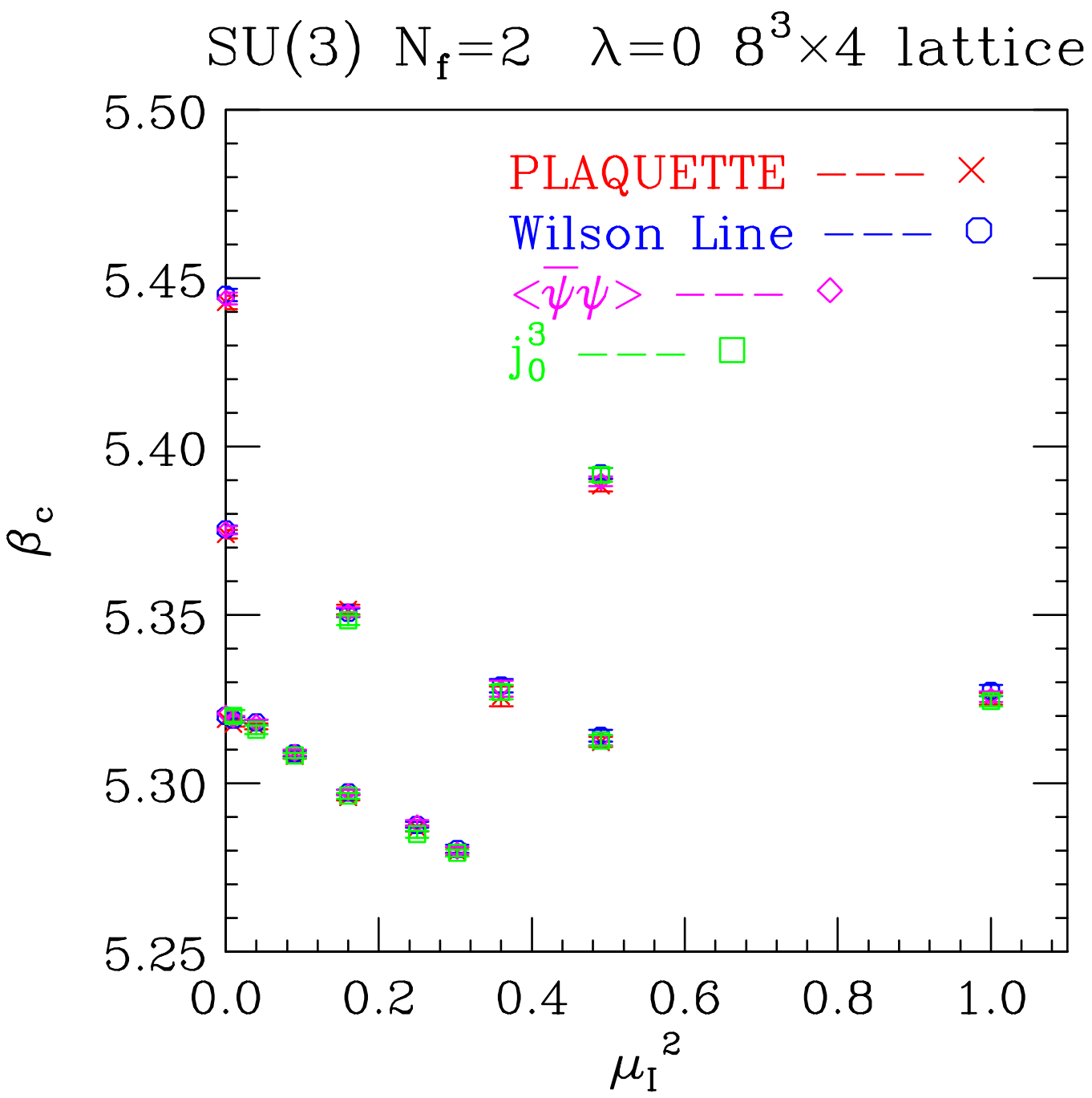

Figure 10: β_c determined from the maxima of the susceptibilities, as a function of μ_I^2. The top points are for $m = 0.2$ the next are for $m = 0.1$, and the bottom set are for $m = 0.05$

The Bielefeld-Swansea collaboration have calculated the phase of the fermion determinant, and find that it is well behaved for small μ in that

$$\langle \cos\theta \rangle \qquad (6)$$

where θ is the phase of the determinant, decreases smoothly from 1 and has an appreciable range of μ over which it is considerably greater than zero, for a $16^3 \times 4$ lattice, which is large enough for sensible studies of the phase diagram.

When this phase is well behaved, one should be able to calculate expectation values of gluonic observables using

$$\langle \mathcal{O} \rangle_\mu = \frac{\langle e^{i\theta} \mathcal{O} \rangle_{\mu_I = 2\mu}}{\langle \cos\theta \rangle_{\mu_I = 2\mu}} \qquad (7)$$

Then, to the extent that the position of the transition is well defined,

$$\beta_c(\mu) = \beta_c(\mu_I = 2\mu) \qquad (8)$$

This is in agreement with the observations of the Bielefeld-Swansea collaboration. A straight line 'fit' to the $m = 0.05$ data gives

$$\beta_c = 5.322 - 0.143\mu_I^2 \qquad (9)$$

which is in good agreement with what de Forcrand and Philipsen obtained from analytic continuations from imaginary μ. We have calculated an unbiased estimate of $\langle\theta^2\rangle$ to lowest non-trivial order in μ_I using the Bielefeld-Swansea formula and our $\mu_I = 0$ simulations:

$$\theta = \frac{1}{4}V\mathrm{Im}(j_0)\mu_I \qquad (10)$$

To this order

$$\langle \cos\theta \rangle \approx 1 - \frac{1}{2}\langle \theta^2 \rangle \qquad (11)$$

The following table indicates that there is indeed a considerable range of μ_I over which the phase of the determinant at the corresponding value of μ is well-behaved.

m	β	$\langle\theta^2\rangle/\mu_I^2$
0.05	5.3000	5.5(2.1)
0.05	5.3075	6.7(1.7)
0.05	5.3125	2.6(1.2)
0.05	5.3190	5.5(1.2)
0.05	5.3250	4.0(1.2)
0.05	5.3300	2.7(1.2)
0.05	5.3375	2.7(0.9)
0.10	5.3500	4.1(1.2)
0.10	5.3625	4.7(0.8)
0.10	5.3750	3.3(0.7)
0.10	5.3875	1.5(0.6)
0.10	5.4000	0.6(1.8)
0.20	5.4250	4.4(0.6)
0.20	5.4375	3.2(0.5)
0.20	5.4500	2.5(0.4)
0.20	5.4625	1.9(0.4)
0.20	5.4750	1.9(0.5)

3-flavour lattice QCD at small μ_I and finite T

We are now extending our studies of the finite temperature transition for small μ_I to 3 flavours. Clearly this does not represent a physical theory, since it has 3/2 up-type flavours and 3/2 down-type flavours. However, since we are really interested in this as a model for the behaviour of 3-flavour QCD at finite μ this should not concern us.

For $\mu = \mu_I = 0$ we know that the finite temperature transition is first order for $m < m_c$, second order with Ising critical exponents for $m = m_c$ and a crossover without an actual phase transition for $m > m_c$. It is believed that as m is increased above m_c (with $\mu_I = 0$), this critical endpoint moves

continuously from $\mu = 0$ to $\mu > 0$. Presumably if μ is fixed at zero and μ_I is varied, this critical endpoint will move to $\mu_I > 0$. If the phase of the determinant is as well behaved as for 2 flavours, then for m sufficiently close to m_c we would expect that these critical endpoints are related by

$$\mu_c = \mu_{Ic}/2 \qquad (12)$$

giving us a way of determining this endpoint.

We are performing simulations on an $8^3 \times 4$ lattice with $m > m_c$, and $\mu_I < m_\pi$. Since an $8^3 \times 4$ lattice is too small to determine the precise nature of the phase transition, we have commenced simulations with the same masses and chemical potentials on a $16^3 \times$

4 lattice. For $N_t = 4$, the Bielefeld group find $m_c \approx 0.033$. Since we want m close to m_c, we have been simulating at $m = 0.035$ and $m = 0.04$. The behaviours of the Wilson line (Polkakov loop) as functions of β for several μ_Is are graphed below.

We have started simulations at $m = 0.035$ and $\mu_I = 0.375$ on a $16^3 \times 4$ lattice to see whether the transition is first order. On an $8^3 \times 4$ lattice there was evidence of a 2-state signal which would suggest that the transition was first order, even at $\mu_I = 0$ where we know it to be a mere crossover.

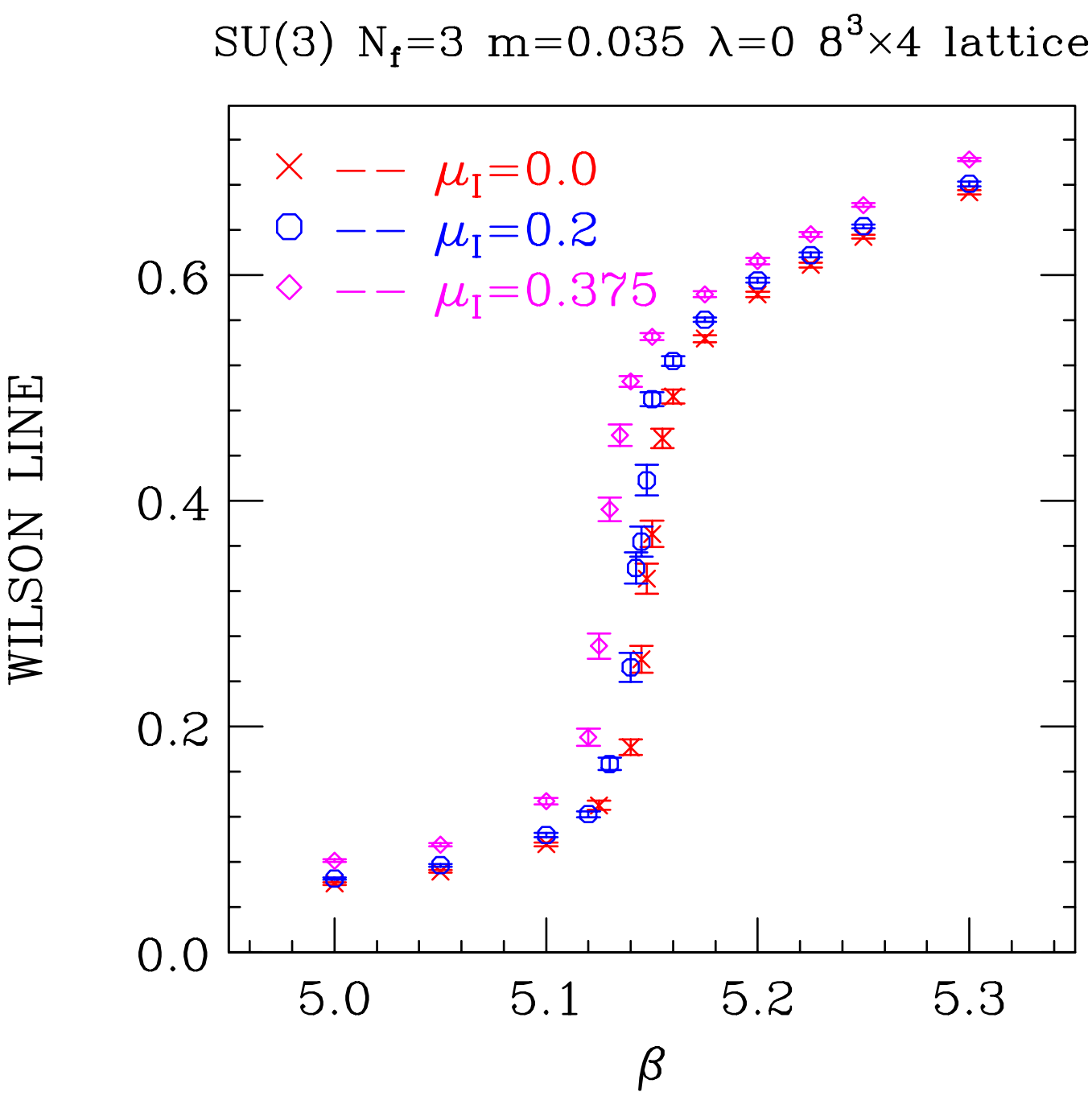

Figure 11: Wilson Line as a function of $\beta = 6/g^2$ for $m = 0.035$ and μ_I values ≤ 0.375.

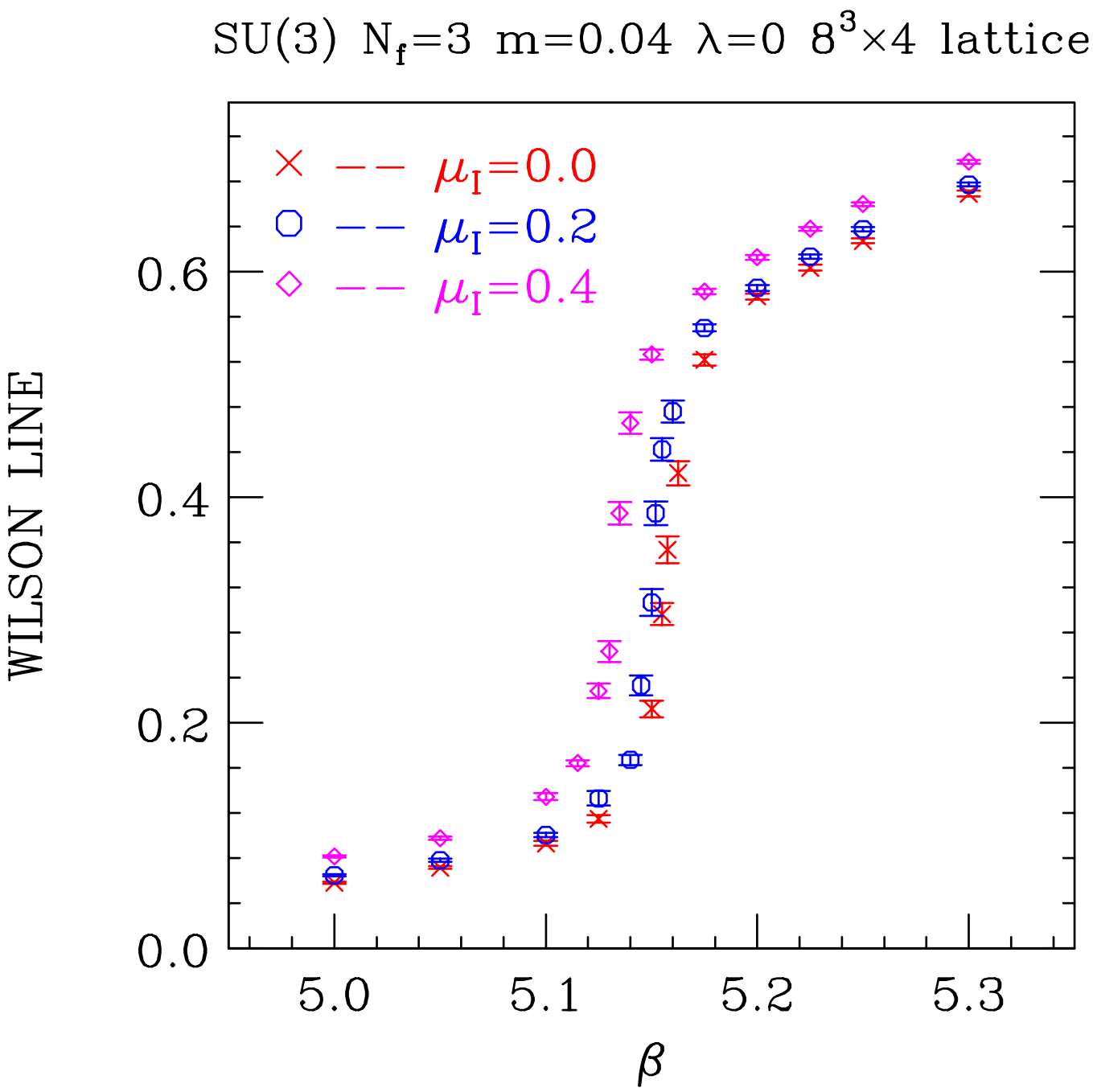

Figure 12: Wilson Line as a function of $\beta = 6/g^2$ for $m = 0.04$ and μ_I values ≤ 0.4.

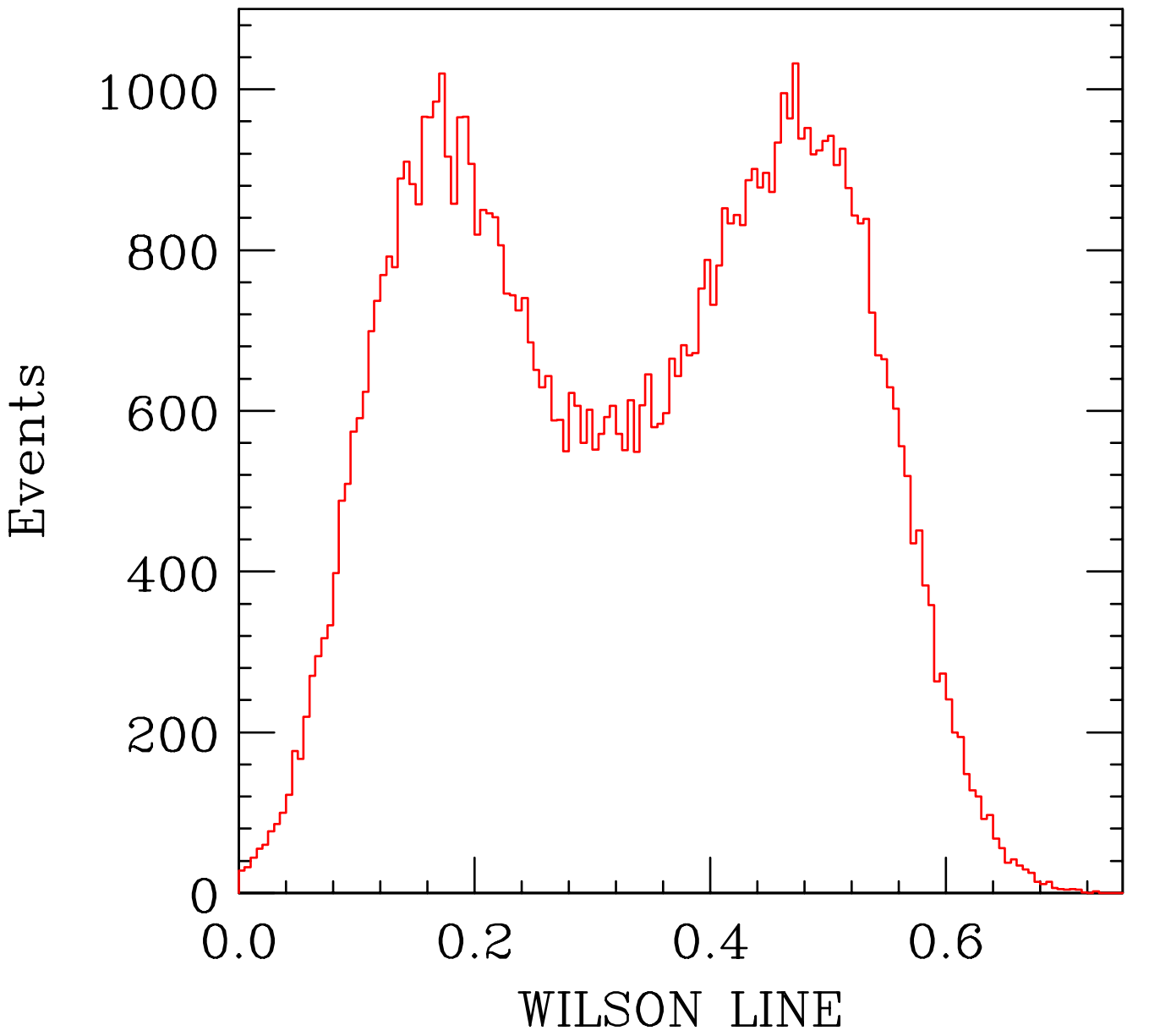

Figure 13: Histogram of Wilson Line 'time' evolution at $\beta = 5.1475$, $m = 0.035$ and $\mu_I = 0$, on an $8^3 \times 4$ lattice with $N_f = 3$.

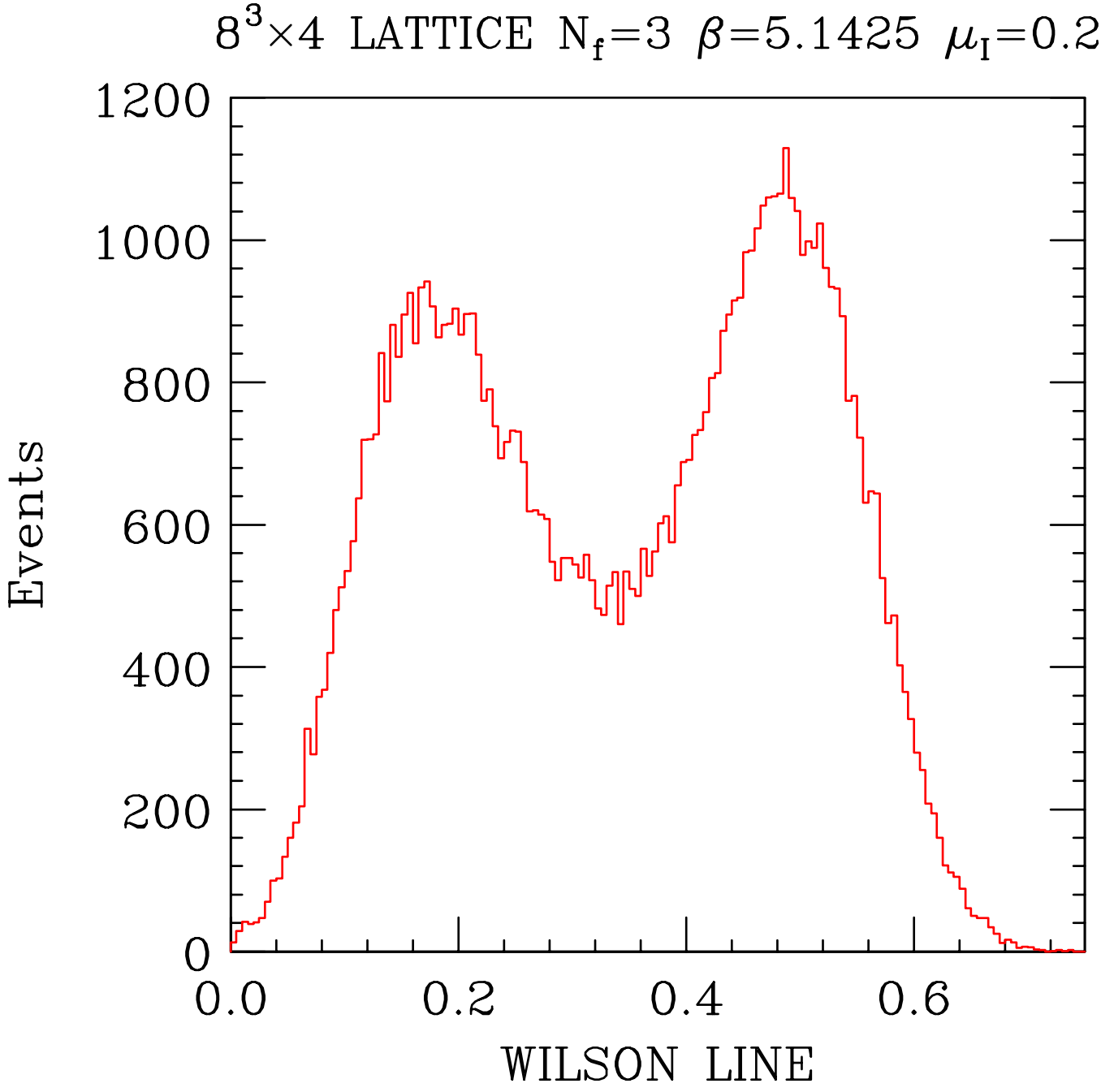

Figure 14: Histogram of Wilson Line 'time' evolution at $\beta = 5.1425$, $m = 0.035$ and $\mu_I = 0.2$, on an $8^3 \times 4$ lattice with $N_f = 3$.

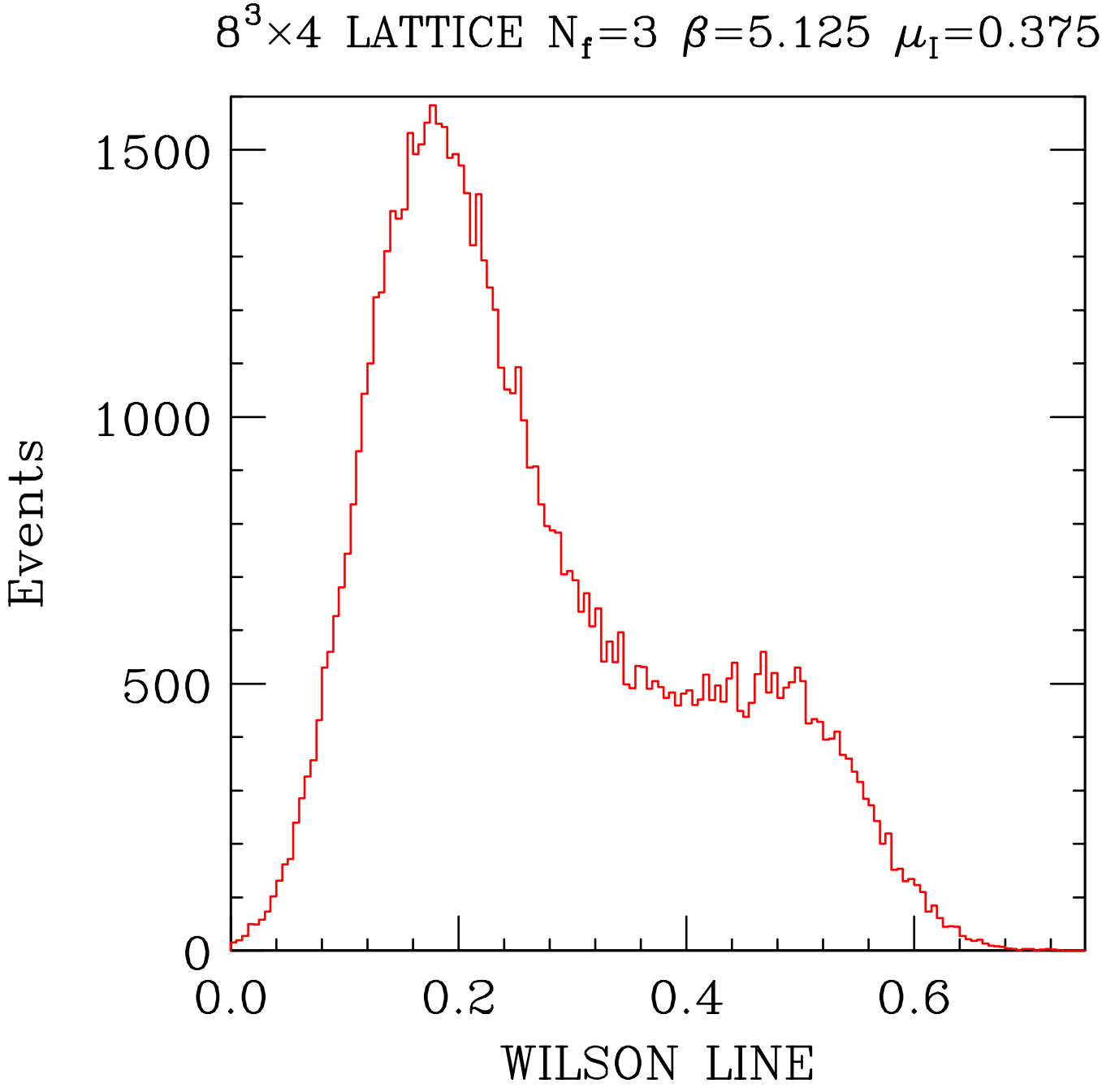

Figure 15: Histogram of Wilson Line 'time' evolution at $\beta = 5.125$, $m = 0.035$ and $\mu_I = 0.375$, on an $8^3 \times 4$ lattice with $N_f = 3$.

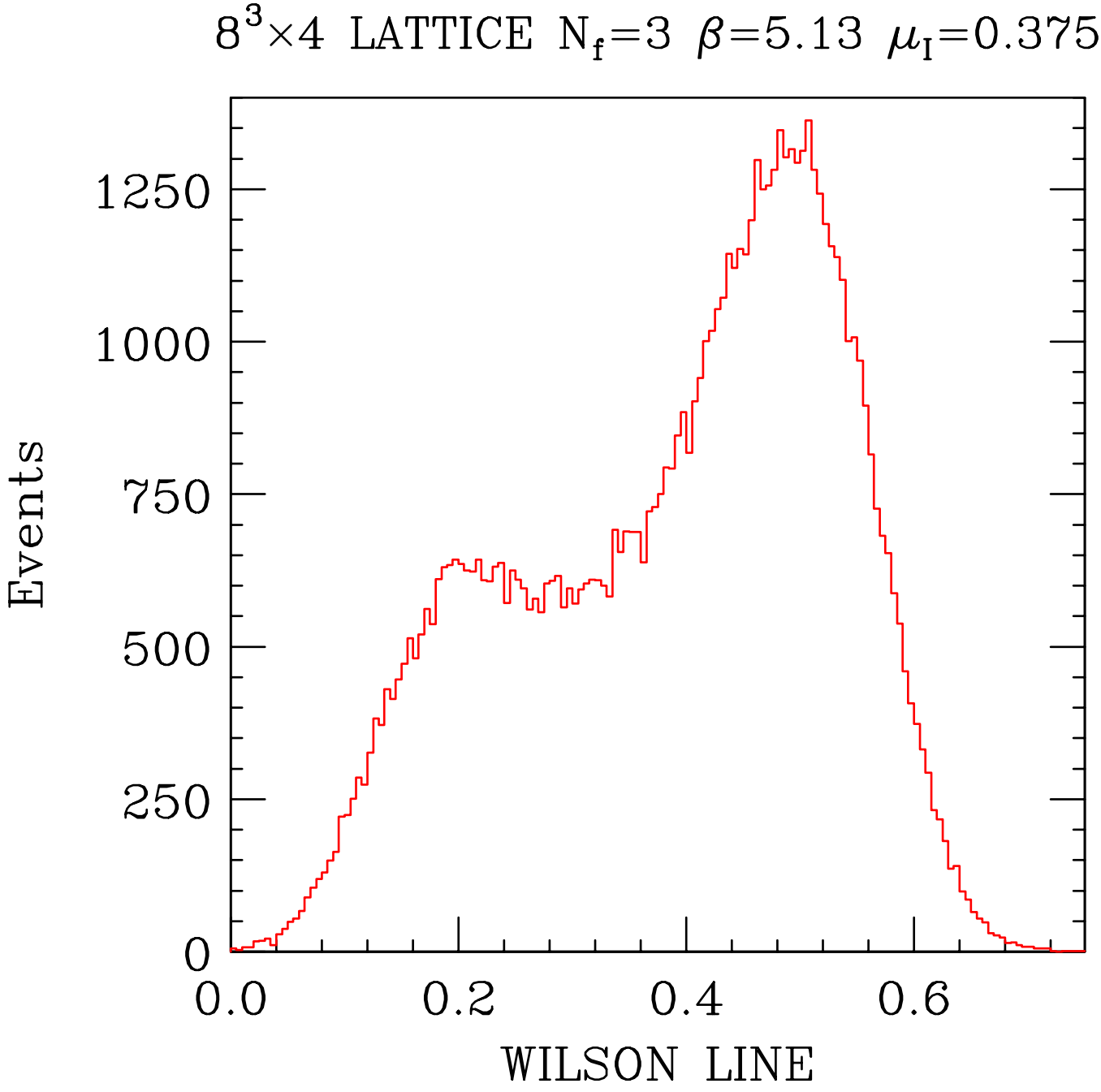

Figure 16: Histogram of Wilson Line 'time' evolution at $\beta = 5.13$, $m = 0.035$ and $\mu_I = 0.375$, on an $8^3\times4$ lattice with $N_f = 3$.

Discussion and Conclusions

- We have studied the finite temperature transition for 2-flavour lattice QCD at small μ_I. The dependence on β_c and hence T_c on μ_I appears to be the same as their dependence on μ. This appears to be due to the fact that the phase of the fermion determinant for small μ (and modest lattice size) is well behaved.
- For the masses we considered the finite temperature transition appears to be a crossover for all $\mu_I < m_\pi$. We found no sign of a critical endpoint. If the relation between the μ and μ_I behaviour of this transition extends to its nature, and is valid over this range, then the critical end-

point (if it exists) must be at $\mu > m_\pi/2$.

- We are now extending these simulations to 3 flavours, where choosing m to be just above m_c should move the critical endpoint as close to $\mu = 0$ as we desire, in particular with $\mu_c << m_\pi/2$. Then there should be a critical endpoint in our μ_I simulations with $\mu_{Ic} \approx 2\mu_c$. We are currently searching parameter space on an $8^3 \times 4$ lattice. Simulations just started on a $16^3 \times 4$ lattice will be needed to determine the nature of the transition.

- Could these simulations at finite μ_I form the basis for a reweighting scheme to get more results at finite μ?

- We will use our lattice QCD action with extra chiral 4-fermion interactions to extend the range of our simulations beyond $\mu_I = m_\pi$.
- These simulations are performed on the IBM SP, Seaborg, at NERSC, the Jazz cluster at the LCRC, Argonne National Laboratory, the Tungsten cluster at NCSA, and Linux PCs in the HEP division at Argonne National Laboratory.