

Toward a precise determination of T_c with 2+1 flavors of quarks

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We present a status report on a new high statistics study of the high temperature transition in full QCD at zero chemical potential. Our simulations use both improved asqtad and p4 staggered quarks on lattices with a temporal extent $N_\tau = 8$ and light quark masses approximately one tenth the strange quark mass. In this report we describe the setup of our calculations and present a preliminary analysis of a variety of sources of systematic error and ambiguity in the determination of the crossover temperature. We propose to present our final analysis with double the current statistics. These calculations were carried out on the IBM BlueGene/L supercomputer at Lawrence Livermore National Laboratory.

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1. Introduction

The high temperature transition in strongly interacting matter is currently being investigated in major experiments at the Brookhaven relativistic heavy ion collider (RHIC) and will soon be studied at the LHC as well. Lattice simulations of QCD provide an *ab initio* characterization of strongly interacting matter in or close to thermal equilibrium and at or close to zero baryon and strangeness chemical potential. By quantifying the behavior of the equation of state, changes in the heavy quark potential and transport coefficients as a function of temperature, lattice results will provide crucial guidance in the phenomenological interpretation of experimental measurements.

The first set of quantities that can be determined precisely using lattice QCD are the transition temperature, strangeness susceptibility, and the equation of state. The importance of a reasonably accurate determination of the transition temperature is obvious since the minimum energy densities required to produce a quark-gluon plasma grow approximately as the fourth power of the temperature. Thus, a 10% error in the threshold temperature corresponds to a 45% error in the threshold energy density.

Thermodynamic simulations face the standard set of challenges inherent in all lattice QCD simulation, *i.e.* of achieving reliable continuum and chiral extrapolations. Our calculations have been carried out with two sets of $\mathcal{O}(a^2)$ improved actions – asqtad and p4 staggered fermions. With these actions an imaginary time extent $N_\tau = 8$ and $m_\pi \approx 215$ MeV represent the state of the art. To check the efficacy of our approach we will compare our results with those of a less improved action at smaller lattice spacing ($N_\tau = 10$) and lower pion mass [3].

Recently three groups have presented results on the transition temperature. The MILC Collaboration obtains $T_c = 169(10)(4)$ MeV [1] based on analyzing the chiral susceptibility, while the RBC-Bielefeld Collaboration reports $T_c = 192(7)(4)$, based on both the chiral susceptibility χ_ℓ and the Polyakov loop susceptibility χ_L [2]. The Budapest-Wuppertal Collaboration carried out simulations closer to the continuum limit with physical quark masses but uses an action that is not $\mathcal{O}(a^2)$ improved and finds $T_c = 151(3)(3)$ MeV, using χ_ℓ , and $T_c = 175(2)(4)$ MeV and $T_c = 176(3)(4)$ MeV from the strange quark number susceptibility χ_s and the renormalized Polyakov loop L_{ren} , respectively [4, 3]. We are working towards developing a quantitative understanding of systematic errors, which were different in the three calculations. Our goal is to resolve the order ± 20 MeV differences in T_c in the current estimates and reduce the uncertainty to ~ 5 MeV.

The Lawrence Livermore National Laboratory houses a 64-rack IBM Blue Gene/L computer. Each rack, consisting of 1024 nodes, is capable of a sustained performance of about one TFlops on lattice QCD codes. Our collaboration (HotQCD) was formed in 2006 after we secured permission from the US DOE (NNSA) to carry out QCD thermodynamic simulations on a portion of this resource. The high-security location of the computer creates an unusual computing environment. Only three of us could supervise the actual simulation, and a very limited set of computational results could be brought out – then only on paper. The detailed logs and gauge configuration files are archived for subsequent analysis but cannot be moved from the secure computing environment. To assure the integrity of the results we matched selected calculations done on identical computers inside and outside the security perimeter and verified checksums for each printed output line.

2. Transition markers

At zero baryon number and strangeness there is a deconfinement phase transition in the limit of infinite quark masses and a chiral symmetry restoring phase transition when the quark masses vanish. Between these extremes we may have a phase transition or simply a crossover. Indeed, it is widely believed that at physical quark masses and zero baryon number and strangeness, the high temperature transition is a rapid crossover, rather than a genuine phase transition [5]. The crossover exhibits characteristics of both deconfinement and chiral symmetry restoration. Different observables are more sensitive to one or the other characteristic. For example, the light-quark chiral condensate $\langle \bar{\psi}\psi \rangle_\ell$ is an order parameter for the chiral phase transition at $m_\ell = 0$. At physical quark masses it is large at low temperature and drops to a low value over a narrow range of temperatures as characteristic of approximate chiral symmetry restoration at high temperature. An inflection point in this crossover as a function of temperature is a marker of a transition in the chiral properties of the medium. Similarly, the associated isosinglet chiral susceptibility χ_{singlet} measures fluctuations in $\langle \bar{\psi}\psi \rangle_\ell$, and a peak in χ_{singlet} also serves as a marker for the chiral transition.

Among indicators more directly related to deconfinement, the Polyakov loop $L \propto \exp(-F_Q/T)$ measures the free energy F_Q of a static quark in the medium. In the confined phase the static quark is screened by a bound light quark, and F_Q reflects the relatively large binding energy of the light quark. In the deconfined phase it can be screened by collective effects in the plasma at a much lower cost in free energy. Thus the Polyakov loop rises at the crossover and its inflection point marks deconfinement. Furthermore, as a result of deconfinement one expects a much reduced cost in free energy to add a light quark or strange quark to the ensemble. So the baryon number and strangeness number susceptibilities rise at the transition and their inflection points also mark deconfinement.

It has long been understood that when there is only a crossover, the transition temperature determined from different markers need not agree¹ – agreement is expected only at a critical point. Our first goal is to quantify the differences at the physical quark masses by determining each marker precisely.

For phenomenological applications, some very important markers are the rapid rise in energy and entropy density as a function of temperature. Locating the crossover in the energy density requires an improved determination of the equation of state to which the above quantities contribute. However, for such a determination analogous measurements at $T = 0$ are needed. These are still in more preliminary stages.

3. Sources of error and ambiguity

A primary purpose of this study is to make a qualitative assessment of some of the important sources of error and ambiguity in the determination of the transition temperature. We discussed sources of ambiguity in determining what T_c to associate with a crossover in the previous section. Here we list additional sources of statistical and systematic error.

1. Finite volume. Fluctuations in the light quark chiral order parameter are long range and sensitive to the lattice spatial volume.

¹For a recent discussion, see [3].

2. Statistics. The current sample sizes are given in Tables 1 and 2.
3. Locating the position of the peak or inflection point. The determination of the location of a peak or inflection point inherits the statistical errors in the observable itself. Compared with peaks, inflection points are determined by the vanishing of a higher order derivative, so require a higher level of accuracy in the data.
4. Extrapolation to physical quark masses and the continuum limit. To obtain the transition temperature at the physical point, one must make measurements at a variety of quark masses and lattice spacings and extrapolate.
5. Error in the determination of the lattice scale. The scale in the Budapest-Wuppertal work is set through separate measurements of the kaon decay constant at zero temperature f_K [3]. We, at present, determine it through a separate measurement of the static quark potential $V(r)$ at zero temperature with the same lattice parameters. The parameters r_0 and r_1 , defined through $r^2V'(r)|_{r=r_0} = 1.65$ and $r^2V'(r)|_{r=r_1} = 1$, are, in turn, determined in physical units from independent measurements of Υ splittings. Thus the values of $r_0 = 0.469(7)$ fm and $r_1 = 0.318(7)$ fm are known to ~ 2 percent [6]. At nonzero lattice spacing, different methods for determining the scale can disagree, but all methods must agree up to statistical errors in the continuum limit.
6. R-algorithm step size error. Earlier calculations done with the R algorithm suffered from a systematic error introduced by a nonzero molecular dynamics step size dt . The more recent RHMC algorithm is exact. We will eventually be combining our current RHMC results with earlier R algorithm calculations. We have, therefore, performed simulations with identical parameter sets to estimate the uncertainty associated with the step size choices in earlier R algorithm calculations.

In this preliminary study we have results bearing on points 1 and 6 in this list and some discussion of $O(a^2)$ errors.

4. Parameter set

The study was carried out on $32^3 \times 8$ lattices at a bare quark mass ratio $m_l/m_s = 0.1$ along lines of approximately constant physics. That is, the bare strange quark mass was adjusted along the trajectory to produce an approximately constant physical value of $m_{\bar{s}s} = 686$ MeV. Resulting parameters for the p4 action simulation are given in Table 1. Parameters for the asqtad action are given in Table 2 and were fixed following the previous R algorithm study, which, in turn were set from parameters used in early ensemble production [7]. The resulting strange quark mass along the asqtad trajectory is now known to be approximately 20% higher than the physical strange quark mass.

5. Results

All results shown here are preliminary.

$\beta = 6/g^2$	am_ℓ	T MeV	Total # of Trajectories
3.460	0.00313	154	10000
3.490	0.00290	169	10000
3.510	0.00259	179	11280
3.540	0.00240	194	11440
3.570	0.00212	209	12460
3.600	0.00192	225	11790
3.630	0.00170	241	12070
3.660	0.00170	256	11190
3.690	0.00150	271	10760
3.760	0.00139	313	10920
3.525	0.00240	186	6510, 6120
3.530	0.00240	189	5450, 5530
3.535	0.00240	191	5140, 5750
3.540	0.00240	194	5410, 6260
3.545	0.00240	196	6280, 6250
3.550	0.00240	199	5790, 6520

Table 1: Simulation parameters for the p4 action. For thermalization 800 trajectories are discarded. The last six were done in two separate streams with trajectory counts indicated.

5.1 Approximate order parameters

The unrenormalized chiral condensate and Polyakov loop suffer from ultraviolet divergences. The chiral condensate $\langle \bar{\psi}\psi \rangle_{\ell,s}$ has an ultraviolet perturbative contribution of the form $m/(a^2)$ at nonzero quark mass, and the static quark free energy F_Q has a self-energy divergence of the form c/a , contributing a factor $\exp(-c/aT)$ to the bare Polyakov loop L_{bare} . We consider the “subtracted” condensate [8] and the “renormalized” Polyakov loop that are free of these divergences:

$$\Delta(T) = \frac{\langle \bar{\psi}\psi \rangle_{\ell}(T) - m_{\ell}/m_s \langle \bar{\psi}\psi \rangle_s(T)}{\langle \bar{\psi}\psi \rangle_{\ell}(0) - m_{\ell}/m_s \langle \bar{\psi}\psi \rangle_s(0)} \quad (5.1)$$

$$L_{\text{ren}} = \exp[-F_{\infty}(T)/(2T)].$$

where $F_{\infty}(T)$ is the renormalized free energy of static quark anti-quark pair separated by infinite distance [9, 8]. The subtracted condensate is shown for both actions as a function of T in Fig. 1. We note that despite slight differences in the lattice parameters, which would lead to different additive and multiplicative renormalization factors, these differences largely cancel in the $\Delta(T)$ ratio as demonstrated by the reasonable agreement between the two actions.

The renormalized Polyakov loop, shown in Fig. 2, is currently available only for the p4 action. Comparing ($N_{\tau} = 4, 6$ and 8) data it is evident that $O(a^2)$ scaling violations are small and the determination of the inflection point has an uncertainty of a few MeV.

$\beta = 6/g^2$	am_ℓ	T MeV	Total # of Trajectories
6.4580	0.00820	141.4	12965
6.5000	0.00765	149.6	12990
6.5500	0.00705	159.8	12720
6.6000	0.00650	170.2	12405
6.6625	0.00624	175.6	12365
6.6500	0.00599	181.0	12445
6.6675	0.00575	186.5	12660
6.7000	0.00552	192.1	12320
6.7600	0.00500	206.0	12530
6.8000	0.00471	215.4	12195
6.8500	0.00437	227.4	12405
6.9000	0.00407	239.8	12470
6.9500	0.00380	252.5	12625
7.0000	0.00355	265.6	12595
7.0800	0.00310	287.6	12790

Table 2: Simulation parameters for the asqtad action. Between 1000-1200 are discarded for thermalization.

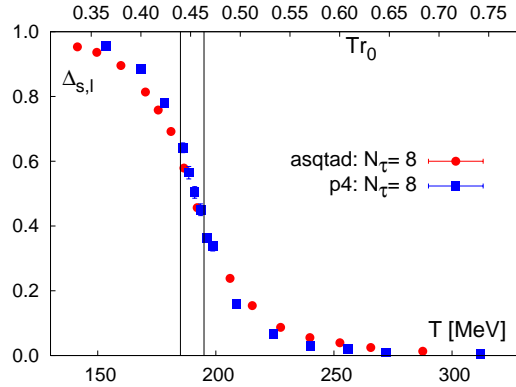


Figure 1: Preliminary results for $\Delta(T)$ for the p4 and asqtad actions as a function of temperature in MeV and in units of r_0 . The vertical lines here and throughout mark the range 185 – 195 MeV for purposes of comparison only.

5.2 Chiral symmetry restoration

The isosinglet chiral susceptibility measures fluctuations in the light quark condensate. It is defined as

$$\chi_s = \chi_{\text{dis}} + 2\chi_{\text{con}} \tag{5.2}$$

$$\chi_{\text{dis}} = \left\langle \int d^4r \langle \bar{\psi}(r)\psi(r) \rangle \langle \bar{\psi}(0)\psi(0) \rangle \right\rangle - V \left\langle \langle \bar{\psi}\psi \rangle \right\rangle^2$$

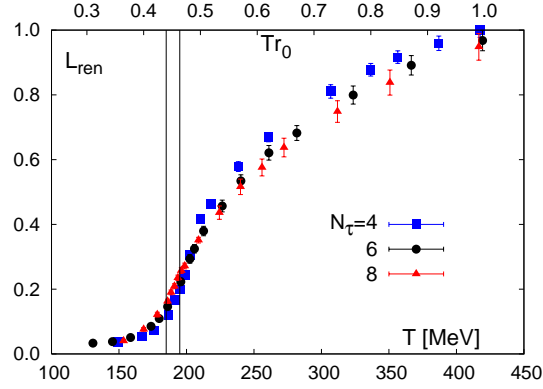


Figure 2: Comparison of the renormalized Polyakov loop data for the p4 action with $N_\tau = 4$ and 6 from [8] and $N_\tau = 8$ (preliminary from this work) as a function of temperature in MeV and in units of r_0 .

$$\chi_{\text{con}} = \left\langle \int d^4r \langle \bar{\psi}(r)\psi(0) \rangle \langle \bar{\psi}(r)\psi(0) \rangle \right\rangle$$

Where $\langle \bar{\psi}\psi \rangle$ includes both up and down flavors and the “connected” and “disconnected” subscripts refer to the two kinds of valence quark line contractions in the correlator. Here the inner angle brackets indicate the quark propagator on a single gauge configuration, and the outer angle brackets denote an average over gauge configurations.

The connected and disconnected light-quark chiral susceptibilities for the two actions are compared in Fig. 3 and the total isosinglet chiral susceptibility is shown in Fig. 4. Since we are now comparing unrenormalized quantities, differences in normalization are not surprising. We are in the process of doubling the statistical sample to resolve some of the discrepancies evident here. Nevertheless, it is unlikely that the location of the peak will shift significantly from the range 185 – 195 MeV at these quark masses and $N_\tau = 8$.

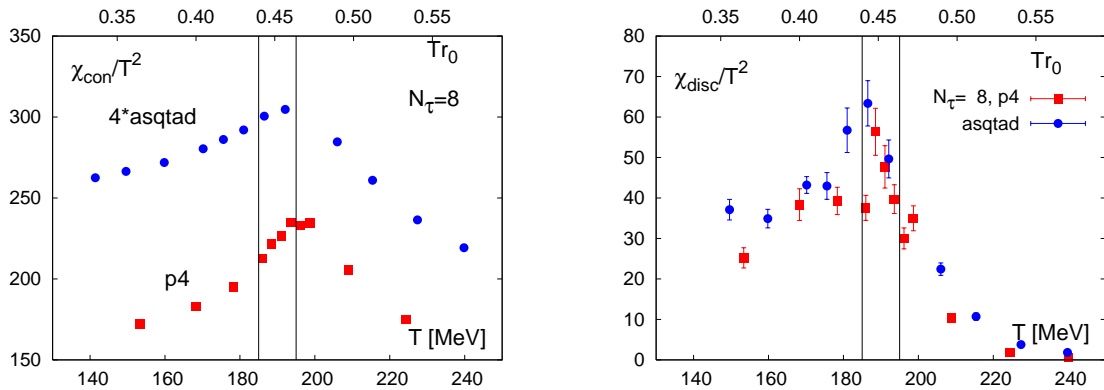


Figure 3: Preliminary results for the connected and disconnected light quark chiral susceptibilities for both p4 and asqtad action. An arbitrary scale factor has been applied to the asqtad connected susceptibility to facilitate the comparison.

To compensate for additive and multiplicative renormalization factors in the chiral suscepti-

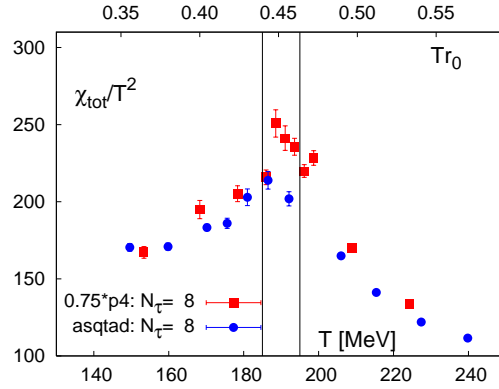


Figure 4: Isosinglet chiral susceptibility for both actions (preliminary). An arbitrary scale factor has been applied to the asqtad value to facilitate the comparison.

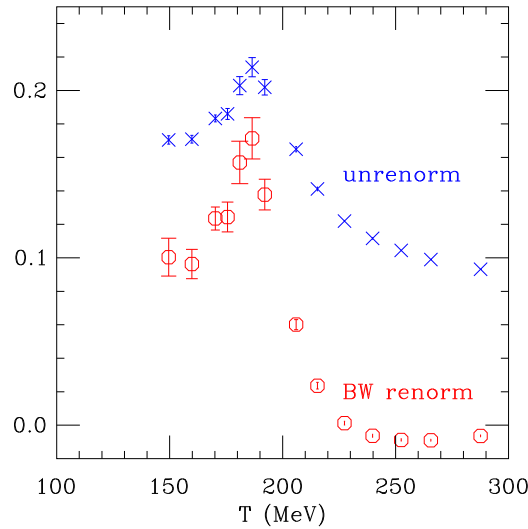


Figure 5: Preliminary unrenormalized isosinglet chiral susceptibility for the asqtad action compared with the proposed Budapest-Wuppertal renormalized quantity. To facilitate the comparison the unrenormalized susceptibility has been rescaled by a factor of 1000.

bility, the Budapest-Wuppertal group has proposed the modified quantity

$$m_\ell^2[\chi_{\text{singlet}}(T) - \chi_{\text{singlet}}(0)]/T^4. \quad (5.3)$$

For the asqtad action we compare this with the unrenormalized quantity in Fig. 5. To compute this modified quantity we have used measurements on a small set of zero temperature (32^4 lattice) runs with parameters matched to the $N_\tau = 8$ ensembles. Since the $T = 0$ data are smooth, dividing by the temperature in this way necessarily shifts the peak towards smaller T , however, the shift appears to be only at the level of a few MeV.

5.3 Crossover in probes of deconfinement

The light quark number and strange quark number susceptibilities measure fluctuations in

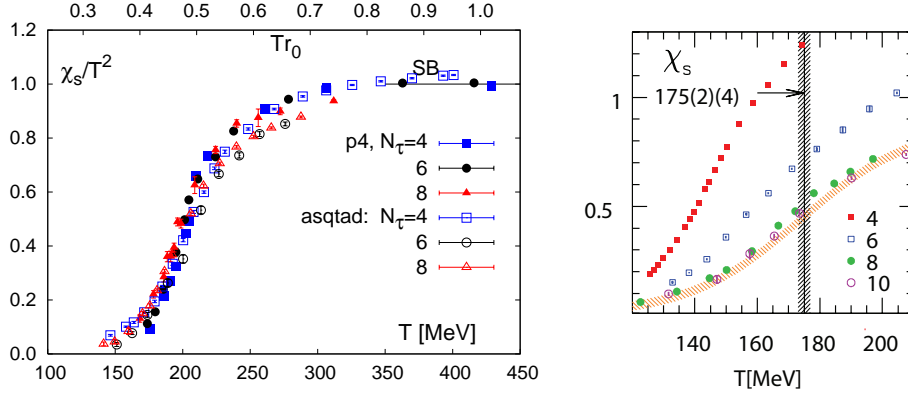


Figure 6: Left panel: preliminary strange quark number susceptibility for the p4 and asqtad actions along the $m_l = 0.1m_s$ line of constant physics. Points for increasing N_τ show scaling trends. Right panel: the same quantity in the crossover region for the one-link stout action of the Budapest-Wuppertal Collaboration with light quark masses approximately at their physical values [3]. Somewhat different conventions were used to set the temperature scales in the two figures.

baryon number and strangeness. They are defined as

$$\chi_{(\ell,s)}/T^2 = \frac{1}{VT} \frac{\partial^2 \log Z}{\partial \mu_{(\ell,s)}^2}. \quad (5.4)$$

Since these susceptibilities measure charge, there are no renormalization issues. We compare the strange quark number susceptibility for the two actions in Fig. 6 as the data are less noisy than those for the light quark. We find good agreement between the two actions. Also shown for comparison are results from the one-link stout action of the Budapest-Wuppertal collaboration. In that case the lines of constant physics are close to the physical quark masses. The similarities and differences in scaling behavior, i.e. $\mathcal{O}(a^2)$ artifacts, of the three actions are evident.

5.4 Comparison of T_c from deconfinement and chiral symmetry restoration markers

A central question that this study addresses is how different is T_c determined from chiral and deconfinement markers? The data are presented in Fig. 7, and we can make the following observations.

1. Locating the inflection point in the strange quark susceptibility is more uncertain than locating the peak in the isosinglet susceptibility. Estimates of the inflection point are sensitive to the number of points in the fit and the functional form of the fit.
2. The peak in the isosinglet chiral susceptibility appears to occur at approximately the same temperature as the inflection point in strange quark number susceptibility. Further statistics are needed to detect and quantify any differences.

5.5 Step size in R algorithm and finite size effects

We would eventually like to combine new and old results at a variety of quark masses and lattice spacings, so we can carry out an extrapolation to the physical point. Many of the older

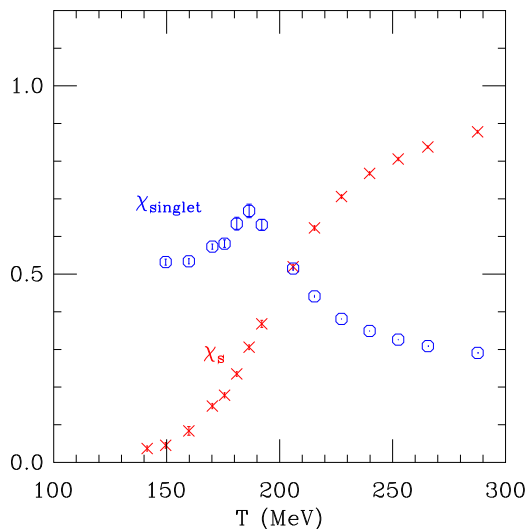


Figure 7: Preliminary results for the strange quark number susceptibility for the asqtad action compared with the isosinglet susceptibility.

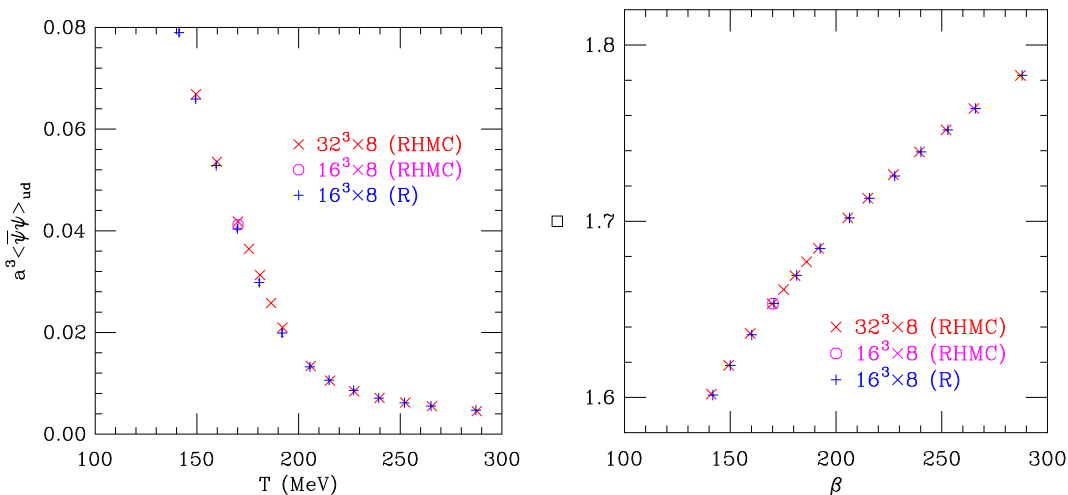


Figure 8: Light quark chiral condensate and plaquette for the asqtad action, comparing results obtained from the R algorithm on $16^3 \times 8$ lattices and the RHMC algorithm (preliminary values) on $32^3 \times 8$. Points for the Polyakov loop have been slightly displaced horizontally for clarity. The $16^3 \times 8$ RHMC point in each case tests sensitivity to the finite spatial size.

simulations used the R algorithm and were done at a smaller aspect ratio N_s/N_t . In Fig. 8 we compare results for the two order parameters from simulations with the R algorithm on $16^3 \times 8$ lattices and the RHMC algorithm on $32^3 \times 8$. Differences are very slight. Although the effect is too small to show in these figures, there are differences at the level of a little more than one standard deviation in the chiral condensate at low temperature but no visible trends in the Polyakov loop.

The light quark susceptibility is more sensitive to differences in the two asqtad calculations, as shown in Fig. 9. Here the connected susceptibility is significantly higher at low temperature in the smaller-volume R-algorithm simulation. To test whether the effect is due to the smaller volume

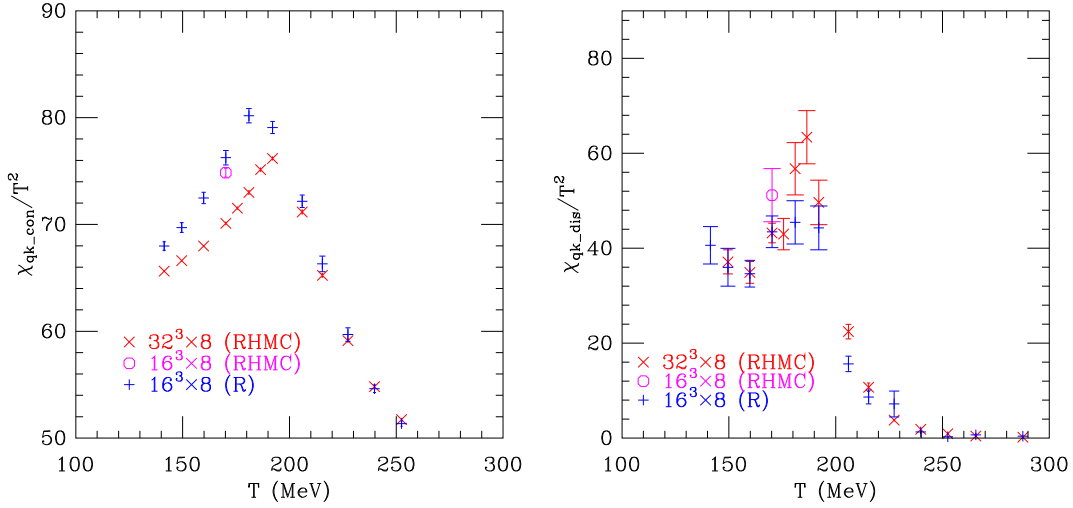


Figure 9: Light quark chiral connected and disconnected susceptibility for the asqtad action, comparing results obtained from the R algorithm on $16^3 \times 8$ lattices, the RHMC algorithm (preliminary results) on $32^3 \times 8$, and one point with the RHMC algorithm on $16^3 \times 8$.

or the algorithm we carried out a simulation of the RHMC algorithm on the smaller volume at one temperature as shown. It is close to the R algorithm result. Thus we conclude that difference in the connected susceptibility is largely a finite volume effect. We also see that the disconnected term appears to have a sharper peak at larger volume.

When the two susceptibilities are combined to form the isosinglet susceptibility, the finite volume effect tends to shift the peak towards higher T by a few MeV with this increase in volume.

5.6 Conclusions and plans

We find good agreement between the p4 and asqtad actions, bearing in mind the small differences in parameter choices. A preliminary assessment of the various crossover markers at $N_\tau = 8$ and $m_\ell = 0.1m_s$ suggests that they may disagree at the level of several MeV, but not at the level of a few tens of MeV. We see similar differences in the peak in the isosinglet chiral susceptibility between the unnormalized and Budapest-Wuppertal-normalized version. We compared asqtad results from the R algorithm and RHMC and do not find evidence of significant step-size effects that would affect the determination of the transition temperature, but we do observe a finite-volume effect that could lower the temperature of the peak in the chiral susceptibility by a few MeV.

Overall, we find the crossover in both the deconfinement and chiral symmetry restoration markers to lie in the range $T = 185 - 195$ MeV at $N_\tau = 8$ and at $m_\ell = 0.1m_s$. Our plans for the immediate future are to double the statistics in the transition region, add data at more values of the quark masses and carry out a detailed quantitative analysis of the effects observed here.

Acknowledgments

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