Thermodynamics with Dynamical Clover Fermions

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Abstract

We investigate the finite temperature behavior of nonperturbatively improved clover fermions on lattices with temporal extent $N_t = 4$ and 6. Unfortunately in the gauge coupling range, where the clover coefficient has been determined nonperturbatively, the finite temperature crossover/transition occurs at heavy pseudoscalar masses and large pseudoscalar to vector meson mass ratios. However, on an $N_t = 6$ lattice the thermal crossover for the improved fermions is much smoother than for unimproved Wilson fermions and no strange metastable behavior is observed.

Simulations with Wilson fermions suffer $O(a)$ scaling violations due to the dimension five operator that Wilson introduced to give the unwanted fermion doublers masses of order the cutoff, $1/a$. These scaling violations are much larger than those in the glue sector, which are $O(a^2)$, and they can be numerically quite large, necessitating use of small lattice spacings at large simulation cost to get results that can be reliably extrapolated to the continuum limit.

The $O(a)$ scaling violations can be reduced to $O(a^2)$ by introducing another dimension five operator into the fermion action, the so called clover term,

$$S_{sw} = c_{sw} \kappa \sum_x \bar{\psi}(x)i\sigma_{\mu\nu}F_{\mu\nu}(x)\psi(x), \quad (1)$$

where $F_{\mu\nu}(x)$ is a lattice transcription of the field strength tensor $F_{\mu\nu}(x)$, usually taken from four open plaquettes looking like a clover leaf, as proposed by Sheikhholeslami and Wohlert [1]. For the reduction of scaling violations to work the clover coefficient, $c_{sw}$, needs to be determined nonperturbatively as a function of the gauge coupling. The ALPHA collaboration developed a method to do so within the Schrödinger functional framework [2]. For quenched QCD the nonperturbative clover coefficient is now known for gauge coupling
$6/g^2 \geq 5.7$, corresponding to lattice spacings $a \lesssim 0.17$ fm \cite{2,3}. A substantial
reduction of scaling violations in this region from $O(a)$ to $O(a^2)$ has been
verified nicely in \cite{3}.

The clover coefficient has recently also been determined by the ALPHA collabor-
ation for full QCD with two flavors of dynamical fermions for gauge coupling
$\beta = 6/g^2 \geq 5.2$, corresponding roughly to lattice spacings $a \lesssim 0.14$ fm \cite{4}. To
be precise, the clover coefficient was determined for $\beta \geq 5.4$ and fitted to a
ratio of polynomials in $g^2$. At $\beta = 5.2$ a numerical consistency check with the
value extrapolated with this function of $g^2$ was performed (see \cite{4} for details).
Preliminary first results of hadron spectroscopy and the heavy quark potential
in dynamical simulations with this nonperturbatively determined clover
coefficient have appeared in \cite{5}.

Arguably the largest lattice artifacts in simulations with dynamical Wilson
fermions have been observed in simulations probing the finite temperature
behavior in the vicinity of the deconfinement/chiral symmetry restoration
transition or (at finite quark mass) crossover. The most likely scenario for
the behavior of two-flavor QCD at finite temperature is a rapid crossover
for finite quark mass, turning into a second order chiral symmetry restoring
phase transition in the massless limit \cite{6}. However, simulations with dynamical
Wilson fermions showed strange, unexpected behavior, \textit{e.g.} first order phase
transition like signals at intermediate quark masses, that softened again at
smaller quark masses \cite{7,8}.

It has been argued \cite{9} that this strange and unexpected behavior is due to
effects of the Wilson pure gauge action in its so called “crossover region”,
where the plaquette varies sharply with changes in the gauge coupling, which
feeds back to the fermions, rather than being due to artifacts in the fermion
action. Indeed, their simulations did not show any evidence for first order like
signals. Similarly, a study using both an improved gauge and a clover improved
fermion action, with so-called tadpole improved coefficients, found a smoother
behavior in the thermal crossover region than the simulations with unimproved
Wilson action for both gauge and fermion sectors \cite{10}. From the point of
view of the Symanzik improvement program both these simulations still have
$O(g^a a)$ errors of unknown magnitude. Furthermore, it is not clear, in the
study where both gauge and fermion action are improved, which improvement
is more important in smoothening out the thermal crossover behavior.

In this letter, we study the effect of the nonperturbative improvement of the
Wilson fermion action on the behavior at the finite temperature crossover.
We are interested in simulations with small lattice extent in the temporal
direction, \textit{i.e.} at large lattice spacing, where the simulations are relatively
cheap.
Table 1
The clover coefficients, $c_{sw}$, used in the simulations and estimates of the $\kappa_c$'s. They were obtained from Ref. [4].

| $\beta$ | $c_{sw}$ | $\kappa_c$ |
|---------|----------|------------|
| 5.4     | 1.82277  | 0.1370     |
| 5.3     | 1.90952  | 0.1370     |
| 5.2     | 2.02     | 0.1370     |

Fig. 1. $\langle \text{Re} P \rangle$ for the simulations with $N_t = 4$ and volume $8^3$ at $\beta = 5.4$ (squares) 5.3 (diamonds) and 5.2 (octagons) and with volume $12^3$ at $\beta = 5.2$ (crosses).

The largest coupling for which the nonperturbative value of $c_{sw}$ is known is $\beta = 6/g^2 = 5.2$. We performed simulations on $8^3 \times 4$ lattices for $\beta = 5.4$, 5.3 and 5.2 and various values of $\kappa$ in the thermal transition/crossover region. The values for $c_{sw}$ used, obtained from Ref. [4] are listed in Table 1. Measurements were taken, after thermalization, over 500 trajectories away from the crossover region, and over up to 4000 trajectories in the middle of the crossover region. We show in Figure 1 the real part of the Polyakov line expectation value and in Figure 2 the average space-like plaquette. A clear crossover is seen for all three gauge couplings, becoming sharper as the coupling is increased (as $\beta$ is decreased). For the largest coupling, $\beta = 5.2$, we also simulated on a larger spatial volume, $12^3 \times 4$. As can be seen from the figures, there is no evidence for finite volume effects.

The thermal crossover appears quite rapid, reminiscent of unimproved Wil-
Fig. 2. Space-like plaquettes, $\langle \text{Tr} U_p/3 \rangle$, for the same lattices and with the same symbols as Fig. 1.

son simulations [7], as compared to thermodynamics with a tadpole improved clover fermion and Symanzik improved gauge action [10]. But, of course, comparisons should not be made in terms of bare parameters, such as $\kappa$. We have therefore computed hadron masses and the heavy quark potential at the thermal crossover points. For $\beta = 5.2$ hadron masses were also computed on both sides of the thermal crossover. Most of these measurements were done on $8^3 \times 16$ lattices. In one case, for $\beta = 5.2$ and $\kappa = 0.1340$, where the meson masses are lightest, we also have preliminary results from a simulation on a larger $16^3 \times 32$ lattice. There, we do see finite size effects on the masses of about 10%, but much less on the mass ratio. We suspect that the masses for the next lightest quark mass, at $\beta = 5.2$, $\kappa = 0.1330$ are also affected by some small finite size effects, while for the other cases the finite size effects are expected to be smaller than the statistical errors. All the results are collected in Table 2.

Even at the strongest coupling, for which the nonperturbative clover coefficient is known, the thermal crossover for $N_t = 4$ lattices occurs at heavy pseudoscalar meson mass and large pseudoscalar to vector meson mass ratio. We therefore also considered thermodynamics on an $N_t = 6$ lattice at $\beta = 5.2$. $\langle \text{ReP} \rangle$ and $\langle \text{Tr} U_p/3 \rangle$ are shown in Figures 3 and 4, where they are compared to the results from $N_t = 4$. The crossover seems somewhat smoother for $N_t = 6$, and it occurs at lighter meson masses. However, at 0.85 the pseudoscalar to vector meson mass ratio is still rather large.
Fig. 3. \(\langle \text{Re} P \rangle\) for the simulations at \(\beta = 5.2\) for lattice size \(8^3 \times 4\) (octagons), \(12^3 \times 4\) (crosses) and \(12^3 \times 6\) (diamonds).

Fig. 4. Space-like plaquettes, \(\langle \text{Tr} U_{ps}/3 \rangle\), for the same lattices and with the same symbols as Fig. 3.
Table 2
Masses of pseudoscalar and vector mesons and their ratio, and values for the string tension from $L^3 \times (2L)$ lattices. Points marked by an asterisk lie on the $N_t = 4$ crossover, and the point marked by a plus on the $N_t = 6$ crossover.

| $\beta$ | $\kappa$ | $L$ | $m_{PS}$ | $m_V$ | $m_{PS}/m_V$ | $a\sqrt{\sigma}$ |
|---------|---------|-----|---------|-------|-------------|----------------|
| *5.4    | 0.1125  | 8   | 2.167(3)| 2.237(4)| 0.968(1)    | 0.479(18)      |
| *5.3    | 0.1215  | 8   | 1.833(3)| 1.948(4)| 0.941(1)    | 0.530(7)       |
| 5.2     | 0.1260  | 8   | 1.656(3)| 1.814(5)| 0.913(2)    |                |
| *5.2    | 0.1270  | 8   | 1.594(2)| 1.757(3)| 0.907(1)    | 0.559(10)      |
| 5.2     | 0.1280  | 8   | 1.506(3)| 1.672(7)| 0.901(3)    |                |
| 5.2     | 0.1320  | 8   | 1.026(5)| 1.185(27)| 0.866(18)  |                |
| +5.2    | 0.1330  | 8   | 0.793(5)| 0.934(7)| 0.849(5)    | 0.304(7)       |
| 5.2     | 0.1340  | 8   | 0.691(4)| 0.877(4)| 0.789(3)    | 0.283(12)      |
| 5.2     | 0.1340  | 16  | 0.631(1)| 0.787(3)| 0.802(3)    | 0.290(8)       |

Comparing Figure 1 with similar plots for unimproved Wilson fermions such as Fig. 5 of [7] the crossover for the improved clover fermions appears to be even more pronounced than for the unimproved Wilson fermions. Comparing as function of the bare hopping parameter $\kappa$, though, can be misleading and we therefore follow the strategy of Ref. [10] and make a comparison as function of the quark mass, or equivalently as function of $m_{PS}^2$. From Ref. [11] we can see that the crossover for Wilson fermions at $\beta = 5.12$ and $\kappa = 0.1700$ occurs at a pseudoscalar to vector meson mass ratio $m_{PS}/m_V = 0.899(4)$. It appears that the unimproved Wilson fermion data at $\beta = 5.1$ of [7] are the set that most closely matches ours at $\beta = 5.2$. In addition, from Ref. [12] we have some mass measurements in the thermal crossover region. While the $m_{PS}/m_V$ ratios at the thermal crossover are comparable, the masses in lattice units are quite different. We therefore decided to plot $\langle \text{Re}P \rangle$ as function of $(m_{PS}/m_V(\kappa_T))^2$, where $m_V(\kappa_T)$ is the vector meson mass at the thermal crossover point $\kappa_T$. The comparison is shown in Fig. 5. It appears that the crossover for the improved fermions with $N_t = 4$ is somewhat sharper than for the unimproved fermions.

The crossover for the improved fermions on the $N_t = 6$ lattice, on the other hand, is much smoother. The pseudoscalar to vector meson mass ratio at the crossover corresponds to that for unimproved Wilson fermion at $\beta = 5.22$, $\kappa = 0.17$ [8]. This is the region where first order like metastable states were observed in [8]. So here the improvement seems to help.

In conclusion, we have carried out finite temperature simulations with non-perturbatively improved Wilson fermion in the region of largest coupling, and hence largest lattice spacing, for which the nonperturbative value of the clover
Fig. 5. Comparison of $\langle \text{Re} P \rangle$ for the simulations with clover improved and non-improved Wilson fermions at similar $m_{PS}/m_V$ ratios at the thermal crossover as function of $(m_{PS}/m_V(\kappa_T))^2$, giving a comparable measure of the quark masses, for $N_t = 4$. Also shown are the clover results for $N_t = 6$.

The coefficient $c_{sw}$ is known. The thermal crossover on $N_t = 4$ lattices occurs at very heavy pseudoscalar meson masses and large pseudoscalar to vector meson mass ratios. The crossover appears somewhat sharper than for unimproved Wilson fermions at comparable $m_{PS}/m_V$ ratios. However, for the improved fermions the masses (in lattice units) are considerably larger, and the thermal crossover could still be significantly influenced by the deconfinement transition in the pure gauge theory. While the thermal crossover on an $N_t = 6$ lattice at the strongest accessible coupling still occurs at a large $m_{PS}/m_V$ ratio, it has become much smoother, in particular compared to unimproved Wilson fermions, which show strange first order like behavior for comparable $m_{PS}/m_V$ ratios. To get the thermal crossover to occur for smaller $m_{PS}/m_V$ ratio, one needs to use lattices with larger temporal extent $N_t$ or try to push the nonperturbative determination of $c_{sw}$ to stronger couplings.

Acknowledgements

This research was supported by DOE contracts DE-FG05-85ER250000 and DE-FG05-96ER40979. Computations were performed on the CM-2 and the workstation cluster at SCRI.
References

[1] B. Sheikholeslami and R. Wohlert, *Nucl. Phys.* **B259** (1985) 572.

[2] M. Lüscher, S. Sint, R. Sommer, P. Weisz, and U. Wolff, *Nucl. Phys.* **B478** (1996) 365, *Nucl. Phys.* **B491** (1997) 323, 344.

[3] R.G. Edwards, U.M. Heller and T.R. Klassen, *Phys. Rev. Lett.* **80** (1997) 3448.

[4] K. Jansen and R. Sommer, *Nucl. Phys.* **B530** (1998) 185.

[5] M. Talevi (The UKQCD Collaboration), hep-lat/9809182; C.R. Allton *et al.* (The UKQCD Collaboration), hep-lat/9808016.

[6] R. Pisarski and F. Wilczek, *Phys. Rev.* **D29** (1984) 339.

[7] C. Bernard *et al.* (The MILC collaboration), *Phys. Rev.* **D49** (1994) 3574.

[8] C. Bernard *et al.* (The MILC collaboration), *Phys. Rev.* **D46** (1992) 4741; T. Blum *et al.* (The MILC collaboration), *Phys. Rev.* **D50** (1994) 3377.

[9] Y. Iwasaki, K. Kanaya, S. Kaya and T. Yoshié, *Phys. Rev. Lett.* **78** (1997) 179.

[10] C. Bernard *et al.* (The MILC collaboration), *Phys. Rev.* **D56** (1997) 5584.

[11] K.M. Bitar *et al.* (The HEMCGC Collaboration), *Phys. Rev.* **D43** (1991) 2396.

[12] K.M. Bitar, R.G. Edwards, U.M. Heller and A.D. Kennedy, *Phys. Rev.* **D54** (1996) 3546.