Thermodynamics of Lattice QCD with massless quarks and chiral 4-fermion interactions.

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We have simulated lattice QCD with an irrelevant 4-fermion interaction and 2 zero mass quarks. The chiral phase transition is observed to be second order and we discuss extraction of critical exponents.

1. The action

We have extended the standard staggered quark QCD action by the addition of a 4-fermion term with a \( U(1) \times U(1) \) chiral flavour symmetry, generated by \( (\xi_5, \gamma_5 \xi_5) \). (For earlier, related work see \[3\].) Introducing the auxiliary fields \((\sigma, \pi)\) to render the action quadratic we have

\[
L = -\beta \sum_i \left[ 1 - \frac{1}{3} \text{Re}(\text{Tr}_U U U U) \right] + \frac{N_f}{8} \sum_i A_i^\dagger A_i
- \sum_i \frac{1}{8} N_f \gamma (\sigma^2 + \pi^2) + \frac{1}{2} \sum_i (\sigma^2 + \pi^2)
+ \frac{1}{2} \sum_i (\hat{\theta}_1^2 + \hat{\theta}_2^2 + \hat{\theta}_1^* \hat{\theta}_1 + \hat{\theta}_2^* \hat{\theta}_2 + \hat{\theta}_3^* \hat{\theta}_3)
\]

for our molecular dynamics lagrangian, where

\[
A = D + m + \frac{1}{16} \sum_i (\sigma_i + i e \pi_i)
\]

The advantage of this action is that the Dirac operator remains non-singular when \( m = 0 \) so that we can work in the chiral limit. Note that we have an exact chiral symmetry generated by \( \gamma_5 \xi_5 \) which means we will have a massless pion at \( m = 0 \) when this symmetry is spontaneously broken.

The 4-fermion term is an irrelevant operator, so this theory should have the same continuum limit — continuum QCD — as the standard action.

2. Application to \( N_f = 2 \) thermodynamics

\( N_f = 2 \) QCD is believed to have a second order finite temperature chiral phase transition for \( m = 0 \) which weakens to a rapid crossover, with no actual phase transition, for \( m \neq 0 \). The critical exponents that describe the neighbourhood of this critical point are expected to be those of an \( O(4) \) spin model in 3 dimensions. (See \[3\] for a recent review of lattice QCD thermodynamics and critical exponents.)

For the staggered lattice formulation the critical exponents are expected to be \( O(2) \) or \( O(4) \). (For recent work on staggered critical exponents see \[4\].) Here the advantage of being able to work at zero quark mass is clear. We can hope to see clear evidence for the second order nature of the phase transition. In addition one can measure certain critical exponents directly. In particular one can measure the exponent \( \beta_m \) from

\[
\langle \bar{\psi} \psi \rangle = \text{const}(\beta_c - \beta)^{\beta_m} = \gamma \langle \sigma \rangle
\]

where \( \beta_m = 0.5 \) for mean field theory, \( \beta_m \approx 0.38 \) for \( O(4) \), and \( \beta_m \approx 0.35 \) for \( O(2) \). In the high temperature phase, the common \( \pi \) and \( \sigma \) screening masses increase from zero as

\[
m_\pi^2 m = \text{const}(\beta - \beta_c)^{\gamma m}
\]

where \( \gamma_m = 1 \) for mean field theory, \( \gamma_m \approx 1.44 \) for \( O(4) \) and \( \gamma_m \approx 1.32 \) for \( O(2) \). The same critical exponent governs the vanishing of the \( \sigma \) mass below the transition. If we now fix \( \beta = \beta_c \) and decrease the mass \( m \) from a finite value to zero, \( \langle \bar{\psi} \psi \rangle \) vanishes as

\[
\langle \bar{\psi} \psi \rangle = \text{const} m^{1/\delta}
\]

where \( \delta = 3 \) for mean field theory, \( \delta \approx 4.8 \) for \( O(4) \), and \( \delta \approx 4.8 \) for \( O(2) \).
Of the fluctuation quantities (susceptibilities), the most accessible is the “magnetic” susceptibility
\[ \chi_\sigma = \frac{1}{V} \left[ \langle (\sum_x \sigma(x))^2 \rangle - \langle (\sum_x \sigma(x)) \rangle^2 \right] \] (6)
which scales as
\[ \chi_\sigma = \text{const} (\beta - \beta_c)^{-\gamma_m}. \] (7)

3. Lattice simulations and preliminary results

Our simulations are being carried out using hybrid molecular dynamics with noisy fermions to accommodate \( N_f = 2 \). Because of the exact flavour \( U(1)_{\text{axial}} \) symmetry at \( m = 0 \), the direction of symmetry breaking in the \( (\langle \bar{\psi}\psi \rangle, i\langle \bar{\psi}\gamma_5\xi_5\psi \rangle) \) space (or \( (\sigma, \pi) \) space is not determined. On a finite lattice, this direction rotates during the run, forcing us to use \( \sqrt{\langle (\bar{\psi}\psi)^2 - \langle \bar{\psi}\gamma_5\xi_5\psi \rangle^2 \rangle} \) or \( \sqrt{\langle \sigma^2 + \langle \pi \rangle^2 \rangle} \) as our order parameter on each configuration. (Here \( \langle \rangle \) should be taken to mean a lattice average, not an ensemble average.) This estimate differs from the true value by \( O(1/\sqrt{V}) \), which can only be removed by working at more than 1 spatial volume for each \( N_t \).

We are currently running on \( 8^3 \times 4, 12^2 \times 24 \times 4, 12^3 \times 6, \) and \( 18^3 \times 6 \) lattices at \( \gamma = 20 \), and on a \( 12^3 \times 6 \) at \( \gamma = 10 \).

Whereas our earlier simulations at \( N_t = 4 \) and \( \gamma = 10 \) showed a first order transition, all \( N_t = 6 \) combinations above show evidence for the expected second order transition. \( \langle \bar{\psi}\psi \rangle \) and the Wilson line show a sharp, but not discontinuous, transition with no sign of metastability, unlike the previous case. Figure 1 shows the \( \beta \) dependence of the chiral condensate for \( N_t = 6 \) and \( \gamma = 20 \). In addition, close to the transition, observables show clear signs of critical slowing down with large fluctuations over many thousands of time units. (We have simulated for as many as 39,000 time units at a single \( \beta \) value.) Such a time evolution for the chiral condensate close to the transition is shown in figure 2. The \( N_t = 4, \gamma = 20 \) runs show signs of critical fluctuations, but the transition occurs over a very narrow range and it will require more statistics to tell if it has become second order or remains first order.

\[ \langle \bar{\psi}\psi \rangle \text{ as a function of } \beta \text{ for } N_t = 6 \text{ and } \gamma = 20. \]

\[ \text{Time evolution of } \langle \bar{\psi}\psi \rangle \text{ at } \beta = 5.42 \text{ on an } 18^3 \times 6 \text{ lattice at } \gamma = 20. \]
It is clear that we will need to extend our runs close to the phase transition. This is a consequence of the critical slowing down close to the second order transition. This currently limits our ability to extract accurate critical exponents due in part to the fact that our errors are poorly determined and partly because it prevents accurate extrapolation to infinite volume. In addition, the scaling window could be very narrow requiring us to consider more $\beta$ values close to the transition. Despite this, the $\langle \bar{\psi} \psi \rangle$ data looks promising, and suggests a critical exponent $\beta_m \sim 0.3$, however, this is on the basis of statistically poor fits. The $N_t = 6, \gamma = 20$ data shows relatively modest finite volume effects. For $N_t = 4, \gamma = 20$, we find $\beta_e \approx 5.288$. For $N_t = 6, \gamma = 10, \beta_e \approx 5.466$, while for $N_t = 6, \gamma = 20$, $\beta_e \approx 5.424$.

Figure 3 shows the $\sigma$ and $\pi$ screening masses for the $18^3 \times 6$, $\gamma = 20$ simulations. The $\sigma$ screening mass shows the correct behaviour, decreasing to zero as $\beta$ is increased through the transition, and increasing from zero, degenerate with the $\pi$ above the transition. Below the transition, the pion mass is consistent with zero. It appears doubtful that these masses can be determined accurately enough to obtain a good estimate for $\gamma_m$.

The $\delta$ mass can be calculated, but even assuming it remains distinct from the $\sigma/\pi$ mass above the transition, it will be difficult to tell how much of this is due to the explicit $U(1)_{axial}$ symmetry breaking provided by the 4-fermion interaction.

4. Summary

$N_f = 2$ lattice QCD with massless quarks and a weak 4-fermion interaction appears to have the expected second order transition, at least for $N_t \geq 6$. More work is needed to clarify the $N_t = 4$ case.

With more statistics the $N_t = 6$ simulations should produce an accurate determination of the critical exponent $\beta_m$. Moving to finite mass at $\beta = \beta_c$ should allow an accurate determination of $\delta$.

Hadronic screening masses need further analysis. Other order parameters remain to be analysed.

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