Finite Temperature Phase Diagramm of QCD with improved Wilson fermions

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We present first results of a study of two flavour QCD with Wilson fermions at finite temperature. We have used tree level Symanzik improvement in both the gauge and fermion part of the action. In a first step we explore the phase diagramm on an $8^3 \times 4$ lattice, with particular emphasis on checking Aoki’s conjecture with an improved action.

1. Introduction

The study of the finite temperature phase transition in QCD with Wilson fermions is much more complicated than in the staggered fermion formulation, because of the absence of an order parameter due to explicit chiral symmetry breaking. This means e.g. that the existence of a massless pion at finite lattice spacing is not at all obvious.

In recent years a detailed picture of the finite temperature phase diagramm of QCD with Wilson fermions has emerged [1]. This picture is based on the idea of spontaneous breakdown of parity and flavour symmetry [2] and has been investigated analytically as well as numerically. The features of this phase diagramm are (i) the critical line $\kappa_c(\beta)$ defined by a vanishing pion screening mass for finite temporal lattice size turns back towards strong coupling forming a cusp, (ii) the region bounded by the critical line represent a phase of spontaneously broken parity and flavour symmetry, (iii) the finite temperature phase transition line $\kappa_l(\beta)$ presumably does not cross the critical line, but runs past it towards larger values of the hopping parameter[3].

From an analysis of the Gross-Neveu model in two dimensions, where three cusps connected to doublers develop, one expects the critical line for QCD in four dimensions to form five cusps moving towards weak coupling with increasing temporal lattice size $N_T$. Simulations with the standard Wilson formulation for quarks and gluons have shown, that at $N_T = 1/(aT) = 4$ the tip of the cusp lies in the strong coupling regime at $\beta \approx 3.9$ and moves only slowly towards weak coupling as $N_T$ is increased.

Since one expects the same features to hold for a wider class of actions including the clover action, which tends to reduce cutoff dependencies, a study of the phase diagramm using improved actions is of practical as well as theoretical importance[4].

2. Results

We have conducted a simulation of 2 flavour QCD on an $8^3 \times 4$ lattice using tree level Symanzik improved actions for quarks and gluons. In the gauge sector this amounts to adding a $2 \times 1$-loop to the standard plaquette action and for the fermions in adding the clover term with $c_{SW} = 1$. We have used a Hybrid Monte Carlo algorithm with a timestep $\delta \tau = 0.01$ and the number of molecular dynamics steps $N_{MD} = 20$, which so far amounts to rather short trajectories. We simulated several $\kappa$ values for each $\beta = 3.00, 3.50, 3.75$ and 4.00. We have measured the Polyakov loop, the pion norm and the average number of iterations it takes to invert the fermion matrix. Each observable is now discussed in detail.

2.1. Locating the critical line

Although not a physical observable in its own right, the average number of iterations it takes to invert the fermion matrix is a very good indica-
tor for criticality. The simulations where done in the following way. At each \( \beta \)-value we started a simulation at \( \kappa = 0.12 \) and used a thermalized configuration from this run as a start configuration at a higher value of \( \kappa \). We continued to do so for higher and higher \( \kappa \)-values. At those \( \beta \)-values, where we saw a drastic increase in the number of iterations, we started a simulation at a much higher \( \kappa \)-value and continued towards smaller \( \kappa \)-values. Our findings are summarized in Fig. 1. At \( \beta = 3.00 \) we were not able to simulate the system for \( 0.1770 < \kappa < 0.1825 \). At \( \beta = 3.50 \) we saw an initial increase of iterations, even after switching from minimal residual to conjugate gradient, which usually decreased the number of iterations. With increasing \( \kappa \) the number of iterations decreased again, only to increase again at fairly high \( \kappa \)-values. At \( \beta = 3.75 \) and 4.00 we saw a similar behaviour as at \( \beta = 3.50 \) but not as pronounced. We experimented with different inversion routines and our conclusions are, that close to the critical line conjugate gradient is superior to overrelaxed minimal residual and BiCGstab1.

2.2. Pion Norm

Since it is not possible to reliably extract the pion screening mass on small lattices, we use the pion norm instead to indicate the existence of a critical line of vanishing pion screening mass. The pion norm is the integrated pion correlator and is defined as follows:

\[
\Pi = \frac{1}{4N_\sigma^3N_\tau} \cdot \text{Tr} \left[ \mathcal{M}^{-1} \gamma_5 \mathcal{M}^{-1} \gamma_5 \right]
\]

(1)

Here \( \mathcal{M} \) is the fermion matrix on a particular gauge configuration. Near the critical line the pion norm behaves as \( \Pi \approx 1/m_{\pi}^2 \), hence a diverging pion norm indicates the existence of the critical line. Our results are displayed in Fig. 2. At \( \beta = 3.00 \) we find a clear signal for two critical lines close to \( \kappa = 0.1770 \) and 0.1825. The difference in \( \kappa \) is already quite small, so we are near the tip of the cusp. At \( \beta = 3.50 \) the pion norm develops a small peak at \( \kappa = 0.1550 \), which is located where the crossover from the low temperature to the high temperature phase starts (see section on Polyakov loop). No divergent behaviour is observed and the critical line ceases to exist in this coupling region. The simulations at \( \beta = 3.75 \) and 4.00 do not even find a peak for the pion norm, but rather a smooth behaviour as a function of hopping parameter. We conclude, that the critical line turns back towards strong coupling and develops a cusp between \( \beta = 3.00 \) and 3.50.

2.3. Polyakov Loop

The Polyakov loop is defined as follows:

\[
L = \frac{1}{N_\tau} \sum_{\vec{x}} \frac{1}{N_c} \text{Tr} \prod_{\tau=1}^{N_\tau} U_4(\vec{x}, \tau)
\]

(2)

This observable is sensitive to the finite temperature phase transition although it is no order parameter in the full theory. Our results are displayed in Fig. 3. At \( \beta = 3.00 \) we find a confined phase for \( \kappa \leq 0.1770 \). For \( \kappa > 0.1825 \), when one approaches the critical line from above, the Polyakov loop decreases to \( |L| \approx 0.1 \). This indicates that the system develops a low temperature behaviour in the vicinity of the critical line. On the other hand we do not see a sharp crossover, so we cannot conclude that one crosses the thermal line as one lowers \( \kappa \) towards \( \kappa_c(\beta) \).
At $\beta = 3.50$ the Polyakov loop displays a sharp crossover phenomenon, which means that the system crosses the thermal line for $0.1550 < \kappa < 0.1600$.

At $\beta = 3.75$ and 4.00 the system is in the high temperature phase down to $\kappa = 0.12$. This is not unexpected, since the finite temperature phase transition in the quenched theory for our choice of action occurs at $\beta_c = 4.07$.

3. Summary and Conclusions

From measuring the pion norm, Polyakov loop and the average number of iterations to invert the fermion matrix we conclude, that the finite temperature phase structure observed with the standard Wilson formulation is preserved for the tree level Symanzik improved formulation of quarks and gluons. We note that the difference in $\beta$ between the location of the cusp and the quenched $\beta_c$ is considerably reduced. What this means in terms of physical scales remains to be investigated by measurements of the lattice spacing. After this preparatory simulation on a small lattice, we will investigate the phase diagramm on larger lattices including a precise measurement of the pion screening mass and quark mass, the latter enabling us to study the chiral condensate as well [5].

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