One-flavour QCD at finite temperature *

Constantia Alexandrou\textsuperscript{a}, Artan Borici\textsuperscript{b}, Alessandra Feo\textsuperscript{a}, Philippe de Forcrand\textsuperscript{c}, Andrea Galli\textsuperscript{d}, Fred Jegerlehner\textsuperscript{e}, and Tetsuya Takaishi\textsuperscript{f}

\textsuperscript{a}Department of Natural Sciences, University of Cyprus, CY-1678 Nicosia, Cyprus
\textsuperscript{b}Paul Scherrer Institute, CH-5232 Villigen, Switzerland
\textsuperscript{c}Swiss Center for Scientific Computing, ETH-Zentrum, CH-8092 Zürich, Switzerland
\textsuperscript{d}ELCA Informatique, HofwiesenStr. 26, CH-8057 Zürich, Switzerland
\textsuperscript{e}DESY-IfH Zeuthen, D-15738 Zeuthen, Germany
\textsuperscript{f}Hiroshima University of Economics, Hiroshima, Japan 731-01

We present results, for heavy to moderate quark masses, of a study of thermodynamic properties of 1-flavour QCD, using the multiboson algorithm. Finite-size scaling behaviour is studied on lattices of size $8^3 \times 4$, $12^3 \times 4$, and $16^3 \times 4$. It is shown that, for heavy quarks, the peak of the Polyakov loop susceptibility grows linearly with the spatial volume, indicating a first order phase transition. The deconfinement ratio and the distribution of the norm of the Polyakov loop corroborate this result. For moderately heavy quarks the first-order transition weakens and becomes a crossover. We estimate the end point of the first-order phase transition to occur at a quark mass of about 1.6 GeV.

1. Introduction

We use the non-hermitian variant of the multiboson method \cite{1} to simulate one-flavour QCD at finite temperature (for more details on the algorithm see \cite{2,3}). We perform a finite-size scaling study for four $\kappa$ values of Wilson fermions. Because we simulate heavy quarks only, we can safely ignore the problem of the sign of the fermionic determinant. Global observables, such as the Polyakov loop, obtained with our multiboson algorithm showed an autocorrelation time $O(10)$ shorter than if obtained with an efficient polynomial variant of HMC, appropriate to simulate 1 flavour \cite{4}. This substantial improvement can presumably be attributed to the additional freedom due to the bosonic fields of the multiboson algorithm enabling movement \textit{around} energy barriers in contrast to HMC where one has to go \textit{over} the barrier.

In Table 1 we collect the parameters of our simulations.

| $\kappa$ | $8^3 \times 4$ | $12^3 \times 4$ | $16^3 \times 4$ |
|-----------|-----------------|-------------------|------------------|
|           | $N_b/\text{acc}$ | $Ksw$             | $N_b/\text{acc}$ | $Ksw$ |
| 0.05      | 8/0.78          | 18                 | 12/0.74          | 20    |
| 0.10      | 16/0.67         | 45                 | 24/0.63          | 50    |
| 0.12      | 24/0.74         | 55                 | 32/0.67          | 40    |
| 0.14      | 32/0.77         | 60                 | 40/0.70          | 37    |

\* indicates that we are still accumulating statistics.

2. Determination of $\beta_c$

To identify the critical line $\beta(\kappa)$ we study the signals for a first order phase transition on a finite lattice (e.g. \cite{5}) using three observables:

- The histogram of the norm of the Polyakov loop, which shows 2 peaks of equal area

\textsuperscript{*} indicates that we are still accumulating statistics.
at criticality. For the lattices under study here we observed enough tunneling events between the two phases to make this a reliable method. This is shown in Fig. 1 for $\kappa = 0.05$ for the three lattice sizes.

- The deconfinement ratio $\rho = 3/2p - 1/2$, where $p$ is the probability for the complex trace of the Polyakov loop to fall within $\pm 20$ deg of a $Z_3$ axis. $\rho$ goes from 0 (uniform angular distribution) to 1 (alignment with $Z_3$ axis).

- The peak value of the susceptibility of the Polyakov loop.

Using these criteria we determined the critical values $\beta(\kappa)$ given in Table 2.

| $\kappa$ | 0.05 | 0.10 | 0.12 | 0.14 |
|----------|------|------|------|------|
| $\beta_c$ | 5.692 | 5.66 | 5.63 | 5.59 |

Table 2
The critical values $\beta(\kappa)$. The estimated error is about one on the last digit.

3. Order of transition

In Fig. 2 we show the deconfinement ratio $\rho$ obtained using reweighting [4] for $\kappa = 0.05, \kappa = 0.10$ and $\kappa = 0.12$. Across the transition region the slope of $\rho(\beta)$ increases with the volume for $\kappa = 0.05$ signaling a first order transition. This is to be contrasted with the behaviour of $\rho$ for $\kappa = 0.12$ indicating that $\kappa = 0.12$ is already in the crossover region. For $\kappa = 0.10$ we observe a qualitative behaviour more appropriate for a weak first order transition.

In Fig. 3 we display the peak of the susceptibility versus the spatial volume $V$. The lines shown are best fits to the form $V^\alpha$. For $\kappa = 0.05$ the best fit yields $\alpha = 0.96(4)$ whereas for $\kappa = 0.14$ $\alpha$ is zero. For $\kappa = 0.10$ and $\kappa = 0.12$ the situation is less clear. The small value of $\alpha = 0.24(4)$ at $\kappa = 0.12$ as well as the absence of tunneling indicate that we are in the crossover region. For $\kappa = 0.10$ $\alpha = 0.54(3)$, increasing with the statistics of the $L = 16$ lattice (still in progress), and tunneling is still observed. If this increasing trend of the peak of the susceptibility for $L = 16$ continues then we will have confirmed that the transition is still first order.

Considering the signals that we have for $\kappa = 0.1$, namely tunneling between the two phases, the behaviour of the deconfinement ratio and the finite size scaling of the susceptibility, we are led to the conclusion that the end point of the first order phase transition occurs very near $\kappa = 0.1$. Taking the end-point value of $\kappa$, $\kappa_{ep} \approx 0.1 \pm 0.01$, we can approximately map to physical units, using the tadpole-improvement property $\kappa_c(\beta)(\Box)^{1/4} \approx 1/8$ to obtain $m_q a \sim 1.8(5)$, and $(4a)^{-1} \sim 220 \text{MeV}$ from the deconfinement temperature. This gives $m_q \sim 1.6(5) \text{GeV}$ at the end-point.
Figure 2. Deconfinement ratio for $\kappa = 0.05$, $\kappa = 0.10$ and $\kappa = 0.12$ for three lattice sizes.

This is in line with phenomenological expectations. The pure gauge deconfinement transition is fairly weak, with a correlation length $O(a \text{ few } \sigma^{-1/2})$. This is the minimum system size necessary to observe the deconfinement transition. Dynamical quarks introduce a new length scale, the distance where the string breaks, $O(2m_q/\sigma)$. Confinement can only be observed up to this distance. When the quark mass is lowered sufficiently that the second length-scale is similar to (or smaller than) the first, one cannot tell if the system is confined or deconfined, and the transition is replaced by a crossover. This occurs for $m_q \sim O(\text{afew}\sqrt{\sigma}/2)$, i.e. $m_q \sim O(1)\text{GeV}$.

Figure 3. Volume dependence of the maximum of the Polyakov loop susceptibility.

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