Thermodynamics of One-flavour QCD

C. Alexandrou, A. Boriçi, A. Feo, Ph. de Forcrand, A. Galli, F. Jegerlehner and T. Takaishi

Department of Natural Sciences, University of Cyprus, CY-1678 Nicosia, Cyprus
Paul Scherrer Institute, CH - 5232 Villigen, Switzerland
SCSC, ETH-Zentrum, CH-8092 Zürich, Switzerland
ELCA Informatique, HofwiesenStr. 26, CH-8057 Zürich, Switzerland
DESY-IFH Zeuthen, D-15738 Zeuthen, Germany
Hiroshima University of Economics, Hiroshima, Japan 731-01

We give a brief introduction on finite temperature phase transitions in lattice QCD including a discussion on the identification of first order transitions. We present a study of the deconfinement phase transition of one-flavour QCD, using the multiboson algorithm on lattice of sizes $8^3$, $12^3$ and $16^3 \times 4$. For heavy quarks our results are characteristic of a first order phase transition which gets weaker as the quark mass decreases and ends at a critical value of $\kappa \sim 0.1$ or in physical units at about 1.6 GeV.

1. Introduction

Twenty years ago Polyakov and Susskind pointed out that, when the temperature is increased, a deconfinement phase transition from normal hadronic matter to quark-gluon plasma can occur. Understanding the properties of QCD under extreme conditions of high temperature and/or pressure has been ever since a challenging problem (for a recent review see for example Ref. [3]).

The nature of the deconfinement phase transition has far-reaching phenomenological consequences: In Astrophysics it is important because such a phase transition is believed to have occurred, in the opposite direction, $10^{-6}$ s after the Big Bang. If of first order, effects due to supercooling should be visible today, possibly as deviations in the light element abundance from values obtained in the standard scenario. Determination of the order is also of importance to model builders of neutron stars and supernovae. In experiments with ultra-relativistic heavy-ions the aim is to create and detect the quark-gluon plasma. A first order phase transition is generally considered easier to detect and many of the proposed signatures assume the existence of a mixed phase. In the planned heavy ion experiments that will start next year at

*Talk presented by C. Alexandrou.
RHIC, Brookhaven and later on at LHC, CERN, the temperature reached will be of the order of 600 MeV and at this temperature one is still dealing with a strongly interactive system. Thus lattice QCD provides the most suitable non-perturbative approach to study such phenomena starting directly from the QCD Lagrangian. In order to use lattice QCD to study these phenomena we need an efficient method for simulating an odd number of flavours, namely the two light \( u \) and \( d \) quarks and the heavier strange quark. The local bosonic algorithm originally proposed by Lüscher for two degenerate flavours\(^5\) can be generalized to any number of flavours\(^6\),\(^7\). Before treating the \((2 + 1)\)-flavour case, we have applied it first to the study of one-flavour QCD\(^8\),\(^9\). In part because of algorithmic difficulties, one-flavour QCD has been largely ignored in spite of its interesting properties. The continuum \( N_f = 1 \) theory contains no pions and is expected to have no chiral phase transition\(^1\), whereas the heavy quark regime of the theory is expected to be qualitatively similar to the three dimensional three-states Potts model in an external magnetic field.

In this talk, after giving a brief overview of how one studies first-order phase transitions on a finite lattice taking as an example the well-studied deconfinement phase transition in quenched QCD, we will present results for heavy to moderately heavy Wilson fermions for one flavour QCD, on lattices of size \( 8^3 \), \( 12^3 \) and \( 16^3 \times 4\).

2. Overview

The deconfinement phase transition was first studied in the case of pure gauge. The basic degrees of freedom here are the \( SU(3) \) link variables \( U_\mu(n) \) located on the link leaving site \( n \) in the direction \( \hat{\mu} \) of a space-time lattice with \( N_s^3 \) spatial size and temporal size \( N_t \), with \( N_s \gg N_t \) if possible. The temperature is given by \( T = (N_t a)^{-1} \) with \( a \) the lattice spacing. The partition function in Euclidean space is given by

\[
Z = \int [dU] \ e^{-S_G} \quad \text{and} \quad S_G = \beta \sum_P [1 - \frac{1}{3} \text{Re} \ Tr \ U_P] \tag{2.1}
\]

where \( U_P \) is the product \( U_\mu(n)U_\nu(n + \hat{\mu})U_\mu^\dagger(n + \hat{\nu})U_\nu^\dagger(n) \) of 4 links around an elementary plaquette \( P \), and we sum over all plaquettes \( P \). We take periodic boundary conditions for the links and, for a given \( N_t \), the temperature is changed by varying \( \beta = 6/g^2 \) with \( g \) the coupling constant. Svetitsky and Yaffe\(^2\) identified the global symmetry that is spontaneously broken at the
deconfinement phase transition as the center symmetry \(Z(3)\) of \(SU(3)\). The pure gauge action is invariant under \(Z(3)\). To see this let us transform all time-like links with a given time coordinate \(n_0\),
\[
U_0(n, n_0) \to zU_0(n, n_0)
\]  
with \(z\) an element of \(Z(3)\). A temporal plaquette at time \(n_0\) necessarily has two transformed links so that \(U_P \to U_P(z)U_0(n + \hat{\mu})U_0^\dagger(n)z^\dagger = U_P\) since \(z\) commutes with all \(U\)’s. While local observables are invariant, the Polyakov line defined as the product of temporal links
\[
L(n) = \frac{1}{3} \text{Tr} \prod_{n_0=1}^{N_t} U_0(n, n_0)
\]  
transforms as \(L \to zL\) under \(Z(3)\). Its expectation value \(\langle L \rangle = 0\) if the symmetry is unbroken whereas \(\langle L \rangle \neq 0\) if the symmetry is spontaneously broken. If \(\langle L \rangle = 0\) the free energy of a static quark, \(F_q = -\frac{1}{\beta} \log(\langle L \rangle)\), becomes infinite and at large distances the correlator
\[
G(r) \equiv \langle L(n) L(n + r) \rangle \sim \exp(-\sigma a^2 |r| N_t)
\]  
should also vanish with an exponential dependence \(\sim \exp(-\sigma a^2 |r| N_t)\) with \(\sigma\) the string tension and \(F_{q\bar{q}}\) the free energy of a static quark-antiquark pair. This behaviour describes the confining phase. If the symmetry is spontaneously broken then \(\langle L \rangle \neq 0\) and \(F_q\) is finite signaling quark liberation. Therefore the Polyakov loop is an order parameter for the \(Z(3)\) symmetry. Constructing an effective action for \(L\) and using universality arguments the authors of Ref. predicted that the phase transition in pure gauge is first order. This has been confirmed by numerical lattice simulations.

Dynamical quarks are included using the standard Wilson discretization procedure. Writing the fermion matrix \(D = 1 - \kappa M\), where \(M\) is the hopping matrix, the Wilson action is
\[
S^{(W)}_F = \sum_{nn'} \bar{\psi}(n) D(n, n') \psi(n') \quad \text{with} \quad 2m_q a = \frac{1}{\kappa} - \frac{1}{\kappa_c}; \quad M \equiv \sum_{\mu=0}^{3} M_\mu;
\]
\[
M_\mu(n, n') = (1 - \gamma_\mu)U_\mu(n)\delta_{n', n+\hat{\mu}} + (1 + \gamma_\mu)U_\mu^\dagger(n')\delta_{n', n-\hat{\mu}}.
\]  
The hopping parameter \(\kappa\) is thus related to the quark mass, \(m_q\), and \(\kappa_c\) is the value of \(\kappa\) for the massless limit. For the fermions we use antiperiodic boundary conditions in the temporal direction and periodic in the spatial directions. Under the \(Z(3)\) transformation \(U_0(n, n_0) \to zU_0(n, n_0)\) and \(S^{(W)}_F\) is no longer invariant. This explicit
symmetry breaking can weaken the first order phase transition, change it to second order or even make it disappear. These possibilities must be investigated by detailed calculations as a function of the quark mass. The order parameter \( \langle L \rangle \) is no longer zero even in the “confined” phase since we can have \( q \bar{q} \) pair creation shielding colour. However it will still show a discontinuity at the phase transition and can still be used as a probe for deconfinement. In the partition function the Wilson fermions can be integrated out yielding

\[
Z = \int d[U] \exp(-S_G^{\text{eff}}[U]) \quad \text{with} \quad S_G^{\text{eff}} = S_G - \text{Tr} \log(1 - \kappa M) .
\]  

(2.5)

\( S_G^{\text{eff}} \) can be expanded in powers of \( \kappa \) and for finite temperature the \( \kappa^N \) term gives a contribution to \( S_G^{\text{eff}} \) of the form

\[
S_h = -h \sum_n \text{Tr} \text{Re} L(n), \quad h > 0
\]  

(2.6)

The effective magnetic field, \( h \propto \kappa^N \) to leading order, induces a magnetization along the positive real axis. Since the transition at \( h = 0 \) is first order the magnetic term is expected to weaken it and above a critical value \( h_{ep} \) the transition may disappear.

Such a behaviour was observed in the three dimensional three-state Potts model in an external magnetic field \( h \):

\[
S = -\sum_{<nl>} \beta \text{Re} z_n^* z_l - h \sum_n \text{Re} z_n
\]  

(2.7)

with \( z_n \) an element of \( Z(3) \). Whereas Fig. 1 may indicate the expected qualitative behaviour for QCD with a dynamical quark, the question of existence of an end-point and its location can only be answered after a detailed calculation.

3. **Local bosonic algorithm for one flavour**

The generalization of the local bosonic algorithm to any number of flavours is made easier by finding a polynomial approximation to the fermionic matrix itself rather than to \( (\gamma_5 D)^2 \). This can be done by constructing a polynomial
of even degree \( n \) defined in the complex plane with complex conjugate roots \( z_k \) such that \( \lim_{n \to \infty} P_n(z) = \frac{1}{2} \) for any \( z \) in the domain containing the spectrum of \( D \) (not including the origin). Since the spectral radius of the hopping matrix \( M \) is bounded by 8 in the free case, less in the interacting one, we are guaranteed that the spectrum of \( D = 1 - \kappa M \) will remain in the complex right half-plane for the heavy to moderately heavy quarks we simulate (\( \kappa \leq 1/8 \)).

Using the property \( D = \gamma_5 D^\dagger \gamma_5 \) we can write

\[
det P_n(D) = c_n \prod_{k=1}^{n/2} \det(D - z_k)^\dagger \det(D - z_k) \tag{3.8}
\]

with \( c_n \) an easily computed constant, obtaining a local representation for \( detD \)

\[
det D = \lim_{n \to \infty} det^{-1} P_n(D) = \int \prod_{k=1}^{n/2} d\phi_k^\dagger d\phi_k e^{-\sum_{k=1}^{n/2} \phi_k^\dagger (D - z_k)^\dagger (D - z_k) \phi_k} \tag{3.9}
\]

The algorithm is made exact with a global Metropolis test at the end of a “trajectory”. The number \( n \) of bosonic fields \( \phi_k \) is chosen so that the correction term leads to an acceptance rate of about 2/3.

For the local updating of the gauge and boson fields we used standard heatbath and over-relaxation algorithms as in Ref.\(^7\). A trajectory is a symmetric combination of \( (2m+1) \) over-relaxation steps applied alternatively to the gauge and boson fields, preceded and followed by a heatbath on the bosons. Ergodicity for the gauge fields is maintained due to their coupling to the bosonic fields. The roots \( z_k \) are distributed on the circle of radius 1 centered at \((1,0)\).

We use even-odd preconditioning to lower the number of bosonic fields needed for a given accuracy, and a quasi-heatbath to initialize the boson fields using thermalized gauge configurations from other \( \kappa \) and \( \beta \) values.\(^9\)

### 4. Order parameters

In section (2) we argued that the deconfinement phase transition is expected to be first order for heavy quarks. Since the discontinuities which characterize a first order phase transition in the continuum are smoothed out on a finite lattice, we must rely on finite size scaling to identify a first order transition. Finite size scaling was first applied to identify transitions in spin systems\(^4\) and later to identify the order of the deconfinement phase transition in quenched QCD\(^2\). The observables that we consider are based on the Polyakov loop (2.3).
Our strategy is to vary $\beta$ at a given quark mass for our three spatial lattice sizes, and look for the following signals:

**Coexistence of the two phases:** A distinctive feature of a first order transition is phase coexistence. On a finite lattice we can look for tunneling between confined and deconfined phase, which occurs over a small temperature range around the critical temperature. We observe enough tunneling events to study the double peak distribution of the norm $|\Omega|$ of the Polyakov loop defined as

$$\Omega = \frac{1}{V} \sum_n L(n) \quad (4.10)$$

with $V$ the spatial volume.

**Deconfinement ratio:** The deconfinement ratio is defined by

$$\rho = \frac{3}{2} p - \frac{1}{2} \quad (4.11)$$

with $p$ the probability for the complex Polyakov loop to be within 20 degrees of a $Z_3$ axis. Therefore if the $Z(3)$ symmetry is unbroken we find $p = 1/3$ and $\rho = 0$, while if it is broken in such a way that the Polyakov loop is distributed around one axis (here the real axis), then $p = 1$ and $\rho = 1$. The value $\rho = 0$ is obtained only in the pure gauge case where the $Z(3)$ symmetry is exact. Since heavy quarks break $Z(3)$ we obtain a value of $\rho$ different from zero in the confined phase but still look for a discontinuity across the phase transition.

**The peak value of the susceptibility:** The susceptibility gives a measure of the fluctuations of the Polyakov loop. We consider the behaviour of

$$\chi_L = V(\langle |\Omega|^2 \rangle - \langle |\Omega| \rangle^2) \quad (4.12)$$

which diverges at criticality for a first order phase transition in the continuum. On a finite lattice the discontinuity is smoothed: the distribution of $\chi_L$ has a width proportional to $1/V$ and a peak value $\chi_L^{\text{peak}} \propto V$. This scaling behaviour changes for a second order transition to $\chi_L^{\text{peak}} \propto V^\alpha$ with $\alpha < 1$. For a crossover behaviour, where no discontinuity occurs even in the thermodynamic limit $V \to \infty$, $\chi_L^{\text{peak}}$ remains constant as $V$ increases.

5. **Results**

The parameters of our simulations are included in Table 1. From the values listed in the table, we find that $n \propto \log(\text{volume})$ for a fixed quark mass and approximately $n \propto 1/m_q$ for a fixed volume, as expected.
Our results for the observables which probe the order of the transition are shown in Figs. (2-4). Tunneling between the confined and the deconfined phase is clearly observed for $\kappa = 0.1$ as shown in Fig. 2. Similar results are obtained for $\kappa = 0.05$ whereas for $\kappa = 0.14$ tunneling is no longer observed. In Fig. 3 we show the deconfinement ratio $\rho$ obtained using reweighting for $\kappa = 0.05, \kappa = 0.10$ and $\kappa = 0.12$. We include for comparison the pure gauge results as well. Across the transition region the slope of $\rho$ increases with the volume for $\kappa = 0.05$ signaling a first order transition in contrast to the behaviour of $\rho$ for $\kappa = 0.12$ indicating that $\kappa = 0.12$ is already in the crossover region. For $\kappa = 0.10$ it is not very clear and one would need a bigger lattice comparable to the correlation length to make a definite decision.

The volume dependence of the peak value of $\chi_L$ is displayed in Fig. 4. The lines shown are best fits to the form $V^n$. For $\kappa = 0.05$ the best fit yields $\alpha = 0.96(4)$ whereas for $\kappa = 0.14$ $\alpha = 0$ and thus we have further evidence that for $\kappa = 0.05$ the transition is first order whereas for $\kappa = 0.14$ we have a crossover. For $\kappa = 0.10$ and $\kappa = 0.12$ the situation is less clear. The small value of $\alpha = 0.22(3)$ at $\kappa = 0.12$ as well as the absence of tunneling leads us to conclude that $\kappa = 0.12$ is in the crossover region. For $\kappa = 0.10$ tunneling is still observed but $\alpha = 0.56(3)$ so that we may conclude that we are near the end point of the first order phase transition.

The critical values $\beta(\kappa)$, given in Table 1 are obtained from the position of the peak value of $\chi_L$. For $\kappa = 0.05$ and $\kappa = 0.1$ the value of $\beta$ where the deconfinement ratios for various volumes cross yields a value consistent with the one obtained from the position of $\chi_L^{peak}$. Not surprisingly, the shift $\beta_c(\kappa) - \beta_c(\kappa = 0)$ from the pure gauge critical coupling is approximately half that of the two-flavour case. Taking the end-point value of $\kappa$, $\kappa_{ep} \sim 0.1$ with 20% uncertainty, we can approximately map to physical units: Using the tadpole-improvement property $\kappa_c(\beta)\langle plaq\rangle^{1/4} \approx 1/8$ we obtain $m_qa \sim 1.8$, with
$(4a)^{-1} \sim 220 MeV$ from the deconfinement temperature. This gives $m_q \sim 1.6 GeV$ at the end-point.

Table 1: We give the $\kappa$ values, the number of bosonic fields $n$ and the average acceptance $acc$ for the three volumes studied. $K_{sw}$ (in kilo sweeps) is the total number of thermalized configurations used in the reweighting procedure. In the last column the critical $\beta$ values obtained from the analysis of the results are listed.

| $\kappa$ | $8^3 \times 4$ | $12^3 \times 4$ | $16^3 \times 4$ | $\beta_c$ |
|----------|----------------|----------------|----------------|---------|
|          | $n/acc$ | $K_{sw}$ | $n/acc$ | $K_{sw}$ | $n/acc$ | $K_{sw}$ | $n/acc$ | $K_{sw}$ |
| 0.05     | 8/0.78 | 18 | 12/0.74 | 20 | 24/0.83 | 20 | 5.690(2) |
| 0.10     | 16/0.67 | 45 | 24/0.63 | 50 | 32/0.67 | 37 | 5.66(1) |
| 0.12     | 24/0.74 | 55 | 32/0.67 | 40 | 40/0.69 | 12 | 5.63(1) |
| 0.14     | 32/0.77 | 60 | 40/0.70 | 37 | 50/0.67 | 12 | 5.59(1) |

6. Summary and Conclusions

In this work we have shown that the multiboson algorithm is well-suited for the study of one-flavour QCD for moderately heavy Wilson quarks. Using an exact algorithm for one flavour we have carried out a detailed finite size scaling analysis and determined the critical value of $\beta$ for $\kappa$ up to 0.14.

We have presented conclusive evidence that the deconfinement phase transition is first order for heavy quarks, with the critical line ending at about $\kappa = 0.1$, i.e. $m_q \sim 1.6$ GeV. This is in line with phenomenological expectations. The pure gauge deconfinement transition is fairly weak, with a correlation length $O(\text{a few } \sigma^{-1/2})$. 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

$$m_q \sim O(\text{a few } \sqrt{\sigma}/2) \quad \text{i.e.} \quad m_q \sim O(1) GeV \quad (6.13)$$

Acknowledgements: We thank SIC of the EPFL in Lausanne, ZIB in Berlin, and the Minnesota Supercomputing Institute for computer time.
Figure 3: The Deconfinement ratio for pure gauge and for $\kappa = 0.05$, $\kappa = 0.10$ and $\kappa = 0.12$ for three lattice sizes.

Figure 4: The volume dependence of the peak of the susceptibility for $\kappa = 0.05$, $\kappa = 0.10$, $\kappa = 0.12$ and $\kappa = 0.14$.

1. A. M. Polyakov, Phys. Lett. B 72 (1977) 477.
2. L. Susskind, Phys. Rev. D 20 (1978) 2610.
3. H. Meyer-Ortmanns, Rev. Mod. Phys. 68 (1996) 473.
4. W. Greiner and D. Rischke, Phys. Rep. 264 (1996) 183.
5. M. Lüscher, Nucl. Phys. B 418 (1994) 637.
6. A. Borici and Ph. de Forcrand, Nucl. Phys. B 454 (1995) 645.
7. A. Borrelli, Ph. de Forcrand and A. Galli, Nucl. Phys. B 477 (1996) 809.
8. C. Alexandrou et al., Nucl. Phys. B (Proc. Suppl.) 53 (1997) 435 and Nucl. Phys. (Proc. Suppl.) 63 (1998) 406.
9. C. Alexandrou et al., in preparation.
10. R. D. Pisarski and F. Wilczek, Phys. Rev. D 29 (1984) 338.
11. T. A. DeGrand and C. E. DeTar, Nucl. Phys. B 225 (1983) 590.
12. L. G. Yaffe and B. Svetitsky, Phys. Rev. D26 (1982) 963; B. Svetitsky and L. G. Yaffe Nucl. Phys. B 210 (1982) 423.
13. B. Svetitsky, Phys. Rep. 132 (1986) 1.
14. M. Fukugita, M. Okawa and A. Ukawa, Nucl. Phys. B 337 (1990). 181.
15. M.S.S. Challa, D.P. Landau and K. Binder, Phys. Rev. B 34 (1986) 1841; K. Binder and D. P. Landau, Phys. Rev. B 30 (1984) 1477; M. E. Fisher and A. N. Berker, Phys. Rev. B 26 (1982) 2507.
16. A. M. Ferrenberg and R. H. Swendsen, Phys. Rev. Lett. 63 (1989) 1195.