THE FINITE TEMPERATURE PHASE TRANSITION IN FOUR FLAVOUR QCD ON AN 8×12^3 LATTICE

MT_c Collaboration

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We present results of a numerical study of lattice QCD with four dynamical flavours of staggered fermions, performed by using a hybrid Monte Carlo algorithm on an 8×12^3 lattice. We find a rapid change in the average value of the Polyakov loop at $\beta_c=5.25\pm0.025$ for a quark mass $ma=0.025$; at this mass value, the behaviour of the chiral order parameter, $\langle\bar{\psi}\psi\rangle$, does not yet allow an independent determination of the transition point. Using existing hadron mass calculations, the value of β_c we have obtained here would lead to a transition temperature $T\sim100$ MeV.

An important prediction which has emerged from numerical simulations of lattice quantum chromodynamics (QCD) is the existence of a phase transition in strongly interacting matter, as one raises its temperature. In principle, such simulations are capable of yielding a variety of information, including the value of the transition temperature, T_c, and the order of the phase transition. This information is very useful in the search for this transition in relativistic heavy ion collisions or in studies of the development of the early universe. For reliable results, however, one first has to establish the presence of scaling and then consider in detail the effects of finite lattice size. This requires large lattices and high statistics. From the experience of pure SU(3) gauge theory simulations at finite temperature, one anticipates that a lattice with at least eight sites in the temporal direction may be needed to reach the scaling region of the full theory. In this letter, we report on first simulations of full QCD on an 8×12^3 lattice and compare these with previous results on smaller lattices.

The inclusion of light dynamical quarks in the simulation complicates the matter further, due to conceptual and technical difficulties which have left the simulations of the full theory lagging behind those of pure gauge theory in both the statistics and the lattice sizes. The emergence of the Hybrid Monte Carlo (HMC) [1] method to incorporate the fermionic loops in the theory has provided us with a reliable fermion algorithm which is free of the systematic errors characteristic of all small step-size algorithms. However, the HMC algorithm has so far been applied only to smaller lattices and intermediate quark masses. It has been argued that, asymptotically, the acceptance can be maintained constant by changing the step-size in the molecular dynamics part of the HMC as $V^{-1/4}m^{3/2}$ [2,3]. Nevertheless, it is far from clear how the algorithm will perform for physically reasonable quark masses and realistic lattices sizes. One anticipates that the tuning of step-size should be much less dependent on the quark mass in the chirally symmetric phase since there are no zero eigenvalues for the Dirac operator in this regime. In addition, for finite temperature QCD, the specific questions of thermalisation, metastabilities and critical fluctuations need to be investigated afresh with

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the new fermion algorithm. Our paper will also address some of these issues.

Finite temperature QCD has been investigated numerically for a variety of input parameters, such as the number of flavours or the value of the quark mass [4]. While the results seem to depend crucially on the quark mass, the flavour dependence is rather weak. The overall picture so far can be summarized as follows. For three or more light flavours, a first order chiral phase transition is observed up to some quark mass m_{ch}. With increasing quark mass the transition seems to become weaker, and beyond m_{ch} the determination of its order becomes ambiguous. There are furthermore indications from simulations at intermediate quark masses ($m/T \simeq 0.4$) [5] that the transition discontinuity decreases with increasing spatial volume. Most of the studies so far used approximate algorithms to include dynamical fermions and lattices with $N_\tau \leqslant 6$, where N_τ is the number of lattice sites in the inverse temperature direction. In ref. [6], the thermodynamics of four flavour QCD with quarks of mass $ma = 0.025$ was studied on a symmetric 8^4 lattice using a hybrid algorithm; a strong first order phase transition was claimed at this mass value. We shall here work on an 8×12^3 lattice with four flavours of staggered fermions of mass 0.025 in lattice units, using the "exact" HMC algorithm. As mentioned above, simulations with this algorithm have so far only been performed on smaller lattices [7,8].

The QCD partition function at finite temperature can be defined in terms of gluonic degrees of freedom,

$$Z = \int \prod_{n,\mu} \mathrm{d}U_{n,\mu} \det Q \exp(-S_G) , \qquad (1)$$

where S_G denotes the standard gluonic Wilson action and the fermion matrix $Q_{n,m}$ is defined as

$$Q_{n,m} = ma\delta_{n,m} + \tfrac{1}{2} \sum_{\mu=0}^{3} \eta_\mu(n) (U_{n,\mu}\delta_{n,m-\hat{\mu}} - U^\dagger_{m,\mu}\delta_{n,m+\hat{\mu}}) , \qquad (2)$$

with phase factors $\eta_\mu(n) = (-1)^{n_0 + \ldots + n_{\mu-1}}$ for $\mu > 0$ and $\eta_0(n) = 1$.

We generate equilibrium configurations by using the HMC algorithm [1] and obtain expectation values of the physical observables of interest by averaging over these configurations. The advantage of the HMC algorithm is that it has no systematic step-size errors. For staggered fermions it is in practice only applicable to QCD with a multiple of four fermion flavours. Using pseudo-fermion fields ϕ_e, ϕ^*_e which occupy only even lattice sites (e) and momenta $\pi^\alpha_{n,\mu}$, $\alpha = 1, \ldots, 8$, the partition function given in eq. (1) can be rewritten in the form

$$Z = \int \prod_{n,\mu} \mathrm{d}U_{n,\mu} \prod_e \mathrm{d}\phi_e \mathrm{d}\phi^*_e \prod_{n,\mu,\alpha} \mathrm{d}\pi^\alpha_{n,\mu} \exp(-H), \qquad (3)$$

where the hamiltonian, H, is given by

$$H = \sum_{n,\mu,\alpha} \tfrac{1}{2} (\pi^\alpha_{n,\mu})^2 + V , \qquad (4)$$

with the potential, V, defined as

$$V = S_G + \tfrac{1}{2} \phi^*_e (Q^\dagger Q)^{-1}_{ee'} \phi_{e'} . \qquad (5)$$

Here e denotes a multiple index $e = (n, \lambda)$, where n designates even sites only and $\lambda = 1, 2, 3$ is the colour index. Similarly we will use a multiple index o for odd sites. Eq. (3) defines the scheme for the molecular dynamics steps of the HMC algorithm. At the beginning of the trajectory complex random numbers R_e, R_o are generated for each lattice site and colour according to the distribution $\exp(-\frac{1}{2} R^\dagger R)$. The ϕ are then calculated from $\phi_e = (Q^\dagger R)_e = maR_e + Q^\dagger_{eo} R_o$, leading to the distribution in eq. (3). The ϕ_e are kept fixed for the remainder of the molecular dynamics trajectory. We use a version of the approximate leapfrog scheme, where the gauge fields $U_{n,\mu}$ are updated according to

$$U_{n,\mu}(\tau_{k+1}) = \exp[\mathrm{i}\Delta\tau \pi^\alpha_{n,\mu}(\tau_k + \tfrac{1}{2}\Delta\tau) T_\alpha] U_{n,\mu}(\tau_k) , \qquad (6)$$

with

$$\pi^\alpha_{n,\mu}(\tau_k + \tfrac{1}{2}\Delta\tau) = \pi^\alpha_{n,\mu}(\tau_k - \tfrac{1}{2}\Delta\tau) - \Delta\tau \partial^\alpha_{n,\mu} V(\tau_k), \qquad (7)$$

where $\partial^\alpha_{n,\mu}$ is to be interpreted as the derivative on the group manifold as defined in ref. [9]. An explicit expression for $\partial^\alpha_{n,\mu} V$ can be found in ref. [7]. For $k = 0$ and N_{MD}, the time step in eq. (7) has to be halved and the initial momenta are chosen for $k = 0$ to be gaussian distributed random numbers.

The new feature of the HMC algorithm comes from the global accept/reject step. This is determined by the change δH of the hamiltonian, defined in eq. (4), during the molecular dynamics trajectory, as calculated using the approximate leapfrog algorithm. The

change in the fields $U_{n,\mu}$ accumulated during the trajectory is accepted with the probability

$$P=\min[1, \exp(-\delta H)] . \quad (8)$$

This removes the systematic $O(\Delta\tau^2)$ errors introduced by the leapfrog scheme.

The HMC algorithm has been tested before on smaller lattices and it has been found that reasonably high acceptance rates can be achieved without making the time step $\Delta\tau$ impractically small. On a 8×12^3 lattice with $ma=0.025$, $5.1\leqslant\beta\leqslant5.6$, we observe that a time step $\Delta\tau$ between 0.0125 and 0.025 is sufficiently small to guarantee acceptance rates of at least 50%. For these $\Delta\tau$ values, we find that the motion through phase space is still rapid enough to take the system from one phase to the other in 1000 trajectories (see below and fig. 1). The acceptance rate depends only weakly on the parameter N_{MD}. Ideally, the latter should be chosen so as to minimize autocorrelations in computer time. Such a tuning is, however, costly, and we have, somewhat arbitrarily, chosen to work with a trajectory length $0.5\leqslant\tau\leqslant1.0$. In table 1, our Monte Carlo parameters are given in detail, together with the acceptance rates achieved. From this table, we see that the acceptance rate exhibits a clear

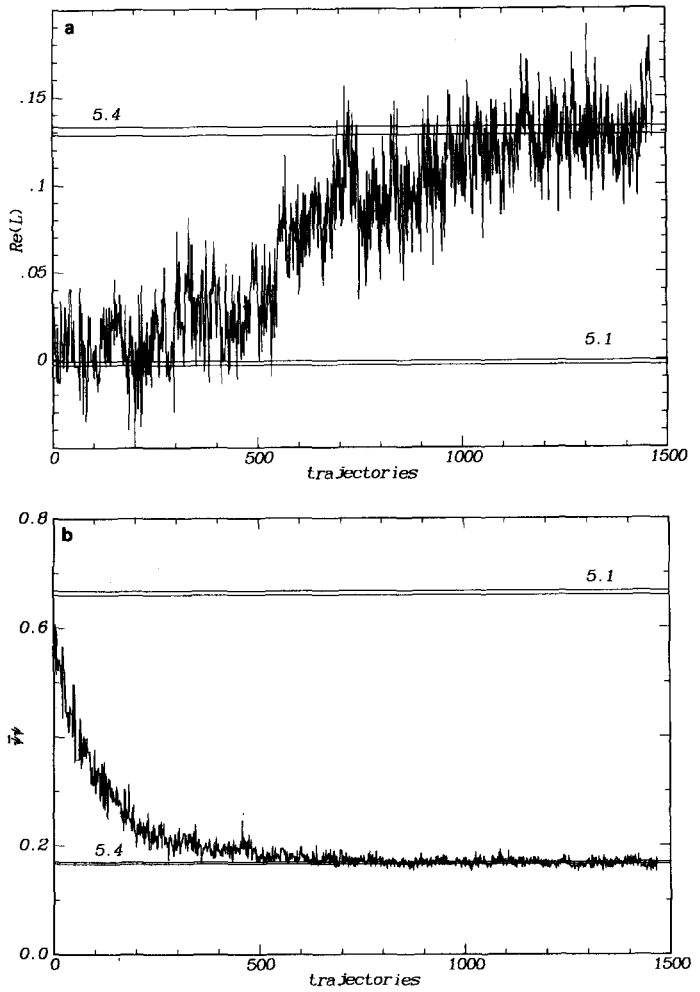

Fig. 1. The run time history for Re L (a) and $\bar{\psi}\psi$ (b) on an 8×12^3 lattice at $\beta=5.4$ starting from a configuration equilibrated at $\beta=5.1$. The bands of straight lines indicate the equilibrated values at $\beta=5.4$ and 5.1.

Table 1
Parameters for the HMC algorithm used in our simulations. The last column gives the acceptance rates achieved.

β	$\Delta\tau$	τ	Acceptance (%)
5.1	0.0125	0.5	51
5.175	0.0125	0.5	70
5.2	0.0125	0.5	72
5.225	0.0125	0.5	76
5.25	0.0125	0.5	84
5.275	0.0125	0.5	83
5.3	0.0250	1.0	43
5.4	0.0125	0.5	90
5.6	0.0250	1.0	75

β dependence. In particular, it is much easier to maintain a high acceptance in the deconfined than in the confined phase. As mentioned above, this is to be expected due to the absence of zero eigenvalues for the Dirac operator in the chirally symmetric phase. For the range of bare parameters we have studied on the 8×12^3 lattice and also from runs on smaller lattices with different quark masses, we further find that in order to keep the acceptance fixed one needs to change $\Delta\tau \sim ma$, unlike the naive expectation $\Delta\tau \sim (ma)^{3/2}$ [3]. In fact, this seems to be also the case for the data presented in ref. [3]. A more detailed presentation of our results for the algorithm performance will be given elsewhere.

For the analysis of the phase structure of QCD at finite temperature, the relevant physical observables are the Polyakov loop L,

$$L = \frac{1}{N_\sigma^3} \sum_{\boldsymbol{n}} \mathrm{Tr} \prod_{n0=1}^{N_\tau} U_{(n0,\boldsymbol{n}),0} \,, \tag{9}$$

and the chiral condensate $\langle \bar{\psi}\psi \rangle$,

$$\langle \bar{\psi}\psi \rangle = \frac{1}{N_\tau N_\sigma^3} \frac{\partial}{\partial ma} \ln Z \,. \tag{10}$$

Monitoring the time evolution of these observables, in addition to others such as plaquette, we checked for thermalisation. Fig. 1 shows the time evolution of $\bar{\psi}\psi$ and L from a random start at $\beta = 5.4$; an equilibrated configuration at $\beta = 5.1$ was used as a random start. One sees that it took approximately 1100 trajectories from the random start to converge to the ordered start value. However, we find that only ~ 700 trajectories are needed for thermalisation if a starting configuration corresponding to a nearby β value is used. Fig. 2a displays the absolute value of the Polyakov loop as a function of β. It shows a clear structure in the range $5.2 \leqslant \beta \leqslant 5.3$ and changes most

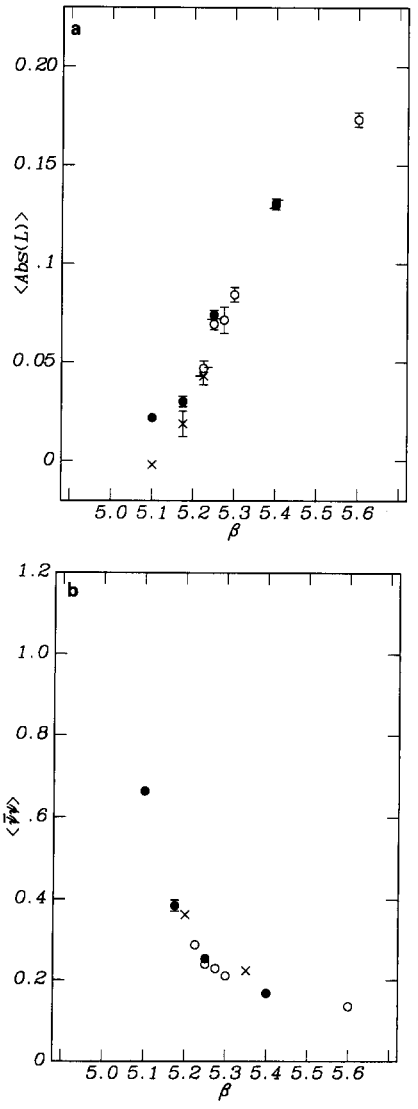

Fig. 2. (a) The average of the absolute value (circles) and the real part (crosses) of the Polyakov loop as a function of β on an 8×12^3 for four flavours of mass 0.025 in lattice units. (b) The order parameter $\langle \bar{\psi}\psi \rangle$ on an 8×12^3 (circles) and 24×12^3 (crosses) lattice for four flavours of mass 0.025. Filled (open) circles denote results obtained from a starting configuration equilibrated at a lower (higher) β.

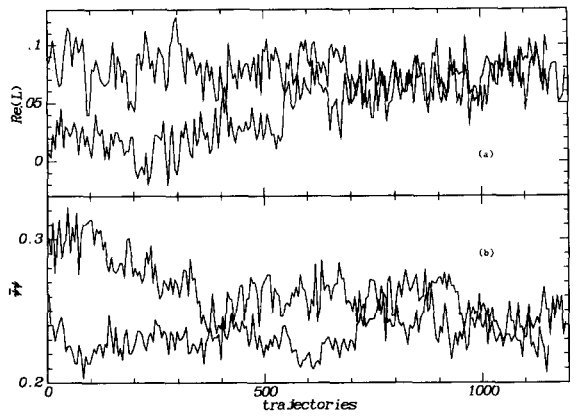

Fig. 3. The run time history for Re L (a) and $\bar{\psi}\psi$ (b) on an 8×12^3 lattice at $\beta=5.25$, originating from random and ordered states.

rapidly around $\beta=5.25$. We estimate from this that the critical coupling, β_c, lies in the region between 5.225 and 5.275. We have reaffirmed the value of Abs L at $\beta=5.25$ by using both a cold and a hot start, as shown in fig. 3. After about 700 trajectories from the respective starts the two runs come close to each other and fluctuate around a mean which is the same for both the runs.

In fig. 2a we also show the expectation value of Re L. As can be seen it starts differing from $\langle \mathrm{Abs}\, L\rangle$ below 5.225. For $\beta>\beta_c$, one expects $\langle \mathrm{Re}\, L\rangle \simeq \langle \mathrm{Abs}\, L\rangle$ for the full theory even on a finite lattice, since fermions explicitly break the Z(3) symmetry present in the gluonic sector. At $\beta=5.1$, however, our data show that $\langle \mathrm{Re}\, L\rangle$ is consistent with zero. This means that the explicit breaking of the Z(3) symmetry in the low temperature phase is small.

In fig. 2b we show the chiral condensate. Our results for $\langle\bar{\psi}\psi\rangle$ are roughly in agreement with measurements on a 24×12^3 lattice [10], i.e., for $T\simeq 0$; these data are shown as crosses in fig. 2b. It thus appears difficult to establish genuine finite temperature effects in our data for $\langle\bar{\psi}\psi\rangle$. In order to see them it seems to be necessary to further reduce the bare quark mass, which will then reduce the large perturbative tail present in our data for $\beta>\beta_c$.

Let us finally discuss the behaviour of the entropy density on the 8×12^3 lattice. It is given by

$$\frac{S}{T^3} = 4\beta N_\tau^4 [1-\tfrac{1}{2}(c'_\sigma - c'_\tau)g^2](\langle P_\sigma\rangle - \langle P_\tau\rangle) + \tfrac{4}{3}N_\tau^4(1+c'_F g^2)(\langle \mathrm{Tr}\, D_0 Q^{-1}\rangle - \tfrac{3}{4}) + \tfrac{1}{3}N_\tau^4 ma\langle \mathrm{Tr}\, Q^{-1}\rangle\,, \quad (11)$$

where $\langle P_\sigma\rangle$ ($\langle P_\tau\rangle$) are the expectation values of space–space (space–time) plaquettes, and D_0 denotes the 0th component of the lattice Dirac operator

$$D_{n,m;0} = \tfrac{1}{2}(U_{n,0}\delta_{n,m-\hat{0}} - U^\dagger_{m,0}\delta_{n,m+\hat{0}})\,. \quad (12)$$

In this formula we have included $O(g^2)$ perturbative results for the derivatives of the bare couplings of the lattice lagrangian with respect to the anisotropy (temperature). For the SU(3) theory with four massless flavours one finds for these corrections $c'_\sigma=0.2002$, $c'_\tau=-0.1474$ and $c'_F=-0.2132$ [11]. Corrections due to finite quark masses are expected to be small. Fig. 4 displays our results for the entropy density. As observed earlier on the smaller lattices, the entropy density appears to overshoot just above the critical region which roughly coincides with the critical region deduced from the Polyakov loop. Although its general features do thus stand out in spite of our enormous error bars (which even compelled us to leave out the data point at $\beta=5.225$ for the sake of clarity), it is clear that one needs a lot more statistics to draw any firm conclusions from this quantity. This is known already from the experience gained from simulations in the pure gauge sector. In fact, also here the main source of errors is the difference in pla-

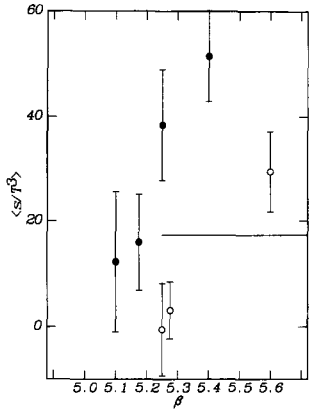

Fig. 4. Same as fig. 2 but for the entropy density s/T^3, defined in eq. (11). The full line gives the result for the entropy density of an ideal gas on a lattice of same size.

quette expectation values. However, the cost of generating independent configurations in the full theory is much higher and consequently any attempt at obtaining the entropy density would require much more computer resources than the ~4000 CPU-hours on a CRAY/XMP utilized in the present work.

Our present work has been performed for a rather large quark mass, $m/T=0.2$. It should be stressed that our simulations do not provide any evidence for strong metastabilities that could be interpreted as a hint for a first order transition, such as those observed in simulations on a 8^4 lattice with the same quark mass [6]. Whether the change in thermodynamic quantities we observe is caused by a genuine second order phase transition or is just related to a rapid crossover behaviour cannot, of course, be decided by the present calculation; this requires a more detailed finite size analysis.

The main aim of our calculations was the determination of the critical coupling for the finite temperature transition on an 8×12^3 lattice. We found $\beta_c=5.25\pm 0.025$. Using the asymptotic scaling relation this corresponds to a critical temperature of $T_c=(2.31\pm 0.09)\Lambda_{\overline{\rm MS}}$. Comparing this with earlier results for $N_\tau=4$ and 6,

$$\begin{aligned} T_c/\Lambda_{\overline{\rm MS}} &= 3.42(25)\,, \quad N_\tau=4,\ m/T=0.20 \quad [12]\,,\\ &= 2.77(15)\,, \quad N_\tau=4,\ m/T=0.15 \quad [13]\,,\\ &= 2.55(10)\,, \quad N_\tau=6,\ m/T=0.15 \quad [14]\,,\\ &= 2.31(9)\,, \quad N_\tau=8,\ m/T=0.20\,, \end{aligned} \tag{13}$$

one finds that in going from $N_\tau=6$ to $N_\tau=8$, the violations of asymptotic scaling are of the order of 10%, which is similar to what has been found in the pure gauge sector. The experience gained from earlier calculations on lattices with $N_\tau=4$ suggests that the critical temperature may further drop by about 20% when one extrapolates to zero quark mass.

We can convert our estimated critical temperature into physical units by comparing with hadron mass measurements. Ideally, one would like to compare with mass calculations performed at β_c using the HMC algorithm. Such data, however, do not exist at present. Thus we can only compare with data obtained with a pseudo-fermion algorithm [10]. As the existing data for m_ρ and m_N at 5.2 and 5.35 show only little β dependence, we can interpolate between them to determine T_c in units of hadron masses. We find

$$\begin{aligned} T_c &= 0.13(1)m_\rho = 100(8)\ \text{MeV}\,,\\ &= 0.083(3)m_N = 78(3)\ \text{MeV}\,. \end{aligned} \tag{14}$$

These values for the transition temperature are much lower (by a factor 2) than estimates for the pure gluon theory. This confirms the tendency seen in calculations at smaller N_τ for $n_f=4$ [12–14] as well as $n_f=2$ [15]. Such a low value of T_c would have serious implications for the experimental search of quark–gluon plasma: it would dramatically reduce the critical energy density relative to the value estimated from pure gauge theory calculations. It is therefore necessary to extend the present calculations to larger lattices and smaller quark masses. We are presently carrying out such a study, using the HMC algorithm, on 8×16^3 and 24×16^3 lattices with quark masses $ma=0.01$. The aim is to determine both T_c and hadron masses, as well as to investigate the relevance of finite size effects for the determination of the transition temperature.

The computations presented here were performed on the CRAY-XMP at CERN, CRAY-YMP at HLRZ, Jülich, the CRAY-2 at NCSA, Urbana-Champaign and the VP400 in Karlsruhe. We are thankful to the staff of the respective computer centers for their assistance. In particular, the friendly support by Dr. E. McIntosh, Dr. H.R. Renshall and Dr. H. Rollnik is greatly appreciated.

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