FIRST-ORDER CHIRAL PHASE TRANSITION IN LATTICE QCD

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Received 23 January 1987

The chiral phase transition in lattice QCD has been studied for light fermions of mass $ma=0.025$ on lattices of size 4^4 and $8^3\times 4$ using the hybrid algorithm. We find evidence for a first-order chiral phase transition with a large latent heat. A comparison with $10^3\times 6$ data shows violations of asymptotic scaling for T_{ch} which are similar in magnitude to those observed in the pure gauge sector.

While the phase structure of pure SU(N) gauge theories at finite temperature is quite well understood by now, the corresponding problem in the presence of dynamical fermions is still subject to much debate. For SU(3) gauge theory it has been found that the first-order deconfining phase transition of the pure gauge sector disappears for intermediate quark masses. A very rapid but smooth cross-over behavior is observed in the intermediate mass regime, $m/T\simeq 0.2$–0.4 (T being the temperature) [1]. However, a recent simulation with even smaller quark masses, $m/T=0.1$, presented evidence for the existence of a first-order chiral phase transition [2]. This is in nice agreement with predictions based on analysis of an effective lagrangian in the chiral limit [3]. The results of Gupta et al. [2] have been obtained with an exact algorithm [4]. This allows large steps in the update from one gauge configuration to the next. Application of this method is in practice, however, restricted to rather small lattices because of its slowness.

In the present letter we analyze the chiral transition for very light quarks, $m/T=0.1$, using the well-tested hybrid algorithm [5,6]. This will allow us to check this algorithm, which by contrast is a "small step" algorithm, against the exact algorithm used in ref. [2]. In addition we will extend the analysis of ref. [2], which has been performed on a 4^4 lattice, to an $8^3\times 4$ lattice. This will give further information about the critical parameters of the transition, i.e. T_c and latent heat.

The hybrid algorithm has been well tested and is described in detailed in the literature (for recent modifications and further references, see ref. [7]). Previously it has been used for a wide range of quark masses, the smallest being $m/T=0.15$ [7]. At this small mass value, indications for a nearby critical point were found, but no metastable states were observed. In the present analysis we have used two versions of the hybrid algorithm, differing in the ways they handle the fermionic sector. The first includes dynamical fermions as bilinear noise and the gauge fields are updated using an exponential update [7]. The second version introduces the fermions through microcanonical equations of motion [7]. The noisy version was used to study the chiral transition on a 4^4 lattice for QCD with $n_f=4$ light fermions of mass $ma=0.025$ ($m/T=0.1$). As in ref. [2] we used anti-periodic boundary conditions in both the spatial and temporal directions for the 4^4 runs.

We have performed runs with ordered and random start configurations at various couplings, $\beta=6/g^2$, in the interval $\beta\in[4.8, 5.0]$. The evolution in Monte Carlo time t was followed up to $t=300$. We noticed a considerable slowing down of the convergence rate around $\beta=4.95$. Indeed clear signals for

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0370-2693/87/$ 03.50 © Elsevier Science Publishers B.V.
(North-Holland Physics Publishing Division)

coexisting states have been found in this region. In fig. 1 we show the time evolution for $\langle\bar{\chi}\chi\rangle$ at various β values and corresponding data for the plaquette expectation values are given in fig. 2. We claim this provides good evidence for a first-order chiral phase transition around $\beta_c \simeq 4.94$. On this small lattice, however, there is a broad region where coexisting states can be found. This makes a precise determination of β_c difficult. Our results are in agreement with those reported in ref. [2]. Our values for $\langle\bar{\chi}\chi\rangle$ agree outside the critical region as does the size of the jump in $\langle\bar{\chi}\chi\rangle$ in the metastble region. The critical coupling itself may be shifted to a slightly higher value.

It has been noted in ref. [2] that in the confined region their algorithm leads to a noticeable systematic error due to the conjugate gradient inversion of the fermion matrix having been truncated after 90 iterations. We used the magnitude of the residual vector r as stopping criterion for the conjugate gradient algorithm. We found that while in the chiral symmetric region ~ 100 iterations yield an acceptable inverse ($r < 0.005$), about 300 iterations were necessary in the confined region to reach this accuracy. This reflects the influence of small eigenvalues in the fermion determinant, which are present in the confined region and are responsible for the nonvanishing chiral condensate, but which are absent in the chirally symmetric phase.

Another qualitative difference between these two regimes can be found in the amount of screening visible in Wilson loop expectation values. In table 1 we

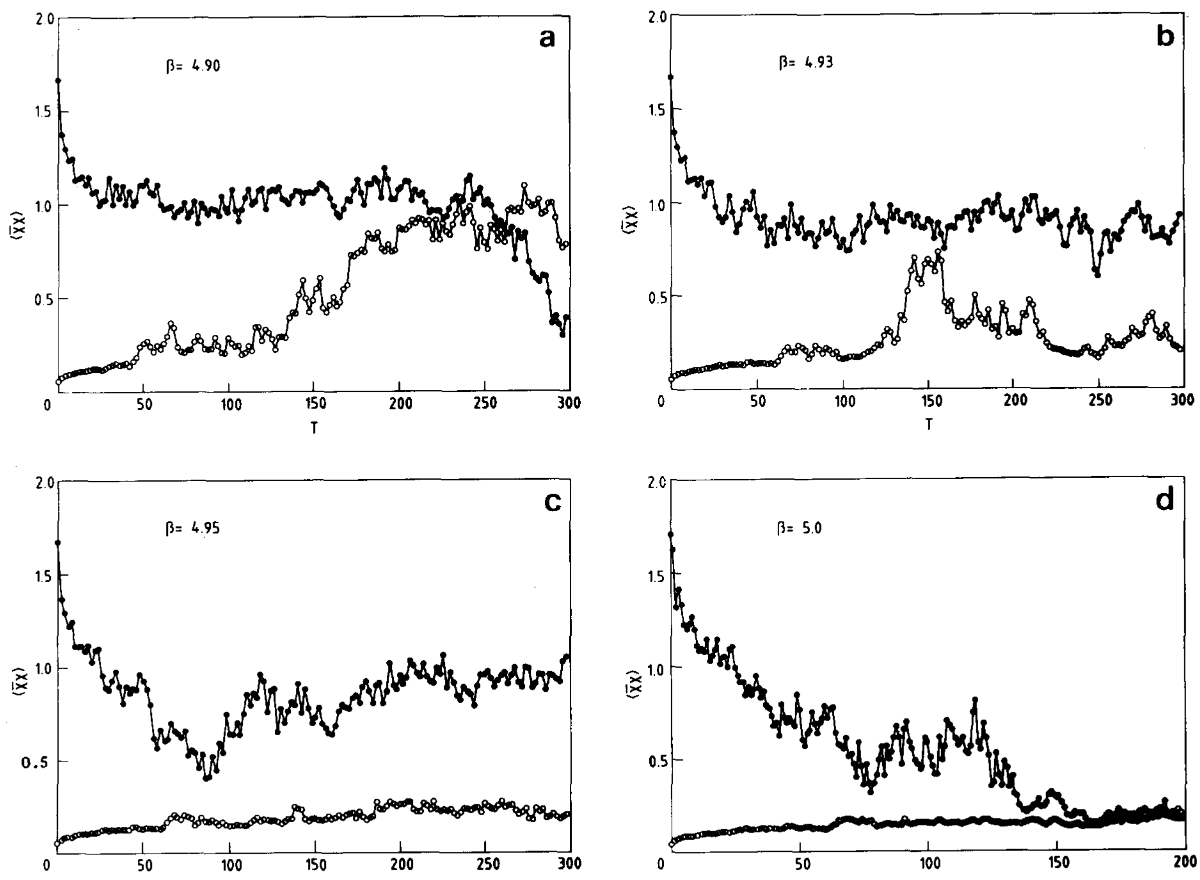

Fig. 1. Time evolution of $\langle\bar{\chi}\chi\rangle$ on a 4^4 lattice at (a) $\beta=4.9$, (b) 4.93, (c) 4.95 and (d) 5.0. Shown are runs with ordered (open circle) and random (full points) start configurations. The increment of the Monte Carlo time T was chosen to be $dt=0.01$.

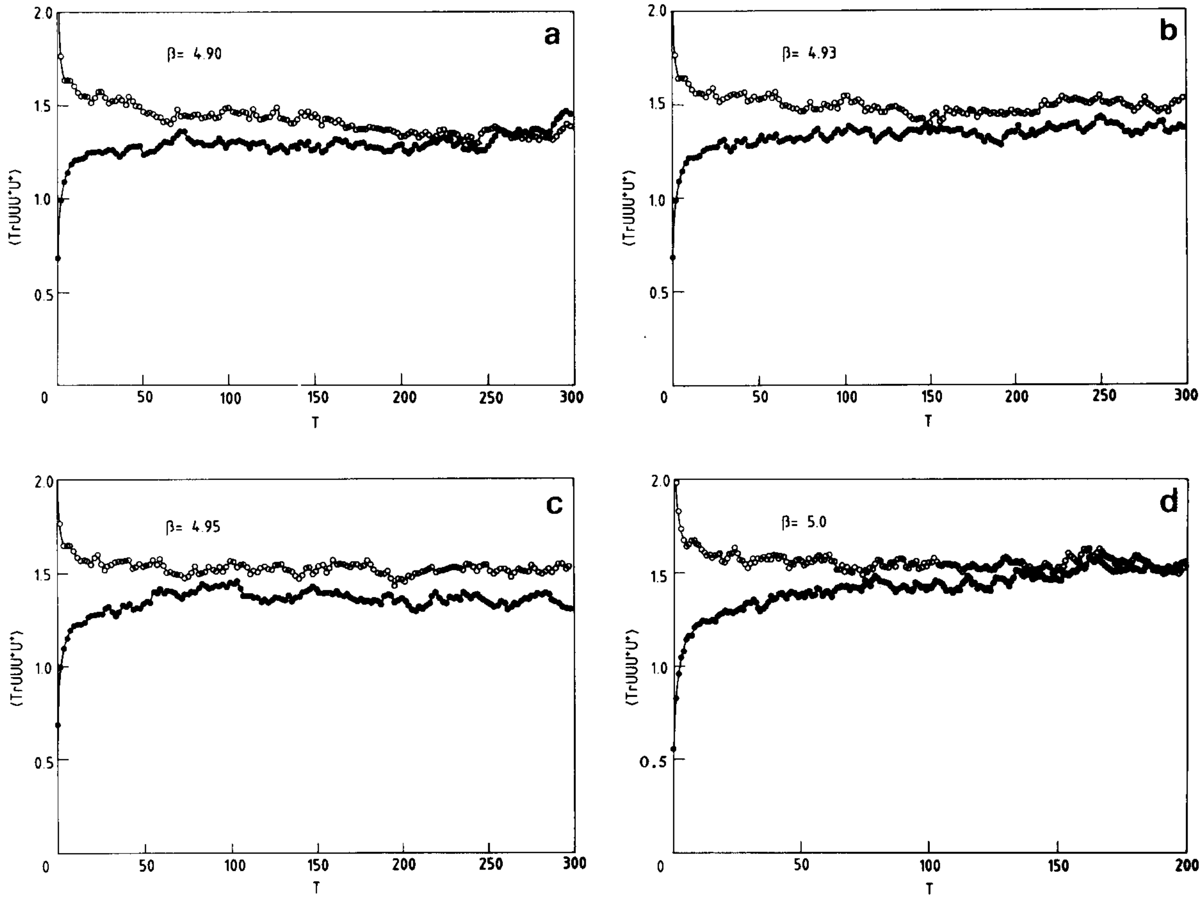

Fig. 2. Same as fig. 1 but for the plaquette expectation value $\langle \mathrm{Tr}\, UU U^+ U^+ \rangle$.

Table 1
Comparison of Wilson loop expectation values on a 4^4 lattice obtained with four flavors of mass $ma=0.025$ and for the pure gauge theory ($ma=\infty$) for various values of β.

Wilson loop	$ma=0.025$ $\beta=4.8$	$ma=\infty$ $\beta=5.0$	$ma=0.025$ $\beta=5.0$	$ma=\infty$ $\beta=5.5$
1×1	0.4067(29)	0.3996(6)	0.5126(24)	0.4996(30)
1×2	0.1699(21)	0.1622(5)	0.2921(36)	0.2633(38)
1×3	0.0712(13)	0.0660(4)	0.1737(36)	0.1402(34)
2×2	0.0297(11)	0.0272(2)	0.1201(40)	0.0819(31)
2×3	0.0049(10)	0.0045(1)	0.0608(39)	0.0271(19)
3×3	−0.0015(14)	0.0007(2)	0.0332(37)	0.0074(9)

compare Wilson loop expectation values below ($\beta=4.8$) and above ($\beta=5.0$) the chiral transition with suitable data from simulations of the pure gauge theory at shifted β-values. These shifted couplings have been selected such that the 1×1 Wilson loops with and without dynamical fermions are in rough agreement. While such a simple shift seems to be sufficient to match all the larger loops in the broken

Table 2
Results for $\langle\bar{\chi}\chi\rangle$ and the plaquette expectation value $\langle \mathrm{Tr}\, UUU^+U^+\rangle/3$ on a 4^4 lattice with four light flavors of mass $ma=0.025$. Where coexisting states were found, separate results are given for the broken (b) and symmetric (s) phases.

β	$\langle\bar{\chi}\chi\rangle$		$\langle \mathrm{Tr}\, UUU^+U^+\rangle/3$	
	b	s	b	s
4.8	1.1000(61)	-	0.4067(29	-
4.9	1.0385(86)	-	0.4256(23)	-
4.93	0.8620(86)	0.2456(276)	0.4475(27)	0.4917(32)
4.95	0.8551(74)	0.2123(86)	0.4487(23)	0.4952(21)
5.0	-	0.1432(57)	-	0.5126(24)

phase too, this is clearly not possible in the chirally symmetric phase. This may be taken as an indication for larger screening effects in the chirally symmetric phase. However, it is partly due also to the smaller coupling, $\beta=4.8$ being still in the strong coupling regime. At larger couplings screening effects, though not that strong, are also visible in the symmetry broken phase [8].

Let us summarize the critical parameters we obtained for the 4^4 lattice:

$$\beta_c = 4.94 \pm 0.04 \, ,$$

$$\Delta p = 0.045 \pm 0.005 \, ,$$

$$\Delta\bar{\chi}\chi = 0.630 \pm 0.020 \, .$$

Detailed results are given in table 2. Notice the large discontinuity in the plaquette expectation value. This is to be compared with the result found in the pure gauge sector, where on an $8^3\times4$ lattice the discontinuity was $\Delta p=0.007$. Of course, this reflects a peculiar feature of the energy density noted already in earlier calculations with dynamical fermions at larger masses: while the fermionic energy density immediately above T_c is quite close to the asymptotic ideal gas value, the gluonic contribution overshoots this limit considerably. This is reflected here in the large jump observed in the plaquette expectation value p.

We now turn to a discussion of our $8^3\times4$ data. Here we used both versions of the hybrid code. Again we find clear indications for coexisting states around $\beta=4.95$. In fig. 3a we show the time evolution of $\langle\bar{\chi}\chi\rangle$ at $\beta=4.95$ obtained with the deterministic algorithm. The Wilson line expectation values obtained with the noisy algorithm are shown in fig. 3b. Both our programs were accurate up to systematic errors of $O(\Delta t^4)$. However, it is known that the systematic errors are larger for the noisy algorithm [9], which thus may require smaller step size than the deterministic algorithm at the same bare mass.

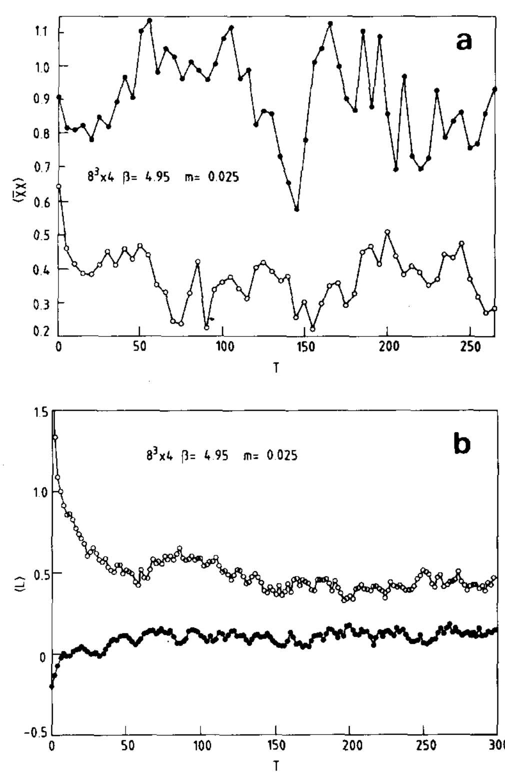

Fig. 3. (a) Time evolution of $\langle\bar{\chi}\chi\rangle$ and (b) the thermal Wilson line $\langle L\rangle$ on a $8^3\times4$ lattice at $\beta=4.95$. Shown are runs with ordered (open circle) and random (full points) start configurations. The increment of the Monte Carlo time T was chosen to be $dt=0.01$.

Outside the transition region these differences are not visible in our simulation, but in the transition region they have the effect that the critical coupling seems to be shifted to slightly higher values for the noisy algorithm.

The results for $\langle \bar{\chi}\chi \rangle$ and the Wilson line obtained at various couplings $\beta \in [4.9, 5.15]$ with both algorithms are shown in fig. 4a and the energy density is given in fig. 4b. From this we get for the critical coupling

$$\beta_c = 4.96 \pm 0.03 .$$

Using earlier data for larger masses [10] on a $8^3 \times 4$ lattice we find for the critical coupling in the $m \to 0$ limit

$$\beta_c = 4.91 \pm 0.03 ,$$

which in units of Λ_{min} corresponds to a critical temperature of $T_c/\Lambda_{min} = 2.77 \pm 0.15$. Note that this is somewhat larger than the value found for $N_t = 6$ [7] and indicates violations of asymptotic scaling in this intermediate coupling regime. Results for the critical temperature obtained for $N_t = 4$ and 6 are summarized in table 3 and compared with corresponding pure gauge data [11]. This shows that the observed scaling violations follow a similar pattern as in the pure gauge sector. A similar observation has been made in MCRG studies of the QCD β-function in the presence of dynamical fermions [8]. We leave it to the interested reader to try on the basis of table 3 a guess where the value for T_c/Λ_{min} will settle down on larger lattices with dynamical fermions.

From the jump in the fermionic and gluonic contribution to the total energy density (fig. 4b) we see that the latent heat of the transition overshoots the

Table 3
Comparison of critical temperatures obtained for QCD with four massless fermions with critical temperatures for the pure gauge sector.

N_t	T_c/Λ_{min}	
	$n_f = 4$	$n_f = 0$
4	2.77 ± 0.15	2.61 ± 0.01
6	2.14 ± 0.10	2.12 ± 0.01
-	-	-
10–14	?	1.68 ± 0.05

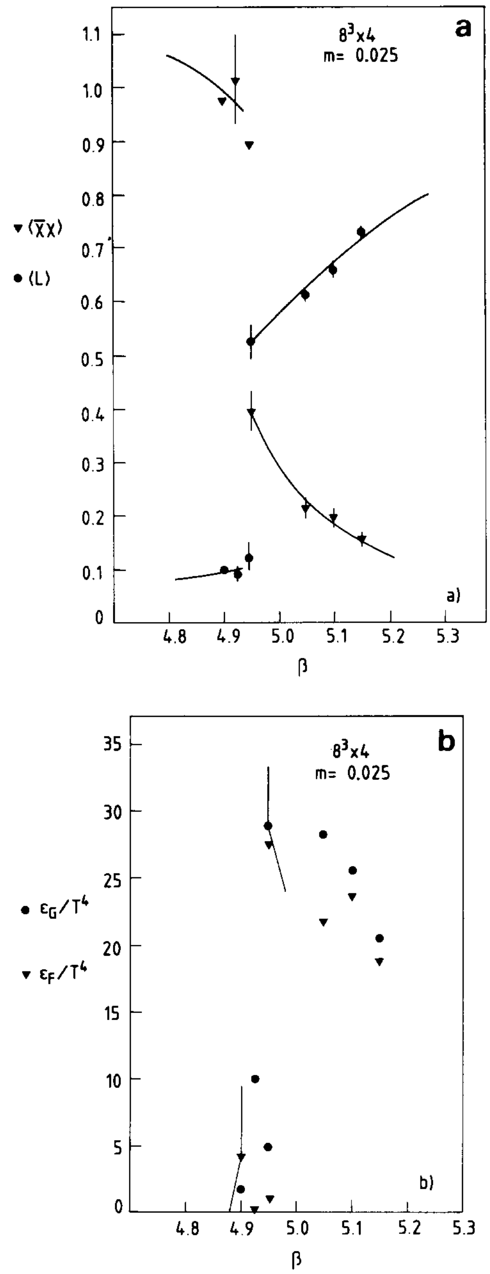

Fig. 4. (a) $\langle \bar{\chi}\chi \rangle$ and thermal Wilson line $\langle L \rangle$ versus β on a $8^3 \times 4$ lattice. (b) Gluonic (dots) and fermionic (triangles) contributions to the total energy density versus β.

Stefan–Boltzmann value considerably. On a $8^3 \times 4$ lattice the Stefan–Boltzmann limit would correspond to a total energy $\epsilon/T^4 = 31.61$ [12], while we find a latent heat $\Delta\epsilon/T^4 = 50 \pm 10$. This overshooting is due to the large gluonic contribution, ϵ_G. Weak coupling expansions for this term [12] suggest that the large overshoot is indeed a finite-lattice effect. Thus much larger lattices will be necessary to get reliable estimates for the size of the latent heat in the presence of dynamical fermions. It is also interesting to note that the discontinuity in the Wilson line has about the same size as for the pure SU(3) gauge theory on an $8^3 \times 4$ lattice [13]. The critical parameters found for the $8^3 \times 4$ lattice are similar to those for the 4^4 lattice:

$$\beta_c = 4.96 \pm 0.03 ,$$

$$\Delta p = 0.06 \pm 0.01 ,$$

$$\Delta \bar{\chi}\chi = 0.6 \pm 0.1 ,$$

$$\Delta \langle L \rangle = 0.35 \pm 0.05 .$$

In conclusion we note that the data obtained with the hybrid algorithm show good agreement with those obtained using the exact algorithm of ref. [2]. The results obtained for the first-order chiral transition for four light flavors of mass $m/T = 0.1$ lead to critical parameters which agree well with those found in the pure gauge sector. This shows that in some sense the transition is as strong as the transition in the quenched limit. Indeed we expect that the gap in physical observables may become even larger once the extrapolation to zero quark mass is possible. This will require more data in the first-order regime for even lighter fermions. Finally we want to stress that the present data have been obtained for a theory with four light flavors. The arguments leading to a prediction of a first-order transition for $n_f \geqslant 3$ are somewhat more subtle for the physically interesting case of two light flavors [3]. This case deserves further study. Moreover, it will be interesting to see whether the introduction of an intermdiately heavy fermion (strange quark) in addition to the two massless u and d quarks can smooth out a first-order chiral transition. Work in this direction is in progress.

This work was partly supported by the grant NSF-PHY-82-1948. The work of D.K.S. was supported by the US Department of Energy, Division of High Energy Physics, under contract W-31-109-ENG-38. We gratefully acknowledge the National Center for Supercomputing Applications at Urbana-Champaign, where the computations presented in this paper were performed.

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