FLAVOUR DEGREES OF FREEDOM AND THE TRANSITION TEMPERATURE IN QCD

MT_c Collaboration

R.V. GAVAI [a], Sourendu GUPTA [b], A. IRBÄCK [b], F. KARSCH [c], S. MEYER [d], B. PETERSSON [b],
H. SATZ [c] and H.W. WYLD [e]

[a] TIFR, Homi Bhabha Road, Bombay 400 005, India
[b] Fakultät für Physik, Universität Bielefeld, D-4800 Bielefeld 1, FRG
[c] Theory Division, CERN, CH-1211 Geneva 23, Switzerland
[d] Fachbereich Physik, Universität Kaiserslautern, D-6750 Kaiserslautern, FRG
[e] Department of Physics, University of Illinois, Urbana, IL 61801, USA

We study the finite temperature transition in QCD with four flavours of dynamical quarks. Our simulation is performed on an 8×16^3 lattice for quarks of mass $ma = 0.01$. At the coupling $\beta_c = 5.15$, we find long-lived metastable states, as well as an abrupt change in the entropy density, suggesting a first order phase transition. Using presently available results from corresponding calculations of the hadron masses and the chiral condensate, this gives us a transition temperature $T_c \simeq 100$ MeV, which is a factor two lower than the transition temperature found in quenched QCD.

The most striking feature in strong interaction thermodynamics is the predicted transition from hadronic matter at low temperature to a plasma of deconfined quarks and gluons at high temperature. In the case of pure $SU(3)$ gauge field thermodynamics, this transition has been extensively studied and appears to be quite well understood: there is a first order phase transition from the $\mathbb{Z}_3$-symmetric confined phase to a deconfined phase with spontaneously broken $\mathbb{Z}_3$ symmetry. Using results from string tension calculations [1], one finds for the transition temperature $T_c / \sqrt{\sigma} = 0.58 \pm 0.04$. With a string tension of $\sqrt{\sigma} \simeq 440$ MeV [2], this implies a deconfinement temperature $T_c \simeq 250$ MeV. What happens in full QCD, when quarks are included? The presence of dynamical quarks makes the dissolution of bound states "easier", since they can directly screen the colour charge of the binding partners. However, their presence breaks the $\mathbb{Z}_3$ symmetry of the lagrangian and hence could weaken the abruptness of deconfinement. On the other hand, for vanishing quark mass the lagrangian becomes chirally symmetric, so that in this limit we can have a phase transition restoring chiral symmetry, which is spontaneously broken in the low temperature phase.

First studies with dynamical quarks on relatively small lattices and with fairly large quark masses show an astonishingly strong flavour dependence. There are hints that the transition temperature, if converted into physical units by utilising hadron mass calculations at the same coupling, decreases as the number of flavours is increased, from about 200 MeV for $N_f = 0$ to values around 100 MeV for $N_f = 4$ [3–6]. This has a dramatic effect on the critical energy density needed for the transition. For an ideal gas of quarks and gluons, the energy density is given by

$$\epsilon = \tfrac{1}{15}\pi^2 (8 + \tfrac{21}{4}N_f) T^4 . \tag{1}$$

Hence ϵ drops at the critical point by more than a factor 4 between $N_f = 0$ and $N_f = 4$. It thus seems that the results for critical temperature obtained for $N_f = 0$ are not directly applicable to the "real world" studied in heavy ion collisions; for an experimental quark matter search, a clarification of the flavour dependence of T_c is clearly very important.

At the transition point, a further flavour dependence appears: for $N_f \geq 2$, the chiral transition seems to be of first order for quark masses below a critical value $m_c(N_f)$. This critical quark mass seems to in-

crease as the number of flavours is increased.

In contrast to this, the ratio $T_c/\Lambda_{\overline{MS}}$ seems to vary little or not at all when N_f is increased [7].

For an understanding of deconfinement and chiral symmetry restoration in full QCD, the flavour dependence of the transition thus becomes of essential importance. Most of the calculations of the transition temperature carried out so far were performed at couplings well below the asymptotic scaling regime, with comparatively large quark masses, and on lattices of volume $V = N_\tau \times N_\sigma^3$ with $N_\sigma \leq 10$, $N_\tau = 4$–6 [3]. It is therefore necessary to push simulations closer to the continuum regime, keeping at the same time the physical quark mass in units of the temperature as small as possible; however, already the extension to $N_\tau = 8$ leads to enormous computational effort, if one attempts to keep the quark mass small in units of the temperature [4–6]. Most useful are calculations at several small quark mass values, allowing an extrapolation to vanishing quark mass.

We have therefore carried out simulations with $N_f = 4$ on an 8×16^3 lattice, for quarks of mass $ma = 0.01$. In a preliminary study [5], we had considered the corresponding case for $ma = 0.025$ on an 8×12^3 lattice, so that we can combine the results for the two investigations in order to estimate the zero quark mass limit. The quark mass $ma = 0.01$ corresponds to $m/T = 0.08$; previous calculations [8] at $N_\tau = 4$ for $m/T = 0.1$ have shown a first order transition. Finally, the choice of $N_f = 4$ allows the use of an exact algorithm for the simulation, thus eliminating systematic errors in the determination of the critical coupling.

The partition function for four flavour QCD can be written in terms of the usual gluonic link matrices U and the Wilson action $S(U)$ as

$$Z = \int dU \det Q(U) \exp[-S(U)], \qquad (2)$$

where

$$Q(U)_{xy} = ma\delta_{xy}$$
$$+ \tfrac{1}{2} \sum_\mu \alpha_{x,\mu} (U_{x,\mu}\delta_{x,y-\mu} - U_{x-\mu,\mu}^\dagger \delta_{x,y+\mu}) \qquad (3)$$

is the staggered fermion matrix with phase factors $\alpha_{x,\mu} = (-1)^{x_1 + \cdots + x_{\mu-1}}$. We have simulated this partition function with the hybrid Monte Carlo algorithm [9]. Our implementation of this algorithm was dis-

cussed in ref. [5]. Even for the large lattice and small quark mass used in this study, we found that a reasonable acceptance rate (of about 70%) could be achieved without making the step size impractically small. We have used $\Delta\tau = 0.004$–0.0125, and adjusted the number of steps in each trajectory so that its length $\tau = 0.3$. The stopping criterion in the conjugate gradient inversion of the matrix Q was that the norm of the residual vector be less than $1.25 \times 10^{-11} V$. Further details about the performance of the algorithm, including a formula giving the dependence of the acceptance on the coupling, quark mass, volume and step size, are given in ref. [10].

In order to look for critical behaviour, we studied the evolution of the Polyakov loop $\mathrm{Re}(L)$ and the chiral condensate $\bar{\chi}\chi$ at the couplings $\beta = 5.1, 5.15, 5.2$ and 5.3. Here

$$L = \frac{1}{N_\sigma^3} \sum_{\boldsymbol{n}} \mathrm{Tr} \prod_{n_0 = 1}^{N_\tau} U_{(n_0,\boldsymbol{n}),0}, \qquad (4)$$

and

$$\bar{\chi}\chi = \frac{1}{V} \mathrm{Tr}\, Q^{-1}. \qquad (5)$$

Fig. 1 shows the run time histories for $\mathrm{Re}(L)$. From an ordered start at $\beta = 5.1$, the system attained equilibrium in a disordered state with $\mathrm{Re}(L)$ close to zero. At $\beta = 5.2$, the runs from ordered and disordered starts converged to the same value $\mathrm{Re}(L) > 0$. We then used
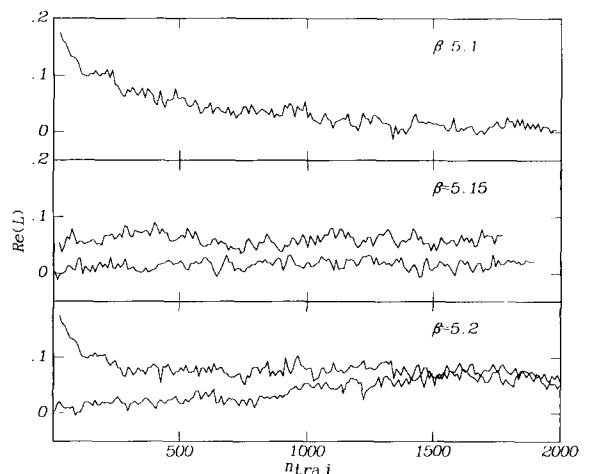

Fig. 1. The run time histories for $\mathrm{Re}(L)$ at the indicated values of β.

equilibrium configurations from runs at 5.1 and 5.2 as "disordered" and "ordered" starts at $\beta = 5.15$. Even after nearly 2000 trajectories did they not converge to a common value. We take this as an indication for long lived metastable states at $\beta = 5.15$, suggestive of a first order phase transition. A similar behaviour was seen in the run time histories for $\bar{\chi}\chi$ (fig. 2). In the simulations at the mass $ma = 0.025$ reported in ref. [5] we did not observe such metastabilities. For $N_\tau = 4$, in contrast, there are metastable states for $ma = 0.025$, and a smooth transition for $ma = 0.05$. This is consistent with the end of the first order transition line scaling with m_c/T_c. It should be noted, however, that only a much more extensive investigation can definitively establish the order of the transition.

In fig. 3 we show the behaviour of the averages, $\langle \mathrm{Re}(L) \rangle$ and $\langle \bar{\chi}\chi \rangle$, as obtained after discarding the transient parts of the runs. For those cases in which the system was started in the phase in which it eventually came to equilibrium, this meant discarding approximately the first 1000 trajectories; when crossing from one phase to another was involved, about 1500 trajectories were discarded. Also shown in fig. 3 are the results of our earlier work at $ma = 0.025$.

At $\beta = 5.1$, a linear extrapolation of the values of $\langle \bar{\chi}\chi \rangle$ obtained at the two masses (fig. 4) gives a finite value at $ma = 0$, whereas for $\beta = 5.2$ and 5.3 the extrapolations lead to vanishing, or even negative, values. This shows that for $ma = 0.01$, the point $\beta = 5.1$
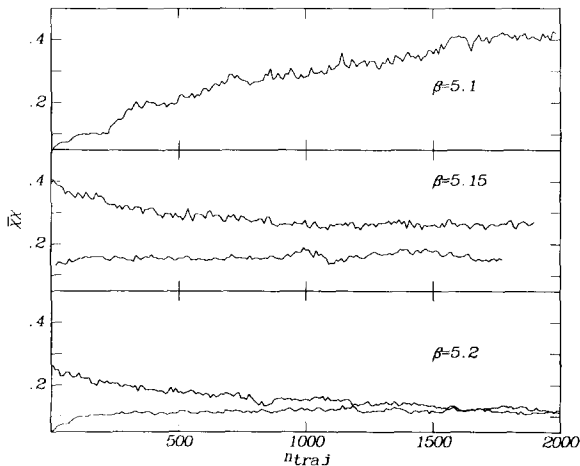

Fig. 2. The run time histories for $\bar{\chi}\chi$ at the indicated values of β.
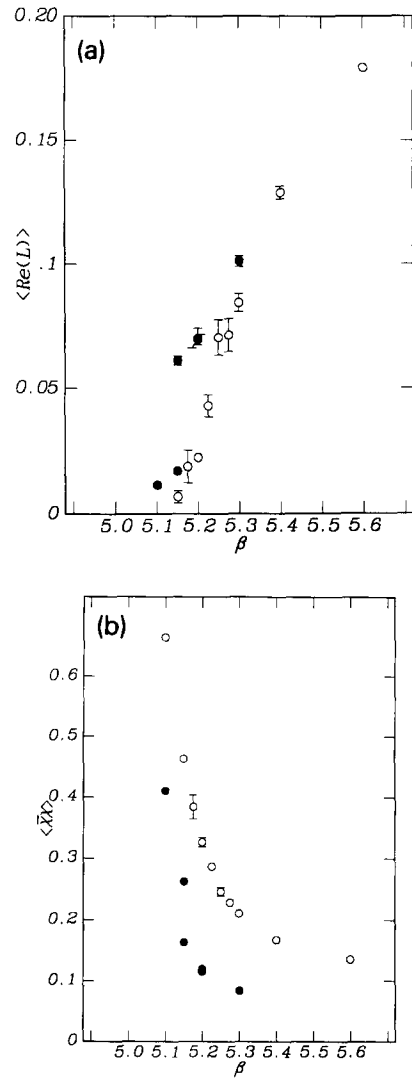

Fig. 3. The averages (a) $\langle \mathrm{Re}(L) \rangle$ and (b) $\langle \bar{\chi}\chi \rangle$. The filled circles are for data obtained on the 8×16^3 lattice with $ma = 0.01$, whereas the open circles are for data with $ma = 0.025$ on an 8×12^3 lattice.

belongs to a phase with spontaneously broken chiral symmetry, whereas for $\beta \geqslant 5.2$ there is no such symmetry breaking. The slightly negative zero-mass extrapolations at $\beta = 5.2$ and 5.15 (disordered start) are readily understood from the dependence of β_c on the quark mass: for $ma = 0.025$, $\beta = 5.2$ is in the broken symmetry phase, whereas for $ma = 0.01$ it is in the symmetric phase. For the same reason, the extrapo-
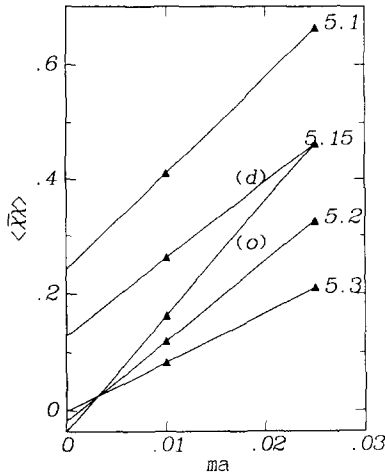
Fig. 4. $\langle \bar{\chi}\chi \rangle$ obtained at $ma = 0.025$ [5] and $ma = 0.01$, plotted against ma. The values of β are as marked.

lation of the data at $\beta = 5.1$ do not necessarily give us the actual value at $ma = 0$.

Turning now to $\langle \mathrm{Re}(L) \rangle$, we note that the rapid change across the transition region seen on the 8×12^3 lattice persists also for 8×16^3. The curves for the two lattice sizes are similar, $\langle \mathrm{Re}(L) \rangle$ being small and nearly zero at small β, but clearly non-zero at larger coupling. Apart from this change of scale, there is also a shift of the whole curve towards lower β for the larger lattice. This behaviour is entirely consistent with that of the phase transition between $\beta = 5.1$ and 5.2 seen from $\langle \bar{\chi}\chi \rangle$.

We have also measured the entropy density, which, for four flavours, is given by

$$\frac{s}{T^3} = 4\beta N_\tau^4 \left(1 - \frac{c'_\sigma - c'_\tau}{2} g^2 \right) [\langle P_\sigma \rangle - \langle P_\tau \rangle]$$

$$+ \tfrac{4}{3} N_\tau^4 (1 + c'_F g^2)$$

$$\times \left(\frac{1}{V} \langle \mathrm{Tr}\, D_0 Q^- \rangle + \frac{1}{4V} ma \langle \mathrm{Tr}\, Q^{-1} \rangle - \tfrac{3}{4} \right), \quad (6)$$

where $\langle P_\sigma \rangle$ and $\langle P_\tau \rangle$ are the expectation values of the space–space and space–time plaquettes, D_0 is the time component of the Dirac operator on the lattice, and the constants c'_σ, c'_τ and c'_F are obtained from a weak coupling computation [11] that yields the formula for the entropy density given above. We note that s/T^3 involves the difference of two plaquette av-

erages. This makes it a difficult measurement, as reflected in the estimates of errors. Nevertheless, the abrupt change at $\beta = 5.15$ (fig. 5) is also consistent with a first order transition. In the high temperature phase the results are in agreement with an ideal gas of quarks and gluons.

In summary, the present data at $\beta = 5.1$ and 5.2 establish lower and upper bounds for β_c at $ma = 0.01$. For the purpose of the following discussion of the critical temperature we therefore take

$$\beta_c (ma = 0.01) = 5.15 \pm 0.05 \qquad (7)$$

as the critical coupling on the 8×16^3 lattice. Combining this result with that for $ma = 0.025$, $\beta_c (ma = 0.025) = 5.250 \pm 0.025$ [5], we can extract the critical coupling in the zero mass limit. A linear extrapolation gives

$$\beta_c (ma = 0) = 5.08 \pm 0.08 . \qquad (8)$$

Using the asymptotic scaling formula at the two-loop level, this gives us

$$\frac{T_c (ma = 0)}{\Lambda_{\overline{MS}}} = 1.8 \pm 0.2 . \qquad (9)$$

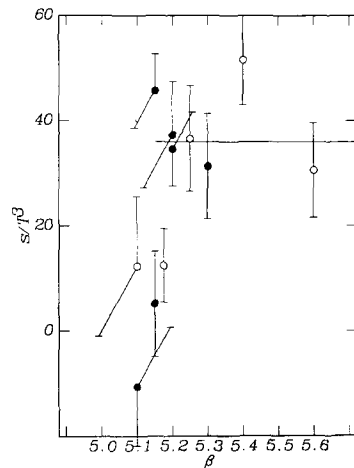The corresponding value for SU(3) pure gauge the-

Fig. 5. The values of s/T^3 as a function of β. The filled circles are for data obtained on the 8×16^3 lattice with $ma = 0.01$, whereas the open circles are for data with $ma = 0.025$ on an 8×12^3 lattice. The value of s/T^3 obtained for a free gas of quarks and gluons on a lattice of this size is marked by the line.

ory is 1.87 ± 0.04 [12]. The observation made at smaller N_τ, that $T_c/\Lambda_{\overline{MS}}$ for the theories with $N_f = 0$, 2 and 4 are nearly equal [7], thus seems to carry over to $N_\tau = 8$. One should note, however, that higher loop corrections to the $T_c/\Lambda_{\overline{MS}}$ value are not yet under complete control. Even in the pure gauge theory, where data have been taken up to $N_\tau = 14$, the functional behaviour of $T_c/\Lambda_{\overline{MS}}$ in β is as well described by the one-loop β-function as it is by the two-loop function. Using the one-loop renormalisation group equation, one finds that $T_c/\Lambda_{\overline{MS}}$ decreases by $(12 \pm 5)\%$ when going from $N_\tau = 8$ to 14, while the two-loop formula gives a decrease of $(15 \pm 5)\%$. For the two different forms, the value for $T_c/\Lambda_{\overline{MS}}$, however, differs by a factor three. Existing data therefore, do not provide a sensitive test of the functional form beyond the one-loop level. In particular, the existence of higher loop contributions which vary little over the presently probed region, but affect the continuum value of $T_c/\Lambda_{\overline{MS}}$ significantly, cannot be ruled out. Furthermore, before we can compare the value of T_c in pure gauge theory with that for four flavour QCD, we must know the flavour dependence of $\Lambda_{\overline{MS}}$.

If we want to extract T_c in physical units without invoking the RG relation, and hence the assumption of asymptotic scaling, then we should compare T_c directly to another observable calculated on the lattice at $T = 0$ with the same quark mass and at the same coupling. Using hadron masses, we can construct the dimensionless ratio

$$\frac{T_c}{m_H^{exptl}} = \frac{1}{N_\tau m_H a} . \tag{10}$$

At the critical coupling determined by us [eq. (7)], such a calculation does not exist at present. For the moment we have to rely on an extrapolation based on calculations performed at nearby couplings with the same bare quark masses [4,13,14]. In particular the hadron mass calculations at $\beta = 5.2$ have been checked with different fermion algorithms, and seem to be rather insensitive to the particular integration scheme used. We obtain an estimate of the critical temperature by a linear extrapolation of the hadron masses, measured for $ma = 0.01$ at $\beta = 5.2$ and 5.35 [14], to our critical coupling. This yields at $ma = 0.01$,

$$\frac{T_c}{m_\rho} = 0.12 \pm 0.02 , \quad \frac{T_c}{m_N} = 0.09 \pm 0.01 , \tag{11}$$

which is consistent with our earlier estimates for $ma = 0.025$ [5]. In contrast, the corresponding ratios for the quenched theory are more than a factor two bigger:

$$\frac{T_c}{m_\rho} = 0.30 \pm 0.05 , \quad \frac{T_c}{m_N} = 0.21 \pm 0.02 . \tag{12}$$

If the lattice spacing a is determined by inserting the experimental hadron masses in eqs. (11) and (12), then $T_c = 1/N_\tau a$ implies approximately the same lattice spacing for $N_f = 4$ at $N_\tau = 8$ as in the quenched theory for $N_\tau = 4$. It has, however, been observed in the quenched theory that these ratios do not vary significantly as N_τ is changed from 4 to 14. We take this to be an indication that the difference between eqs. (11) and (12) is a general feature.

Inserting the experimental values of the hadron masses into eq. (11) we find that for four flavour QCD at $N_\tau = 8$ and $ma = 0.01$,

$$T_c = 93 \pm 15 \text{ MeV} \quad \text{(from } m_\rho) ,$$

$$= 85 \pm 11 \text{ MeV} \quad \text{(from } m_N) . \tag{13}$$

The error estimates given here take into account the uncertainties in our determination of β_c, as well as the propagation of the statistical errors in the masses on extrapolating to β_c. In contrast, using the experimental hadron masses in eq. (12) results in a transition temperature around 200 MeV. We thus find that in four flavour QCD the finite temperature phase transition is about a factor of two lower than in quenched theory.

We can also perform a similar computation using the chiral condensate $\langle \bar{\chi}\chi \rangle$ at $T = 0$ instead of the hadron masses. Since this is a bulk quantity, finite size effects may influence it less than the correlation lengths $1/m_H$. For four flavour QCD, we can estimate $\langle \bar{\chi}\chi \rangle$ at $\beta_c(N_\tau = 8, ma = 0) = 5.08 \pm 0.08$ from two different evaluations. One estimate comes from calculations at $\beta = 5.2$ and 5.35 [13,14]. Extrapolating to zero quark mass and $\beta = 5.08$ gives $\langle \bar{\chi}\chi \rangle = 0.35 \pm 0.06$. The second estimate is based on results obtained at $\beta = 5.1$ on an 8^4 lattice at larger quark masses [15]. A linear extrapolation down to $ma = 0$ yields $\langle \bar{\chi}\chi \rangle = 0.40 \pm 0.06$. Using the average of these, we extract the renormalisation group invariant chiral condensate per quark flavour, $\langle \bar{\chi}\chi \rangle_{RGI}$, as defined in ref. [16], to obtain

$$\frac{T_c}{\langle \bar{\chi}\chi \rangle^{1/3}_{\mathrm{RGI}}} = 0.4 \pm 0.1 \ . \tag{14}$$

Combining this with the estimate given in ref. [17], $\langle \bar{\chi}\chi \rangle^{1/3}_{\mathrm{RGI}} = 190 \pm 20$ MeV, we find that our computation at $N_\tau = 8$ yields for $ma = 0$ in four flavour QCD

$$T_c = 80 \pm 20 \text{ MeV} \ . \tag{15}$$

In quenched QCD, we can use the values of the chiral condensate at $\beta = 5.7$ and 5.9, corresponding to the critical couplings for $N_\tau = 4$ and 6 respectively, from ref. [18]. Converting again to the RG invariant value, we get, instead of eq. (14), the ratio

$$\frac{T_c}{\langle \bar{\chi}\chi \rangle^{1/3}_{\mathrm{RGI}}} = 0.82 \pm 0.03 \tag{16}$$

for $N_\tau = 4$ and a 10% larger value for $N_\tau = 6$. We thus note that, like the ratios $T_c / \sqrt{\sigma}$ and T_c / m_{H}, this ratio too is fairly independent of N_τ. Hence we can compare this estimate with that given in eq. (14). We find, once more, a factor of two between the values of T_c obtained for four flavour QCD and the quenched theory.

In conclusion, we have determined the critical coupling $\beta_c = 5.15 \pm 0.05$ for the finite temperature transition in four flavour QCD on an 8×16^3 lattice with dynamical quarks of mass $ma = 0.01$. At this value of β the quantities $\langle \mathrm{Re}(L) \rangle$, $\langle \bar{\chi}\chi \rangle$ and s/T^3 change abruptly; within our statistics, their behaviour is that expected of a first order transition. Combining our present results with those for larger quark mass, $ma = 0.025$, we find that this transition separates phases of spontaneously broken and restored chiral symmetry.

Using existing results from calculations of the hadron masses and the chiral condensate in this region of β, we have two different ways of determining T_c in physical units. Both result in $T_c \simeq 100$ MeV for four flavour QCD; this value lies a factor two below that obtained in the quenched theory. Let us stress again, however, that neither value can be applied directly to the physical world of two light and one or more heavy quark flavours.

References

[1] E. Marinari, Nucl. Phys. B (Proc. Suppl.) 9 (1989) 209.

[2] S. Jacobs, M.G. Olsson and C. Suchyta III, Phys. Rev. D 33 (1986) 3338.

[3] M. Fukugita, S. Ohta, S. Oyanagi and A. Ukawa, Phys. Rev. Lett. 58 (1987) 2515;
S. Gottlieb, W. Liu, R.L. Renken, R.L. Sugar and D. Toussaint, Phys. Rev. D 38 (1988) 2245;
E.V.E. Kovacs, D.K. Sinclair and J.B. Kogut, Phys. Rev. Lett. 58 (1987) 751; Nucl. Phys. B 290 (1987) 431.

[4] M.P. Grady, D.K. Sinclair and J.B. Kogut, Phys. Lett. B 200 (1988) 149.

[5] MT$_c$ Collab., R.V. Gavai, S. Gupta, A. Irbäck, F. Karsch, S. Meyer, B. Petersson, H. Satz and H.W. Wyld, Phys. Lett. B 232 (1989) 491.

[6] S. Gottlieb, W. Liu, R.L. Renken, R.L. Sugar and D. Toussaint, QCD thermodynamics with eight time slices, preprint IUHET-168 (1989).

[7] A. Ukawa, Nucl. Phys. A 498 (1989) 227c.

[8] F. Karsch, J.B. Kogut, D.K. Sinclair and H.W. Wyld, Phys. Lett. B 188 (1987) 353.

[9] S. Duane, A.D. Kennedy, B.J. Pendleton and D. Roweth, Phys. Lett. B 195 (1987) 216.

[10] S. Gupta, A. Irbäck, F. Karsch and B. Petersson, The acceptance probability in the hybrid Monte Carlo method, preprint BI-TP 90-05, CERN-TH.5662/90, Phys. Lett. B, to be published.

[11] F. Karsch and I.O. Stamatescu, Phys. Lett. B 227 (1989) 153.

[12] A.D. Kennedy, J. Kuti, S. Meyer and B.J. Pendleton, Phys. Rev. Lett. 54 (1985) 87;
S.A. Gottlieb, A.D. Kennedy, J. Kuti, S. Meyer, B.J. Pendleton, R.L. Sugar and D. Toussaint, Phys. Rev. Lett. 55 (1985) 1958;
N.H. Christ and A. Terrano, Phys. Rev. Lett. 56 (1986) 181;
N.H. Christ, Nucl. Phys. B (Proc. Suppl.) 1A (1987) 95.

[13] K.D. Born, E. Laermann, T.F. Walsh and P.M. Zerwas, Proc. XXIV Intern. Conf. on High energy physics (Munich, 1988), eds. R. Kotthaus and J.H. Kühn (Springer, Berlin, 1989) p. 797.

[14] E. Laermann, R. Altmeyer, K.D. Born, W. Ibes, R. Sommer, T.F. Walsh and P.M. Zerwas, QCD with dynamical fermions, Aachen preprint PITHA 89/29 (October 1989).

[15] J.B. Kogut, Phys. Lett. B 168 (1986) 367.

[16] A. Gonzalez Arroyo, F.J. Yndurain and G. Martinelli, Phys. Lett. B 117 (1982) 437;
M. Göckeler, Phys. Lett. B 142 (1984) 197;
M.F.L. Golterman and J. Smit, Phys. Lett. B 140 (1984) 392.

[17] J. Gasser and H. Leutwyler, Phys. Rep. 87 (1982) 77.
[18] I.M. Barbour, P. Gibbs, K.C. Bowler and D. Roweth, Phys. Lett. B 158 (1985) 61;
G. Salina and A. Vladikas, The scaling of the quenched chiral condensate, preprint Rom 2F/89/026.