LATTICE QCD WITH SMALL NUMBER OF FLAVOURS

A. IRBÄCK
Department of Physics, University of Lund, Sölvegatan 14 A, S-223 62 Lund, Sweden

F. KARSCH
CERN, CH-1211 Geneva 23, Switzerland

B. PETERSSON
Fakultät für Physik, Universität Bielefeld, D-4800 Bielefeld 1, Fed. Rep. Germany

and

H.W. WYLD
Department of Physics, University of Illinois at Urbana-Champaign, 1110 W. Green Street, Urbana IL 61801, USA

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The finite temperature behaviour of lattice QCD with dynamical quarks for small number of flavours N_f is investigated. Simulations have been performed on lattices of size $N_\sigma^3 \cdot 4$ with $N_\sigma = 8$ and 12 and staggered fermions of mass $ma = 0.1$ using a hybrid algorithm. We find that the two state signal at the critical point of the pure gauge theory, which is taken as sign for a first order phase transition, persists for the values of N_f we have investigated, namely $N_f = 0.5$, 1 and 2. It is, however, considerably weaker for $N_f = 1$ and 2. Moreover, for $N_f = 2$ the discontinuity at β_c decreases with increasing lattice size. This puts doubt on the first order nature of the $N_f = 2$ transition at intermediate masses.

1. Motivation and results

The phase structure of lattice QCD at finite temperature has been the subject of several numerical investigations. In the pure gauge sector the existence of metastable states, usually taken as a signal for a first order deconfining transition, seems to be well established. Corresponding studies with dynamical fermions have by now been performed with different number of flavours N_f and for a wide range of quark masses ma on intermediate sized lattices, $N_\sigma^3 \cdot N_\tau$, typically with $N_\sigma / N_\tau \leq 2$. The situation here is less clear [#1]. For $N_f = 8$ there is a clear signal for metastable states for $m/T = 0.4$ [2]. For $N_f = 4$ the first order transition in the large mass limit has been shown to weaken as the fermion mass is decreased [3]. When further decreasing the mass, evidence for a first order chiral transition has been obtained [4], in agreement with predictions for the chiral limit based on a σ-model analysis [5]. Whether the transition stays first order in the entire mass regime [6] or whether it is continuous in an intermediate regime of masses around $m/T \sim 0.5$ is uncertain. Results obtained by different groups using different algorithms do not agree completely. The strength of the first order signal seems to weaken as N_f is decreased further. Similar uncertainties about the order of the transition thus persist for all $1 \leq N_f \leq 4$ [7–10] at intermediate quark masses. It should be noted that the analysis of the order of the transition in this "unphysical" intermediate mass regime is not only of academic interest. It is for instance of importance in an attempt to understand the analytic properties of finite temperature Green functions and their continuation from the low

[#1] For recent review see ref. [1].

temperature confining phase to the plasma phase at high temperature [11].

In this letter we concentrate on the nature of the chiral transition at quark mass $m/T=0.4$, i.e. we study QCD with quark mass $ma=0.1$ on lattices of size $N_\sigma^3 \cdot 4$. For $N_f=2$ we perform a high statistics finite size analysis of the transition on lattices of size $N_\sigma^3 \cdot 4$ with $N_\sigma=8$ and 12. In addition we attempt to clarify the relation between the transition at $N_f=2$ and the strong deconfinement transition in the pure gauge sector ($N_f=0$). To this extent we have performed simulations at $N_f=0$, 0.5, 1 and 2 on an $8^3 \cdot 4$ lattice. At all these N_f values we find evidence for the existence of metastable states. Whereas the strength of the transition in the $N_f=0.5$ case seems to be approximately the same as in the pure gauge sector, it is markedly weaker for $N_f=1$ and 2. Our observation of metastabilities in the two-flavour case is in agreement with the Langevin results of ref. [8], but differs from the findings of ref. [9]. In addition we find that the signal for metastability weakens when going to larger lattices. This puts doubt on the first order nature of the transition at $N_f=2$, $m/T=0.4$.

2. The algorithm

The partition function for the theory we study is

$$Z=\int\left[\prod_{x,\mu} \mathrm{d}U_{x,\mu}\right]\exp[-S_G(U)] \times [\det M(U)]^{N_f/4}, \qquad (1)$$

where $U_{x,\mu}\in SU(3)$ is a link variable, S_G is the standard Wilson action for the gauge fields and M is the staggered version of the fermion matrix, which in the continuum limit represents four degenerate flavours of quarks. Following Hamber et al. [12], we take eq. (1) to define the theory for $N_f\neq 4$. Using the fact that $M^\dagger M$ does not connect even and odd lattice sites and that its determinant is the same on both sublattices [13], we can write

$$Z=\int \prod_{x,\mu} \mathrm{d}U_{x,\mu}\exp[-S_{\mathrm{eff}}(U)], \qquad (2)$$

with

$$S_{\mathrm{eff}}(U)=S_G(U)-\tfrac{1}{4}N_f\,\mathrm{tr_e}\ln[M^\dagger(U)M(U)]. \qquad (3)$$

Here $\mathrm{tr_e}$ denotes the trace over even lattice sites only.

We have simulated the theory by use of a hybrid scheme [14], which is a mixture of the microcanonical [15] and Langevin [9,16] algorithms. In this scheme configurations distributed according to eq. (2) are generated by letting the system evolve in a fictitious time τ. A convenient choice of discrete microcanonical equation of motion is

$$U_{x,\mu}(\tau+\Delta\tau)=\exp[-\mathrm{i}f_\alpha(\tau)\cdot T^\alpha]\,U_{x,\mu}(\tau), \qquad (4)$$

where T^α are SU(3) generators and the force f_α is given by

$$f_\alpha(\tau)=f_\alpha(\tau-\Delta\tau)+(\Delta\tau)^2\delta_\alpha S_{\mathrm{eff}}. \qquad (5)$$

We estimate the fermionic contribution to $\delta_\alpha S_{\mathrm{eff}}$ by a bilinear noise term [17]

$$-\tfrac{1}{4}N_f X^\dagger\delta_\alpha[M^\dagger(U)M(U)]X,$$

where M is taken at time τ and X is chosen according to the prescription in the improved algorithm by Gottlieb et al. [18]:

$$X=[M^\dagger(U)M(U)]^{-1}\Phi_e, \quad \Phi=M(\bar{U})R,$$
$$\bar{U}=\exp[\mathrm{i}\tfrac{1}{8}N_f f_\alpha(\tau-\Delta\tau)\cdot T^\alpha]\cdot U(\tau). \qquad (6)$$

Here R is a vector of complex gaussian random numbers and Φ_e is the restriction of Φ to even lattice sites. With this prescription the systematic errors in expectation values are expected to be $O((\Delta\tau)^2)$ [18]. For the calculation of X in eq. (6) we employed the conjugate gradient method with stopping criterion that the residue $r<0.005\sqrt{V}$, V being the lattice volume. In all our simulations we used a step-size $\Delta\tau=0.05$. This choice of stopping criterion and step-size was based on the investigations of ref. [19]. Langevin updatings were incorporated in order to insure ergodicity and were applied every 25th iteration. Our program has been tested in the pure gauge sector and also for QCD with various quark masses. In particular it reproduces the known critical coupling for $N_f=2$, $ma=0.025$ on lattices with temporal extent $N_\tau=4$ [20].

3. Calculations

Let us first discuss the fate of the deconfinement phase transition of the pure gauge sector when the number of flavours is increased from 0 to 2. To this extent we performed simulations on a $8^3 \cdot 4$ lattice for

Table 1
Critical couplings and discontinuity in the absolute value of the Polyakov loop on the $8^3\cdot 4$ lattice for different values of N_f.

N_f	β_c	ΔL
0.0	5.6970(30)	0.35(3)
0.5	5.6335(30)	0.39(3)
1.0	5.53(1)	0.19(3)
2.0	5.3825(50)	0.20(2)

quark masses $ma=0.1$. In order to determine the nature of the transition we study the evolution of the system from completely ordered and disordered initial configurations. Preliminary shorter runs ($\tau=150-500$) were used to localize the transition region. The critical couplings we obtained for $N_f=0$, 0.5, 1 and 2 are given in table 1. In the vicinity of the transition we used a step-length $\Delta\beta\leqslant 0.005$. As can be seen from table 1 the dependence on N_f is approximately linear with

$$\beta_c \simeq 5.697-0.15N_f\,. \tag{7}$$

Out of the several measured observables the spatial average of the Polyakov loop

$$L=\frac{1}{N_\sigma^3}\sum_x L_x\,,\quad L_x=\mathrm{Tr}\prod_{x_0=1}^{N_\tau} U_{(x_0,x),0} \tag{8}$$

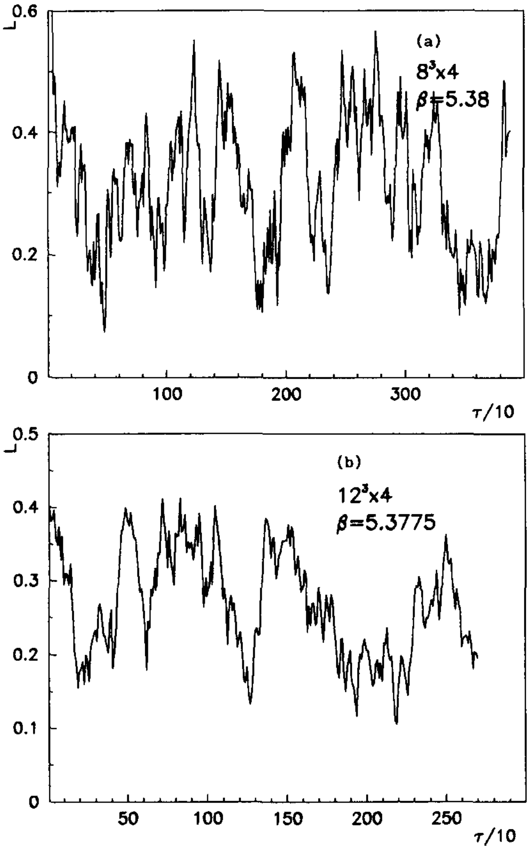

Fig. 2. Time history for $|L|$ for $N_f=2$ on a $8^3\cdot 4$ lattice at $\beta=5.38$ (a) and on a $12^3\cdot 4$ lattice at $\beta=5.3775$ (b).

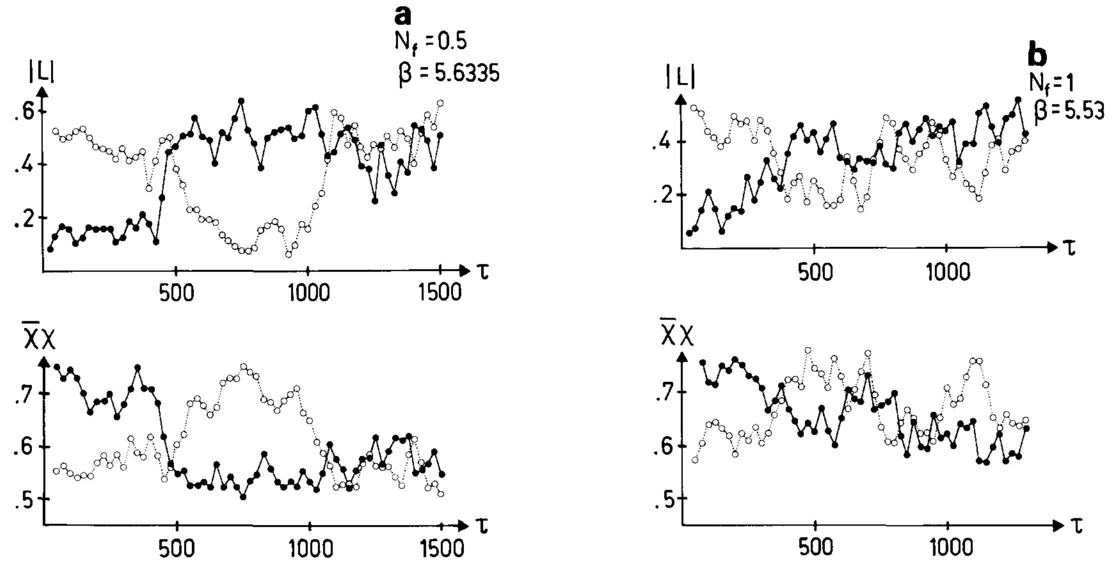

Fig. 1. Time history for $|L|$ and $\bar{\chi}\chi$ and the critical point for $N_f=0.5$ (a), and 1.0 (b). Each point corresponds to an average over 500 iterations or a Monte Carlo time interval $\Delta\tau=25$.

Table 2
Statistics collected on the $8^3 \cdot 4$ and $12^3 \cdot 4$ lattices for various values of β for the $N_f=2$, $ma=0.1$ case.

N_σ	β	τ
8	5.3875	3300
	5.38	3830
	5.375	3050
	5.37	4250
12	5.385	2600
	5.38	3500
	5.3775	2700
	5.375	2800
	5.37	1200

and the chiral condensate $\bar{\chi}\chi$ turned out to provide the clearest signals. Time histories for these two quantities from extended runs at the critical couplings are shown in fig. 1 for $N_f=0.5$ and 1. The runs shown in these figures extend over a simulation time $\tau=1300$–2400 corresponding to 26 000–48 000 iterations. Each 2000 iterations required approximately one CPU-hour on a Cray X-MP.

Also given in table 1 are the discontinuities in $|L|$ at the critical point. They were calculated by averaging over periods (typically of length $\Delta\tau \sim 500$) during which the system certainly was in one of the two states, possibly leading to an overestimate of the gap. For $N_f=0.5$ the gap is as big as in the pure gauge sector ($N_f=0$). However, for $N_f=1$ and 2 the gap is considerably smaller.

For the two-flavour case it became difficult to judge the existence of coexisting states on the basis of the fig. 2 where we show the time history of the absolute value of Polyakov loop for runs at the critical couplings on the $8^3 \cdot 4$ and $12^3 \cdot 4$ lattices. We thus at-

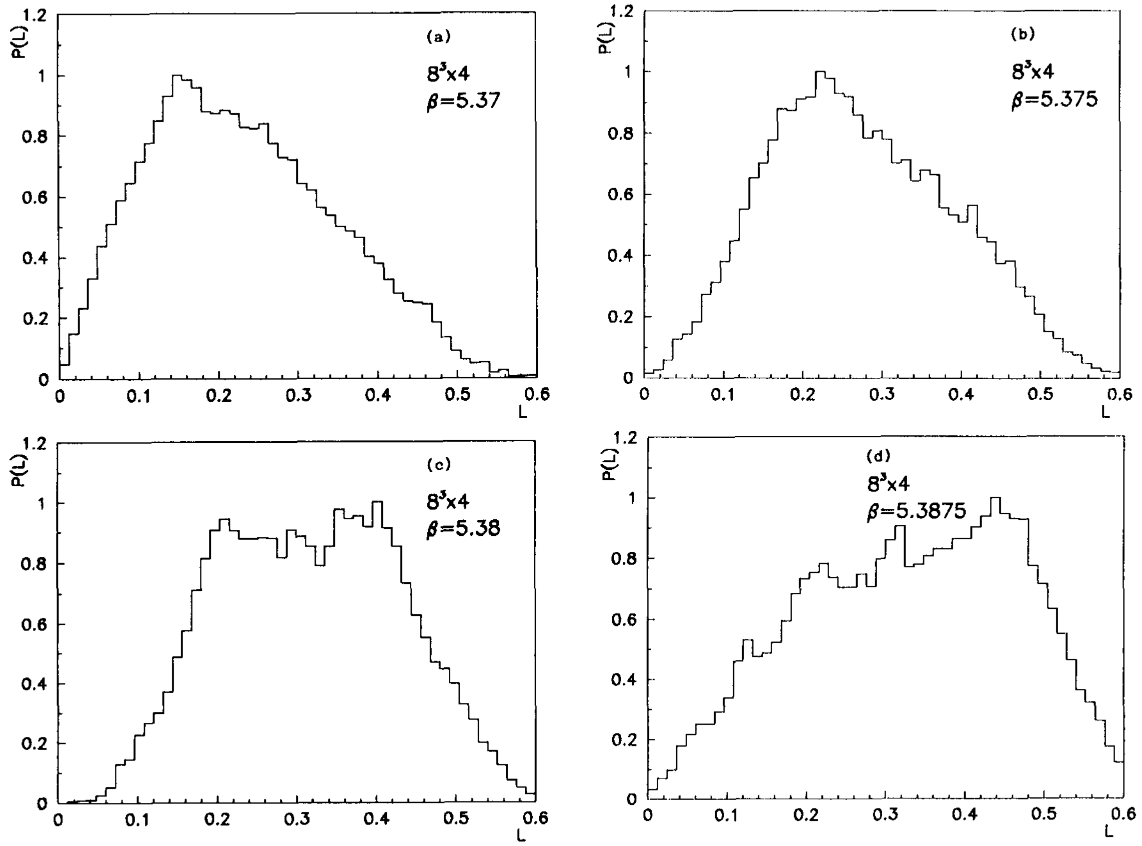

Fig. 3. Probability distribution of $|L|$ on the $8^3 \cdot 4$ lattice at $\beta=5.37$ (a), 5.375 (b), 5.38 (c) and 5.3875 (d).

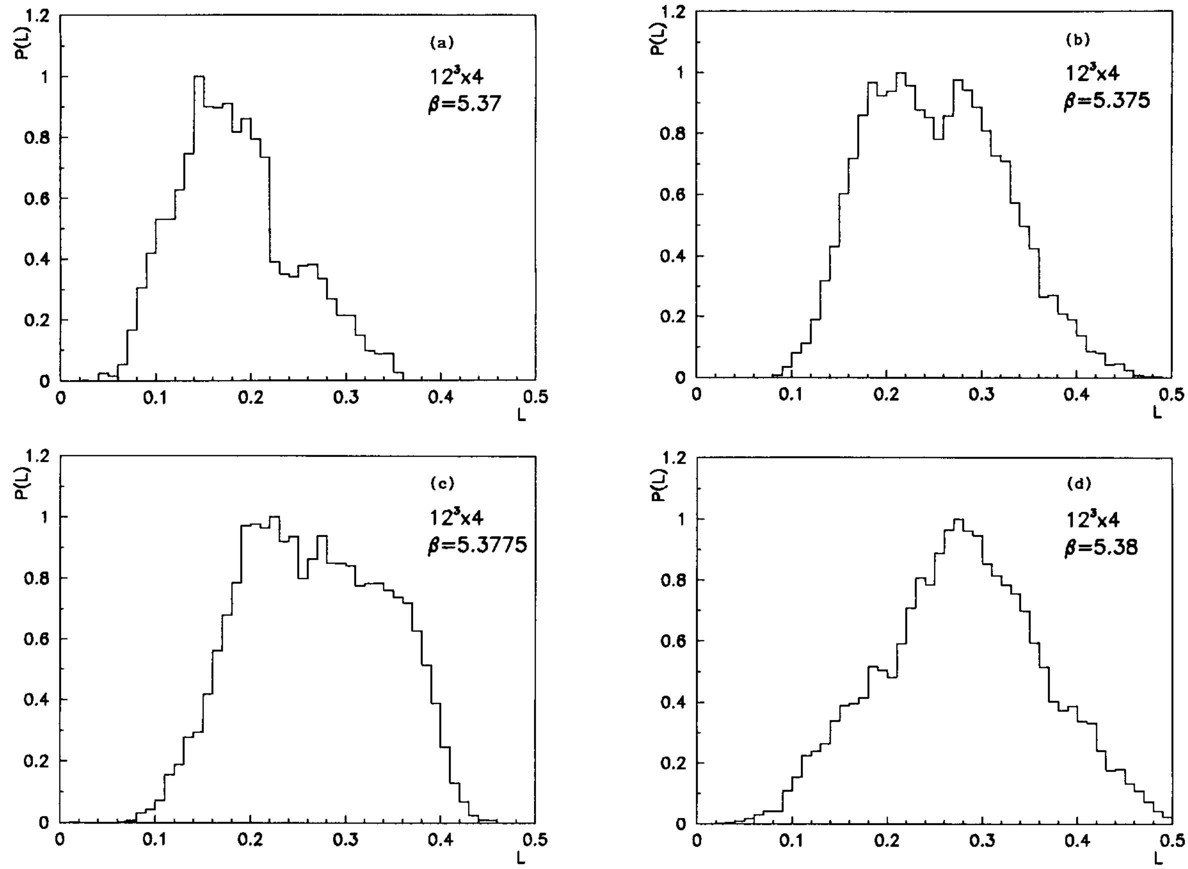

Fig. 4. Probability distribution of $|L|$ on the $12^3 \cdot 4$ lattice at $\beta=5.37$ (a), 5.375 (b), 5.3775 (c) and 5.38 (d).

tempted to analyze the probability distribution of observables and looked for a double-peak structure as indicator for coexisting states. A detailed analysis for $ma=0.1$ has been performed on lattices with spatial extent $N_\sigma=8$ and 12. We performed long runs of time evolution of observables. This is apparent from $\sim 70\,000$ iterations ($\tau \sim 3500$). Details of the statistics collected for the different couplings and lattice sizes are summarized in table 2. The numerical results we are going to discuss in the following are summarized in figs. 3 and 4. These figures show the Polyakov loop probability distribution

$$P(L)=N\int \prod_{x,\mu} \mathrm{d}U_{x,\mu}\,\delta\left(L-\frac{1}{N_\sigma^3}\sum_x |L_x|\right) \times \exp[-S_G(U)]\,, \tag{9}$$

with normalization factor N chosen such that $\max_L P(L)=1$. First of all we note that these distribution functions become narrower with increasing lattice size. For the critical couplings we find from these runs

$$\beta_c=5.3825\pm 0.005\,, \quad 8^3\cdot 4\,,$$
$$\beta_c=5.376\pm 0.003\,, \quad 12^3\cdot 4\,.$$

On both lattices the critical couplings agree within errors and in both cases we find a double-peak structure in the distribution function $P(L)$. This is usually taken as an indication for a first order phase transition. We note, however, that the separation between the two peaks in the distribution function at β_c becomes smaller as the lattice size increases. For the gap, ΔL, in L at β_c we estimate

$$\Delta L=0.20\pm 0.02\,, \quad 8^3\cdot 4\,,$$
$$\Delta L=0.15\pm 0.02\,, \quad 12^3\cdot 4\,.$$

The decrease found in the gap with increasing lattice size is in agreement with observations made in ref. [6] on smaller lattices. From our present analysis it remains unclear whether in the infinite volume limit the discontinuity in the Polyakov loop will persists or will go to zero. The order of the transition for the $N_f=2$, $ma=0.1$ case thus remains uncertain.

We also monitored the probability distribution of the chiral condensate $\bar{\chi}\chi$. In this case we observe a broadening of the distribution at β_c but did not find a clean double-peak structure. However, this may be related to the fact that we do not perform an exact measurement of $\bar{\chi}\chi$ on individual configurations but rather get only a noisy estimator from our bilinear noise algorithm. This makes the observation of a discontinuity in $\bar{\chi}\chi$ difficult. Nonetheless we still find a very strong correlation between individual measurements of L and $\bar{\chi}\chi$. This is already apparent from the strongly correlated fluctuations in L and $\bar{\chi}\chi$ present in the time histories shown in fig. 1. In fig. 5 we show the correlation between L and $\bar{\chi}\chi$ for $N_f=2$ in the transition region. Measurements represented by dots in these figures have been averaged over a time interval of length $\Delta\tau=10$. In the critical region the correlation is well described by a straight line,

$$(\bar{\chi}\chi)_{av}=0.93-0.55(L)_{av}\,, \tag{9}$$

where $(\ )_{av}$ denotes the average of the observables over a time interval $\Delta\tau=10$. It is thus evident that L and $\bar{\chi}\chi$ show the same critical behaviour at β_c.

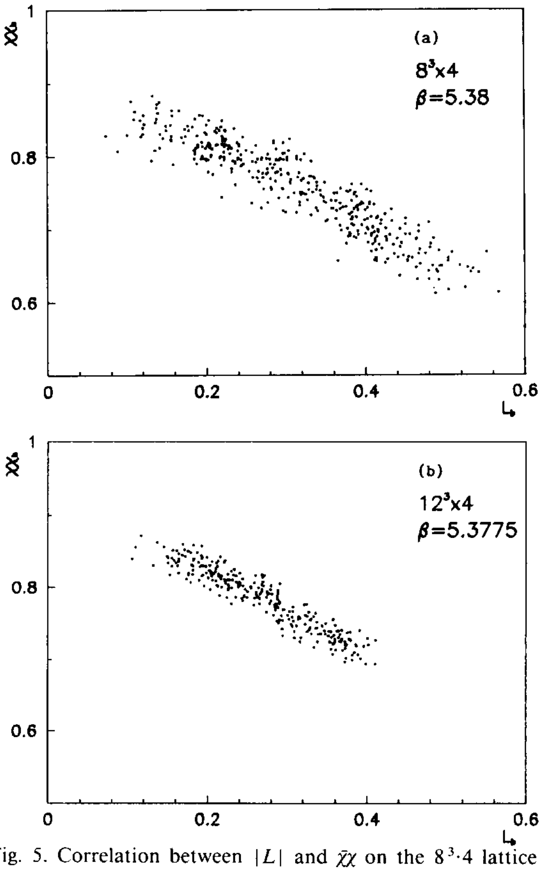

Fig. 5. Correlation between $|L|$ and $\bar{\chi}\chi$ on the $8^3\cdot 4$ lattice at $\beta=5.38$ (a) and on the $12^3\cdot 4$ lattice at $\beta=5.3775$ (b). Each point represents an average over 200 iterations ($\Delta\tau=10$).

4. Summary

In the small N_f region we find that the dependence of the critical coupling on N_f is approximately linear, see eq. (7). Our results indicate that for a quark mass $m/T=0.4$ the discontinuity in the observables present in the pure gauge theory persist for all $N_f\leqslant 2$ on lattices of size $8^3\cdot 4$. The transition is, however, considerably weaker for $N_f=1$ and 2 than for $N_f=0$ and 0.5. Moreover, for $N_f=2$ we find that the transition weakens further when the lattice size is increased from $8^3\cdot 4$ to $12^3\cdot 4$. The present analysis thus puts doubt on the first order nature of the transition for the two flavour theory at intermediate masses. Larger spatial lattices are required in order to judge whether in the infinite volume limit the effective potential, $V_{eff}(L)=-\ln[P(L)]$, will have an extended flat minimum, characteristic for a first order transition, or whether the minimum will shrink to a point.

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