

## THE ACCEPTANCE PROBABILITY IN THE HYBRID MONTE CARLO METHOD

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We study the acceptance probability in the hybrid Monte Carlo method applied to lattice QCD with dynamical fermions. We investigate in detail its dependence upon the step-size and the parameters  $\beta$ ,  $m_q$  and  $V$ , and suggest a simple phenomenological formula for this dependence.

### 1. Introduction

The recently developed hybrid Monte Carlo (HMC) method [1] has become an important tool for numerical investigations of lattice QCD. While in principle equally applicable to pure gauge theories, its most significant role is in simulations of the full theory. As in earlier fermion algorithms which have been widely used, the key to its success is that it requires only  $O(1)$  (incomplete) fermion matrix inversions per update of the entire lattice. The additional attractive feature of the HMC method is that, in contrast to these earlier methods, it is free from systematic finite-step-size errors. Among existing "exact" algorithms it also appears to be superior in efficiency. While the computer time  $T$  required to generate independent configurations grows quadratically with increasing system size  $V$  for other "exact" algorithms, it has been argued that  $T \sim V^{5/4}$  for the HMC method [2,3]. In addition to an overall volume factor, this estimate takes into account the fact that the step-size  $\Delta\tau$  used in the discretized equations of motion has to be reduced as the volume is increased in order to maintain a reasonable acceptance probability in the global Metropolis step. One expects that  $\Delta\tau_A \sim V^{-1/4}$  [2,3], where  $\Delta\tau_A$  denotes the step-size needed to achieve a given acceptance.

Crucial for the performance of QCD algorithms is also the scaling of the computer time requirement with decreasing quark mass  $m_q$ . An increasing num-

ber of iterations for fermion matrix manipulations, by today's methods, gives rise to a factor  $m_q^{-1}$ . In addition, one is confronted with the problem of critical slowing down, associated with a diverging correlation length  $\xi_\pi = m_\pi^{-1}$ . From random walk arguments one would expect the autocorrelation time to grow like  $\xi_\pi^2$ , i.e. like  $m_q^{-1}$  as  $m_q \rightarrow 0$  at fixed coupling. Quantitative verifications of this are, however, still missing. Note that both these estimates are for the phase with broken chiral symmetry. As we will discuss below, in the symmetric phase, the dependence on  $m_q$  is expected to be much weaker. Further slowing down of the HMC algorithm arises from the reduction of step-size needed for constant acceptance. At fixed gauge coupling it has been proposed that  $\Delta\tau_A \sim m_q^{3/2}$  [4]. In recent simulations at small quark masses on lattices of sizes up to  $8 \times 16^3$  we observed, however, a less severe dependence on  $m_q$  [5-7]. In particular, we found a very weak dependence in the chirally symmetric phase, which, as we argue below, might be expected due to the lower density of small eigenvalues of the Dirac operator. Besides the effects of critical slowing down, it thus seems that the acceptance problem still is a major uncertainty in evaluating the performance of the HMC algorithm.

In this note we give a detailed discussion of our observations on the acceptance probability and its dependence upon  $V$ ,  $m_q$  and  $\beta$ . Parts of these results were presented in refs. [5,6]. Extending the analysis in ref. [2], we show that in the large volume limit the

acceptance probability is a simple function of the average energy violation  $\langle \Delta H \rangle$ ;

$$\langle P_{\text{acc}} \rangle = \text{erfc}(\langle \Delta H \rangle^{1/2}/2),$$

where  $\text{erfc}$  is the complementary error function. This allows us to deduce  $\Delta\tau_A$  from the scaling behaviour of  $\langle \Delta H \rangle$ . Our analysis confirms the volume dependence suggested in refs. [2,3], whereas the quark mass dependence is shown to be weaker than proposed in ref. [4]. Finally, we give phenomenological results for the  $\beta$  dependence, which has not been investigated before and which turns out to be strong. Putting our findings together, we arrive at an approximate expression for the acceptance probability which is found to apply to a wide range of bare parameters.

## 2. The algorithm

In our numerical work we apply the hybrid Monte Carlo method to QCD with four flavours of staggered fermions. We briefly describe the algorithm for this case. The partition function can be written in terms of the usual gluonic link matrices  $U$  and pseudo-fermion fields  $\phi_e$ , defined on even sites only. It takes the well-known form

$$Z = \int [dU d\phi_e d\phi_e^\dagger] \exp[-S(U, \phi_e, \phi_e^\dagger)],$$

$$S(U, \phi_e, \phi_e^\dagger) = S_G(U) + \phi_e^\dagger (Q^\dagger(U)Q(U))_{ee}^{-1} \phi_e. \quad (1)$$

Here, and often later, we suppress site, link and colour indices for readability. Subscripts  $e$  are used for restrictions to even sites.  $S_G(U)$  denotes the standard Wilson action for the gauge fields and  $Q(U) = D(U) + m_q$  is the staggered fermion matrix, in which

$$D(U)_{xy} = \frac{1}{2} \sum_{\mu} \alpha_{x,\mu} (U_{x,\mu} \delta_{x,y-\mu} - U_{x-\mu,\mu}^\dagger \delta_{x,y+\mu}), \quad (2)$$

with phase factors  $\alpha_{x,\mu} = (-1)^{x_1 + \dots + x_{\mu-1}}$ .

The update of the  $\phi_e$  fields for fixed gauge fields  $U$  can be performed by a computationally simple heat bath procedure [8]. From a vector  $R$  of independent complex random numbers drawn from a distribution  $P(R) \sim \exp(-R^\dagger R)$ , pseudo-fermion fields weighted according to eq. (1) are obtained as  $\phi_e = (Q^\dagger R)_e$ . A tentative  $U$  update is generated by using molecular

dynamics at fixed  $\phi_e$ 's. Starting from new momenta  $\pi_j$  distributed according to  $P(\pi_j) \sim \exp(-\pi_j^2/2)$ , the leapfrog discretized equations of motion

$$U' = \exp\{i[\Delta\tau\pi_j - \frac{1}{2}\Delta\tau^2 \partial_j S(U)] T_j\} U,$$

$$\pi_j' = \pi_j - \frac{1}{2}\Delta\tau[\partial_j S(U) + \partial_j S(U')] \quad (3)$$

are iterated  $N_{\text{MD}}$  times. This constitutes one so-called trajectory whose length we denote by  $\tau = N_{\text{MD}} \times \Delta\tau$ . The  $T_j$ ,  $j=1, \dots, 8$ , are  $SU(3)$  generators and  $\partial_j$  is a derivative on the group manifold [8]. Explicit expressions for  $\partial_j S(U)$  can for instance be found in ref. [3]. The new feature of the HMC algorithm is that the final  $U$  configuration is subject to a global Metropolis update, where this configuration is accepted with probability

$$P_{\text{acc}} = \min(1, \exp(-\Delta H)),$$

$$H = \frac{1}{2} \sum_{n,j} \pi_{n,j}^2 + S(U). \quad (4)$$

This final Metropolis step removes errors due to the discretisation of the equations of motion.

## 3. The acceptance probability

Non-vanishing reject probabilities in the Metropolis step arise because of discretisation errors in the equations of motion. In one leapfrog step, defined by eq. [3], energy conservation is violated at order  $O(\Delta\tau^3)$ :

$$\Delta H = \Delta\tau^3 \times \left( \frac{1}{4} \pi_i \partial_j S \partial_i \partial_j S - \frac{1}{12} \pi_i \pi_j \pi_k \partial_i \partial_j \partial_k S \right) + O(\Delta\tau^4). \quad (5)$$

As the volume is increased the step-size has to be decreased in order to keep the extensive quantity  $\Delta H$ , and thereby the acceptance rate, at a reasonable level. To estimate the required reduction of step-size we use the identity  $\langle \exp(-\Delta H) \rangle = 1$  [2], which follows from the area-preserving property of eq. (3). This equality can conveniently be expanded into cumulants

$$\langle \Delta H \rangle = \frac{1}{2} \langle (\Delta H - \langle \Delta H \rangle)^2 \rangle + \text{higher cumulants}. \quad (6)$$

At volumes large compared to the relevant correlation length  $\xi$ , i.e.  $V^{1/4} \gg \xi$ , the cumulants grow line-

arly with  $V$  or slower. The step-size dependence, on the other hand, is different: higher cumulants are of higher order in  $\Delta\tau$ . To achieve a finite  $\langle\Delta H\rangle$  in the infinite volume limit, it is thus evident from eq. (6) that  $\Delta\tau$  should be varied so as to keep the variance fixed,  $\sigma(\Delta\tau)^2 \equiv \langle(\Delta H - \langle\Delta H\rangle)^2\rangle = \sigma_0^2 = \text{constant}$ . Higher cumulants will then vanish and the limiting  $\Delta H$  distribution will be a gaussian with mean and width related through

$$\langle\Delta H\rangle = \frac{1}{2} \langle(\Delta H - \langle\Delta H\rangle)^2\rangle, \quad V \rightarrow \infty, \sigma(\Delta\tau)^2 = \sigma_0^2. \quad (7)$$

Using this distribution we can evaluate the average acceptance rate at large volumes

$$\begin{aligned} \langle P_{\text{acc}} \rangle &= \frac{1}{\sqrt{2\pi}\sigma_0} \int_{-\infty}^{\infty} \min(1, \exp(-x)) \\ &\times \exp\left(-\frac{(x - \langle\Delta H\rangle)^2}{2\sigma_0^2}\right) dx \\ &= \text{erfc}\left(\frac{1}{2}\langle\Delta H\rangle^{1/2}\right). \end{aligned} \quad (8)$$

To test the convergence towards this result we have analyzed a system of  $N$  coupled oscillators. Results for the acceptance rate as a function of  $\langle\Delta H\rangle$  are shown in fig. 1a. The line in this figure corresponds to the result in eq. (8). As can be seen, the large volume ( $\sim$  large number of degrees of freedom) result is rapidly approached for fixed  $\langle\Delta H\rangle$  and increasing number of oscillators. In fig. 1b we show some results from our QCD simulations on a  $4 \times 6^3$  lattice. Apparently the agreement with eq. (8) is excellent also in this case, showing that already on a  $4 \times 6^3$  lattice the number of degrees of freedom is large enough for the infinite volume result to apply. In order to determine the step-size required for constant acceptance,  $\Delta\tau_A$ , it is thus sufficient to study the scaling of  $\langle\Delta H\rangle$ .

Combining eqs. (5) and (7), we find immediately for one molecular dynamics step ( $N_{\text{MD}}=1$ ) that  $\langle\Delta H\rangle \sim \Delta\tau^6$ . When iterating the equations of motion  $N_{\text{MD}}$  times, we expect  $\Delta H$  to increase linearly up to some point  $\tilde{N}_{\text{MD}} \times \Delta\tau = \lambda_c$ , beyond which there is no systematic increase in  $\Delta H$ <sup>#1</sup>. Such a behaviour is consistent with the observations made in ref. [9]. For

<sup>#1</sup> This happens provided  $\Delta\tau$  is not too large. On the other hand, if  $\Delta\tau$  exceeds a certain limit then  $\Delta H$  will generically grow exponentially.

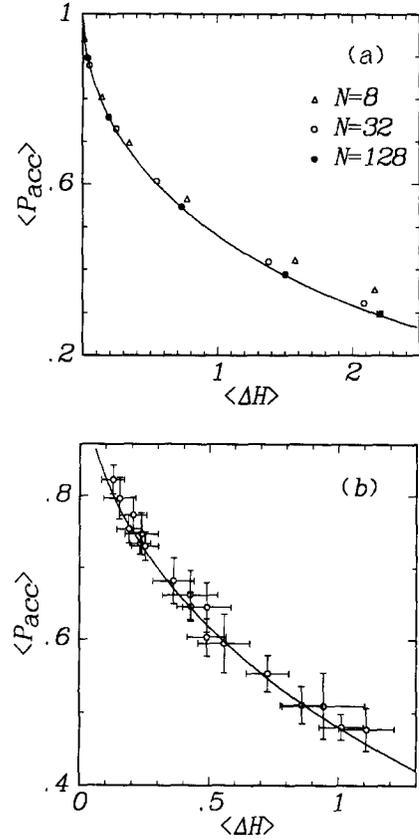


Fig. 1. Acceptance probability as a function of  $\langle\Delta H\rangle$ . In (a) we show data for a chain of  $N$  coupled oscillators,  $N=8, 32$  and  $128$ . The action is  $S(\phi) = \sum \frac{1}{2} [\phi_i^2 - \phi_i(\phi_{i+1} - 2\phi_i + \phi_{i-1})]$  and we use periodic boundary conditions. In (b) data for QCD on a  $4 \times 6^3$  lattice are given. The lines show the large volume result given in eq. (8).

trajectories longer than this characteristic length  $\lambda_c$ , or for trajectories of fixed length  $\tau$ , this means that  $\Delta H \sim \Delta\tau^2$  rather than  $\sim \Delta\tau^3$ . From eq. (7), which like eq. (8) is valid also for  $N_{\text{MD}} > 1$ , we therefore expect that

$$\langle\Delta H\rangle \sim V\Delta\tau^4. \quad (9)$$

This behaviour is verified by our data, as discussed in connection with fig. 2 below, and leads to the relation  $\Delta\tau_A \sim V^{-1/4}$ .

We finally note that our result for the volume dependence of the average acceptance,  $\langle P_{\text{acc}} \rangle \approx \text{erfc}(c\Delta\tau^2 V^{1/2})$ , is valid for arbitrary values of  $\langle\Delta H\rangle$  as long as the volume is large enough. Approximate

expressions have previously been obtained for large [2,3] and small [10] values of  $\langle \Delta H \rangle$ ,

$$\langle P_{\text{acc}} \rangle \sim \exp(-c\Delta\tau^4 V), \quad \langle \Delta H \rangle \text{ large,} \\ \sim \exp(-c\Delta\tau^2 V^{1/2}), \quad \langle \Delta H \rangle \text{ small.} \quad (10)$$

These expressions are easily obtained from eq. (8) if the appropriate limits of the error function are taken.

#### 4. $m_q$ dependence

Apart from the volume and step-size dependence of  $\Delta H$ , it is also important to analyse its dependence on the quark mass  $m_q$ . While  $H$  itself has a non-singular  $m_q$  dependence, its derivatives, which contribute to  $\Delta H$ , behave differently. As discussed in the previous section, we obtain the mass dependence of  $\langle \Delta H \rangle$  in the large volume limit from the square of the leading term in eq. (5). Let us consider one generic contribution, namely

$$(\Delta H)^2 \propto \Delta\tau^6 \times (\partial_i \partial_j \partial_k S_F \partial_i \partial_j \partial_k S_F + \dots) \\ + \text{higher orders in } \Delta\tau, \quad (11)$$

where  $S_F = \phi^\dagger (-D^2 + m_q^2)^{-1} \phi$  and where we have averaged over the momenta  $\pi_i$ . To give an explicit example, we consider the gauge group  $U(1)$ , for which the derivatives have a simple structure. In this case one has

$$\partial_i \partial_j \partial_k S_F \partial_i \partial_j \partial_k S_F \\ \propto \sum_{ijklabcd} (D + m_q)_{i+\hat{\mu}j}^{-1} (D^\dagger + m_q)_{j\hat{\mu}i}^{-1} \\ \times (D + m_q)_{j+\hat{\mu}k}^{-1} (D^\dagger + m_q)_{k\hat{\mu}j}^{-1} \\ \times \phi_a^* (D + m_q)_{a\hat{i}}^{-1} (-D^2 + m_q^2)_{k+\hat{\mu}b}^{-1} \phi_b \\ \times \phi_c^* (-D^2 + m_q^2)_{c\hat{k}+\hat{\mu}k}^{-1} (D^\dagger + m_q)_{i\hat{d}}^{-1} \phi_d \\ + \text{similar terms.} \quad (12)$$

Averaging over the pseudo-fermion fields we get

$$\partial_i \partial_j \partial_k S_F \partial_i \partial_j \partial_k S_F \\ \propto \sum_{ij} (-D^2 + m_q^2)_{ii}^{-1} (-D^2 + m_q^2)_{j+\hat{\mu}j+\hat{\mu}j}^{-1} \\ \times (D + m_q)_{i+\hat{\mu}i}^{-1} (D^\dagger + m_q)_{j\hat{i}+\hat{\mu}i}^{-1} \\ + \dots, \quad (13)$$

where only the most singular part has been kept. By counting powers of the inverse Dirac operator, it was argued in ref. [4] that  $(\Delta H)^2$  diverges as  $m_q^{-6}$ . However, it is clear from the structure of eq. (12) that this eigenvalue singularity will be significantly weakened after integration (summation) over the full eigenvalue spectrum. This is most easily seen in the free case,  $U=1$ , in which the factors  $(-D^2 + m_q^2)_{ii}^{-1} = \bar{\chi}\chi/m_q$  are translationally invariant. The summations are then trivial and one gets  $(\Delta H)^2 \propto V(\bar{\chi}\chi/m_q)^3$ . Since  $\bar{\chi}\chi$  vanishes linearly with  $m_q$ , this, in fact, suggests that  $(\Delta H)^2$  is constant as  $m_q \rightarrow 0$ . We therefore expect a very weak mass dependence in the chirally symmetric phase, where the eigenvalue spectrum is expected to be similar to that of the free case ( $U=1$ ). To the extent that the first two factors in eq. (12) effectively remain translationally invariant, we would further get the estimate  $(\Delta H)^2 \sim m_q^{-3}$  for the broken phase. We have verified this result at strong coupling,  $\beta=0$ . Using the techniques of ref. [11], we have calculated the expression in eq. (13) in a  $1/d$  expansion. To leading order it becomes the product of three free pion propagators at momentum zero. Thus it diverges as  $m_\pi^{-6}$ , which indeed corresponds to  $m_q^{-3}$ . For QCD at  $\beta=0$  in  $d=4$  we have also verified this behaviour numerically.

To study the  $\beta$  dependence of the mass exponent and its variation across the chiral phase transition, we have performed additional simulations with various quark masses at  $\beta=4.5, 4.9$  and  $5.4$  on a  $4 \times 6^3$  lattice. In order to check also the step-size dependence, we studied three different values of  $\Delta\tau$  varying by 50% at several fixed values of  $(\beta, m_q)$ . The step-sizes used by us led to acceptance rates between 0.5 and 0.8. Since the trajectory length was kept constant ( $\tau=1$ ), we expect from the discussion in section 3 that  $\langle \Delta H \rangle \sim \Delta\tau^4$  at fixed  $(\beta, m_q)$  independent of whether we are in the chirally symmetric or broken phase. This behaviour is confirmed by the data shown in fig. 2. The dependence on the quark mass, however, is found to be markedly different in the two different phases. At fixed coupling, it is seen to be consistent with  $\langle \Delta H \rangle \propto \Delta\tau^4 m_q^{-\alpha}$ . Fitting the data to this form, we find exponents  $\alpha=3.0 \pm 0.1$  at  $\beta=4.5$  and  $4.9$  and  $0.3 \pm 0.1$  at  $\beta=5.4$ . Note that for our smallest quark mass,  $m_q=0.025$ , the transition takes place at  $\beta_c=4.95 \pm 0.03$  [12].

The data thus clearly demonstrates the effect of the

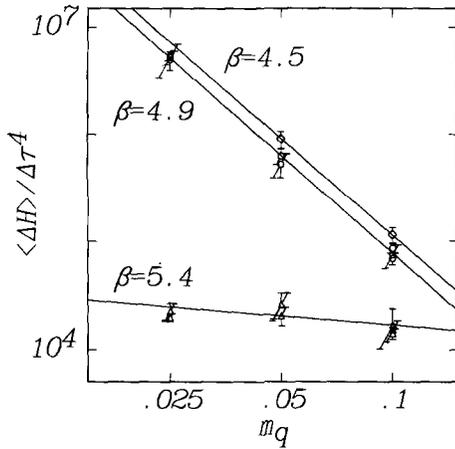


Fig. 2. The mass dependence of  $\langle \Delta H \rangle$  on a  $4 \times 6^3$  lattice at the couplings  $\beta=4.5$  (diamonds), 4.9 (circles) and 5.4 (triangles). Points with the same  $\beta$  and  $m_q$  are for different step-sizes  $\Delta\tau$ . The lines are fits for fixed  $\beta$  to  $\langle \Delta H \rangle = c \Delta \tau^4 m^{-\alpha}$ . The step-sizes vary between 0.0125 and 0.085.

integration over the distribution of eigenvalues. In the symmetric phase the eigenvalue singularity is almost completely cancelled and in the broken phase it is also significantly weakened, i.e. we find  $\alpha \approx 3$  instead of  $\alpha = 6$  as one would have expected from a naive power counting argument.

In the chirally broken phase of QCD we thus find excellent agreement with the analytical strong coupling calculation, while  $\langle \Delta H \rangle$  seems to be approximately independent of  $m_q$  in the chirally symmetric phase. The above analysis suggests that this difference between the two phases arises because of the different eigenvalue spectra for the Dirac operator. An operator which reflects changes in the eigenvalue spectrum and which is easily obtained in lattice simulations is the chiral order parameter

$$\bar{\chi}\chi = \frac{1}{V} \text{Tr}(D + m_q)^{-1}. \quad (14)$$

In general we would expect  $\langle \Delta H \rangle$  to depend on the eigenvalue spectrum in a more complicated way than just through  $\langle \bar{\chi}\chi \rangle$ . Our discussion of the free case and its extension to  $U(1)$  suggests, however, that the dependence of  $\langle \Delta H \rangle$  on  $m_q$  is to a large extent described by the mass dependence of  $\langle \bar{\chi}\chi \rangle$ . In fact, we see that our results for the dependence of  $\langle \Delta H \rangle$  on  $m_q$  at different couplings are well described by the relation

$$\langle \Delta H \rangle \sim \left( \frac{\langle \bar{\chi}\chi \rangle}{m_q} \right)^3. \quad (15)$$

### 5. $\beta$ dependence

The discussion in the previous sections has shown that the volume, step-size and quark mass dependence of  $\Delta H$  is well under control. We are therefore left with an analysis of the  $\beta$  dependence of  $\Delta H$ . We parametrize this by an unknown function  $c(\beta)$ ,

$$\langle \Delta H \rangle = c(\beta) \left( \frac{\langle \bar{\chi}\chi \rangle}{m_q} \right)^3 V \Delta \tau^4. \quad (16)$$

We note that the  $\beta$  dependence of  $\Delta H$  is partly hidden in the  $\beta$  dependence of  $\langle \bar{\chi}\chi \rangle$ . Note also that the phase of the system can change as the lattice size is varied at fixed  $\beta$ . This can lead to deviations from the simple form used in the above ansatz. Such deviations are, in fact, likely to occur close to a phase transition. In that region  $\Delta H$ , which is a sum of  $O(V)$  correlated terms, should grow large because of a long correlation length  $\xi$ . Naively, one would expect  $\langle \Delta H \rangle \propto \xi^4$ .

In fig. 3 we plot the coefficient  $c(\beta)$  for data ob-

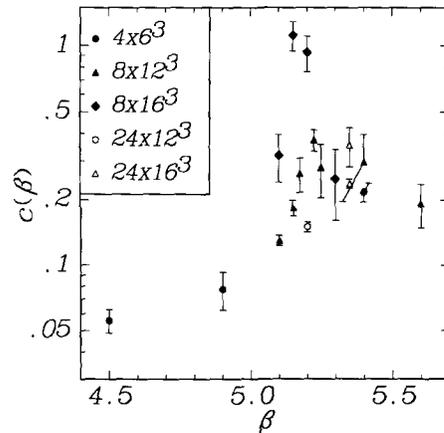


Fig. 3. The coefficient  $c(\beta)$  defined in eq. (16). Data from the  $8 \times 12^3$  [5] and  $8 \times 16^3$  [7] lattices are for  $m_q=0.025$  and 0.01, respectively. On the  $4 \times 6^3$  lattice the different masses studied (see section 4) give consistent values for  $c(\beta)$ . The points shown are for the smallest mass at each  $\beta$ . The data for the  $24 \times 12^3$  ( $m_q=0.025$ ) and  $24 \times 16^3$  ( $m_q=0.01$  and 0.025) lattices are taken from ref. [13].

tained on different lattices and in both phases (values for  $m_q$ ,  $\langle \bar{\chi}\chi \rangle$  and  $V$  given here and below are in lattice units). On the  $8 \times 16^3$  lattice ( $m_q=0.01$ ), we see a clear peak at the phase transition, which is at  $\beta_c=5.15 \pm 0.05$  [7]. Also there is an indication of a peak at the transition/crossover coupling  $\beta_c=5.25 \pm 0.025$  [5] on the  $8 \times 12^3$  lattice ( $m_q=0.025$ ). The presence of these peaks makes a systematic study of  $c(\beta)$  using the present data set difficult. Outside these regions, we see, however, that data from different lattices agree reasonably well. It is furthermore important to note that the increase of  $c(\beta)$  with  $\beta$  is fairly moderate. In fact, the variation in  $c(\beta)$  should be compared with that in  $X \equiv \langle \Delta H \rangle m_q^3 \Delta \tau^{-4} V^{-1}$ , which reflects the full  $\beta$  dependence of  $\langle \Delta H \rangle$  and which we plot in fig. 4 against  $\langle \bar{\chi}\chi \rangle$ . The much larger variation in the latter quantity shows that  $\langle \Delta H \rangle$  has a strong  $\beta$  dependence and that a major part of this dependence is absorbed into  $\langle \bar{\chi}\chi \rangle^3$ . The line drawn in fig. 4 corresponds to  $X = \bar{c} \langle \bar{\chi}\chi \rangle^3$  with  $\bar{c}=0.2$ . As can be seen from fig. 3, using a constant value  $\bar{c}$  rather than the function  $c(\beta)$ , over-estimates the value of  $c(\beta)$  at small  $\beta$ . This leads to the deviations seen at large values of  $\langle \bar{\chi}\chi \rangle$  in fig. 4.

We want to stress again that the strong  $\beta$  dependence of  $\langle \Delta H \rangle$  does not only show up across the transition and that it is to a large extent described by the  $\beta$  dependence of  $\langle \bar{\chi}\chi \rangle$ . To show this explicitly let us compare the behaviour of  $\langle \Delta H \rangle$  at two couplings

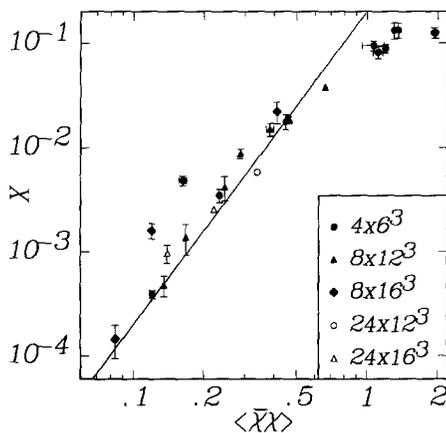


Fig. 4.  $X = \langle \Delta H \rangle (m_q^{-3} \Delta \tau^4 V)^{-1}$  plotted against  $\langle \bar{\chi}\chi \rangle$ . The line corresponds to  $X = \bar{c} \langle \bar{\chi}\chi \rangle^3$  with  $\bar{c}=0.2$ .

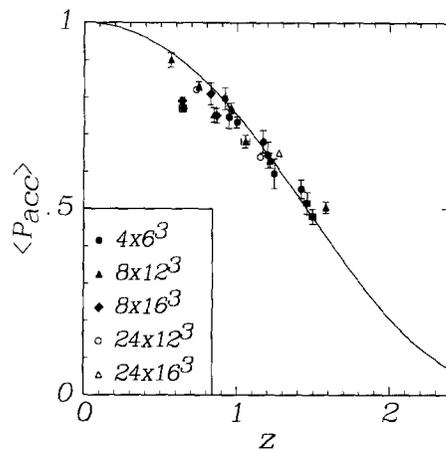


Fig. 5. The acceptance rate as a function of  $z$ , defined in eq. (17), for data in the interval  $5.1 \leq \beta \leq 5.6$ . The curve shows the result in eq. (18).

in the broken phase: Between  $\beta=5.1$  and  $5.35$  for  $m_q=0.025$ , the average  $\langle \bar{\chi}\chi \rangle$  drops from  $0.66$  to  $0.22$ , i.e.  $\langle \bar{\chi}\chi \rangle^3$  drops by a factor  $27$ . In the same interval  $\langle \Delta H \rangle$  decreases by a factor  $13$ . The coefficient  $c(\beta)$  takes care of the mismatch between these different  $\beta$  dependences, which is relatively small, i.e.  $c(\beta)$  changes only by a factor of  $2$ .

By reformulating eq. (16) in terms of the acceptance rate, we can get a useful guide for the choice of step-size in actual simulations. Restricting ourselves to the interval  $5.1 \leq \beta \leq 5.6$ , over which the change in  $c(\beta)$  is negligible, we plot in fig. 5 the acceptance rate as a function of

$$z = \left( \frac{\langle \bar{\chi}\chi \rangle}{m_q} \right)^{3/4} V^{1/4} \Delta \tau. \tag{17}$$

According to eqs. (8) and (16), the acceptance rate should be entirely determined by

$$\langle P_{acc} \rangle = \text{erfc}(c' z^2). \tag{18}$$

Using  $c' = \frac{1}{2} \sqrt{c(\beta)} \approx 0.22$ , we get an excellent description of the acceptance rate in this range of  $\beta$  values. We further note that an acceptance rate of approximately  $75\%$  is achieved for  $z \approx 1$ .

## 6. Summary and discussion

Our results show that the acceptance probability

exhibits very different mass dependences in the two different phases of QCD. Numerical data at different couplings in the chirally broken phase are in favour of a scaling law  $\Delta\tau_A \sim m_q^{3/4}$ , which, furthermore, is the behaviour we find in a  $1/d$  expansion at strong coupling. From this result, together with the volume dependence,  $\Delta\tau_A \sim V^{-1/4}$ , we can estimate the computer time requirement in the limit of small quark mass, assuming a fixed coupling and a fixed ratio  $\xi_\pi/V^{1/4}$ . Taking into account critical slowing down and an increased time for fermion matrix inversions, as discussed in the introduction, we find that the total computer time,  $T$ , grows like  $T \sim m_q^{-21/4}$ . Here the requirement of constant acceptance rate with changing quark mass and lattice volume has contributed with a factor  $m_q^{-5/4}$ . In the symmetric phase, the behaviour at small quark mass is different, due to the different spectrum of the Dirac operator. We find that the acceptance rate is approximately  $m_q$  independent. Furthermore, the time needed for fermion matrix inversions should grow only slowly as  $m_q \rightarrow 0$ , as also observed in our simulations. Finally, if the lowest mode is massive, as indicated in ref. [14], then the increase in autocorrelation time should also be only weakly dependent on  $m_q$ . We thus expect that the explicit dependence of  $T$  on  $m_q$  in the chirally symmetric phase is rather weak.

Finally, we would like to discuss the implications of our phenomenological results for the  $\beta$  dependence. While a change of  $m_q$  and  $V$  in the directions of physical interest leads to smaller acceptance probabilities, our results show that the opposite is true for changes in  $\beta$ . To illustrate the consequences of this, we consider decreasing the lattice spacing  $a$ , while keeping at the same time physical parameters constant. We then get the relation  $\Delta\tau_A \sim \langle \bar{\chi}\chi \rangle^{-3/4} m_q^{3/4} V^{-1/4} \sim a^{-1/2}$ . Here we have ignored the variation of  $c(\beta)$  with  $\beta$ , which probably shifts the exponent of  $a$  to a larger value. Our data indicate, however, that this shift is moderate, possibly leading to an exponent zero. This means that the effects of smaller  $m_q$  and larger  $V$  (in lattice units) are to large extent compensated for by the  $\beta$  dependence in this limit. This suggests that the extra cost for making the algorithm exact is not very sensitive to changes of the lattice spacing at fixed quark mass and lattice volume in physical units.

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