STRONG EVIDENCE FOR SPONTANEOUS CHIRAL SYMMETRY BREAKING IN (QUENCHED) QCD ☆

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We calculate the chiral condensate $\langle\bar{\psi}\psi\rangle$ for all quark masses using Kogut–Susskind fermions in lattice-regularized quenched QCD. The *large* volume behaviour of $\langle\bar{\psi}\psi\rangle$ at *small* quark masses demonstrates that the explicit U(1) chiral symmetry is spontaneously broken. We perform the calculation for $\beta = 5.1$ to 5.9 and find very good continuum renormalization group behaviour. We infer that the spontaneous breaking we observe belongs to continuum QCD. This constitutes the first unambiguous demonstration of spontaneous chiral symmetry breaking in continuum quenched QCD.

Spontaneous chiral symmetry breaking is one of the most striking features of the strong interactions [1], and if QCD is to be a successful candidate theory it must reproduce this phenomenon. Whether it does or not has not yet been established: the problem is made difficult by its non-perturbative nature. If it does *not* then the spectrum predicted by QCD will possess parity doubling and no very light pions, in damaging contrast to the experimental situation. In a previous paper [2] we discussed this problem within the context of a Monte Carlo [3] simulation of lattice-regularized [4] QCD and presented preliminary numerical evidence that chiral symmetry is consistent with being broken spontaneously. In this letter we shall make the evidence convincing: continuum QCD in the quenched approximation, where one neglects vacuum fermionic fluctuations, breaks its (zero quark mass) chiral symmetry dynamically.

The usual criterion for chiral symmetry breaking is that the chiral condensate $\langle\bar{\psi}\psi(m)\rangle$ should not vanish as $m \to 0$. One has to be careful when using this criterion on a lattice of finite volume, V. A finite system will, given enough time, rotate through all the degenerate minima of the effective potential, so that one obtains $\langle\bar{\psi}\psi(m \to 0)\rangle = 0$ even if the symmetry is dynamically broken. The correct criterion is that

$$\lim_{m\to 0} \lim_{V\to\infty} \langle\bar{\psi}\psi(m)\rangle \neq 0, \qquad (1)$$

if we are to have spontaneous breakdown. To check whether (1) holds (or not) one proceeds as follows. Calculate $\langle\bar{\psi}\psi(m)\rangle$ for several different lattice volumes. The condensate should tend to an envelope, which for $m \ll O(\Lambda_{\mathrm{mom}})$ (Λ_{mom} being a rough measure of the energy) is linear in m and has a non-zero

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intercept at $m = 0$. For the largest volumes the mass at which $\langle\bar{\psi}\psi(m)\rangle$ breaks away from the envelope to collapse to zero should be so much smaller than the gauge theory energy scale, $O(\Lambda_{\mathrm{mom}})$, that it is obviously a kinematic rather than a dynamic effect. It is clear that such a calculation requires great accuracy at very small quark masses. We emphasize that unless one calculates for quark masses much less than the energy scale of the non-abelian gauge theory, one cannot say anything about whether the theory breaks chiral symmetry spontaneously or not. Especially so in a numerical lattice calculation, where $\langle\bar{\psi}\psi(m)\rangle$ at larger quark masses possesses a large (ultraviolet) perturbative component. We shall illustrate this explicitly with our data below.

To show that the spontaneous breaking is a *continuum* property one must then repeat the calculation over a range of β and demonstrate the correct continuum renormalization group behaviour for $\langle\bar{\psi}\psi\rangle$.

To demonstrate continuum behaviour is especially important since it is known that one has spontaneous breakdown in various modified strong-coupling limits [5–7]. One also finds spontaneous chiral symmetry breaking whenever one has confinement, in the large N_c and mean-field (space–time dimension $d \to \infty$) approximation [8]. This situation is rather weaker than the one for confinement: there has been no direct demonstration of chiral breaking for SU(3) in $d = 4$ at large g^2. In this paper we shall in fact show that quenched QCD breaks chiral symmetry at strong coupling, and our results are in beautiful agreement with the analytic expressions of ref. [7], but only if one includes their $1/d$ corrections.

There have also been numerical calculations claiming to provide evidence for continuum chiral breaking. In refs. [9] and [10] the cases of SU(3) and SU(2) are considered. Unfortunately these claims are typically based on naive extrapolations of measurements of $\langle\bar{\psi}\psi(m)\rangle$ at large quark masses, $m \gtrsim O(\Lambda_{\mathrm{mom}})$. In addition they use periodic fermionic boundary conditions, which misleadingly simulate [2] chiral symmetry breaking on small lattices, even for the free theory. The dangers of such procedures are highlighted by the apparent appearance [9] of continuum chiral breaking on small lattices at values of β where they are deconfining and there is in fact no spontaneous chiral breaking [11]. An interesting calculation on small lattices with quark loops and at $m = 0$ appears in ref. [12]; it is suggestive but hardly definitive. This is the rather unsatisfactory situation we now try to remedy. (As we were completing this work we received a paper by Kogut et al. [13], which studies the high-temperature recovery of chiral symmetry in the SU(2) case. Although these authors do not attempt to systematically demonstrate chiral symmetry breaking at zero temperature, their emphasis on calculating at small quark masses is realistic. They use the conjugate gradient algorithm, which we have also used both in this context [2] and in that of hadron spectrum calculations [14]. While it is much better than the popular Gauss–Seidel method, it does not compare, for the present purposes, with the Lanczos algorithm [2] we use herein.)

The euclidean lattice QCD action may be decomposed in gluonic and fermionic pieces

$$S = S_G + S_F . \tag{2}$$

For S_G we take the well-studied Wilson action [4]

$$S_G = \tfrac{1}{6}\beta \sum_{n,\mu,\nu\neq\mu} \mathrm{Tr}(U_{n,\mu} U_{n+\mu,\nu} U^{\dagger}_{n+\nu,\mu} U^{\dagger}_{n,\nu}) \tag{3}$$

and impose periodic boundary conditions. For S_F we want an action with chiral symmetry. This disqualifies the $(r \neq 0)$ Wilson-type fermions, which explicitly break all chiral symmetries by irrelevant operators, and there is no evidence that they have recovered chiral symmetry (enough to break it spontaneously) in the region of couplings accessible to Monte Carlo studies. The naive action

$$\begin{aligned} S_F &\equiv -\bar{\psi}[M(U) + 2ma]\psi \\ &= -\sum_{n,\mu} \bar{\psi}_n \gamma_\mu (U_{n,\mu}\psi_{n+\mu} - U^{\dagger}_{n-\mu,\mu}\psi_{n-\mu}) \\ &\quad - 2ma \sum_n \bar{\psi}_n \psi_n \end{aligned} \tag{4}$$

has an obvious explicit chiral symmetry when $m = 0$ but describes 16 "flavours". If we decompose the (antihermitean) matrix M into

$$M = \Gamma \mathcal{M} \Gamma^{\dagger} , \tag{5}$$

where Γ is a unitary block-diagonal matrix containing all the γ matrices [6], and write

$$\psi = \Gamma\chi , \tag{6}$$

the fermion action (4) becomes

$$S_F = \bar{\chi}[\mathcal{M}(U) + 2ma]\chi, \tag{7}$$

where the different components of χ decouple. This allows us to work with a single component fermion field, thereby reducing the number of degrees of freedom by a factor of 4. The fermion action (7) reduced to a single component χ is the action for staggered fermions [15], which we shall employ in this paper. The remaining quark degrees of freedom may be interpreted as 4 flavours [16,17]. The matrix $\mathcal{M}$ is an $N \times N$ sparse complex matrix, where $N = 3L_s^3 L_t$ (where L_s, L_t are the spatial, temporal extents of the lattice). We shall use antiperiodic boundary conditions for the fermion fields: the importance of this choice is discussed in ref. [2].

The action for staggered fermions has a U(4) $\times$ U(4) symmetry for $m = 0$ in the naive continuum limit. At finite lattice spacing the U(4) chiral symmetry is explicitly broken down to U(1) by an irrelevant operator, which mixes flavours. For a quenched calculation such as ours the important point is that there is an explicit U(1) chiral symmetry, for which $\langle\bar{\psi}\psi\rangle$ is an order parameter, and this U(1) is *not* the anomaly afflicted piece of U(4), but belongs to the SU(4) [17].

Let λ_i, $i = 1, ..., N$, be the eigenvalues of the (reduced) matrix $i\mathcal{M}$. These eigenvalues come in pairs of equal and opposite sign (because $\gamma_5 M = -M\gamma_5$), so we can write

$$\langle\bar{\psi}\psi(m)\rangle = (3/N)\langle\mathrm{Tr}(\mathcal{M} + 2ma)^{-1}\rangle$$

$$= \frac{3}{N}\left\langle\sum_{i=1}^{N} \frac{2ma}{\lambda_i^2 + (2ma)^2}\right\rangle$$

$$\xrightarrow[V\to\infty]{} 3\left\langle\int_{-\infty}^{+\infty} d\lambda \frac{2ma\rho(\lambda)}{\lambda^2 + (2ma)^2}\right\rangle, \tag{8}$$

where $\rho(\lambda)$ is the normalized spectral density. We can see explicitly in (8) how for a finite lattice $\langle\bar{\psi}\psi(0)\rangle = 0$, while

$$\lim_{m\to 0} \lim_{V\to\infty} \langle\bar{\psi}\psi(m)\rangle = 3\pi\rho(0) \tag{9}$$

demonstrates that it is the volume dependence of the eigenvalues of $i\mathcal{M}$ close to zero that will determine whether the chiral symmetry is broken spontaneously or not.

The numerical problem we are presented with in (8) is that of finding inverse elements and/or eigenvalues of a very large sparse complex $N \times N$ matrix. A numerical algorithm must satisfy two major constraints if it is to be suitable for use here. The first is that it should require the storage of only a few N-vectors at each step of the calculation; the second is that it should have stability against rounding errors. The best method we know at present for obtaining (selected rows of) the inverse is the conjugate gradient method (see ref. [2] for the algorithm and ref. [14] for detailed references). The best method we know for eigenvalues is the Lanczos algorithm. In the present context there are good reasons for preferring the latter method: we only need to calculate one set of eigenvalues [those of $i\mathcal{M}(U)$] to obtain $\langle\bar{\psi}\psi(m)\rangle$ for *all* quark masses. The conditioning of an eigenvalue problem is in general much better than that of an inversion problem – which means we shall have accurate results even at zero quark mass. In exact arithmetic the Lanczos algorithm [2] generates recursively a sequence of N orthonormal vectors, $v_1, v_2, ..., v_N$ which when put into an $N \times N$ matrix V will tridiagonalize the hermitean matrix $i\mathcal{M}$ by a unitary similarity transformation, $T = iV\mathcal{M}V^\dagger$. The eigenvalues of a tridiagonal matrix can be found quickly and accurately from the Sturm sequence of the principal minors of the matrix (there are standard library routines for this). When one has rounding errors the global orthogonality of the vectors $v_1, v_2, ..., v_N$ is lost, the procedure tends to repeat itself, and the resulting eigenvalues include only some of the correct ones plus several copies of the extreme eigenvalues and also some incorrect eigenvalues, which have not yet converged. Although we still will usually get the extreme eigenvalues correctly, for (8) we need essentially *all* the eigenvalues for accurate results. For small matrices (such as for a $4^3 \times 8$ lattice) one can maintain the global orthogonality explicitly by reorthogonalization. This is, however, a *very* slow procedure. At this level the Lanczos algorithm, as presented by us in ref. [2], would seem to be of limited use and certainly inferior for large lattices to the conjugate gradient method. Hence presumably the similar remarks by Kogut et al. [13]. There has, however, been a recent numerical analysis breakthrough [18] [‡1]

‡1 For a more recent variation of the method see ref. [19]. See also ref. [20].

(which has not yet percolated through to particle physics), that enables one to identify *all* the correct eigenvalues. The procedure is to generate *more* than N vectors v_i, say $\tilde{N}$. One then has a $\tilde{N} \times \tilde{N}$ tridiagonal matrix $\tilde{T}$. Construct also the $(\tilde{N}-1) \times (\tilde{N}-1)$ matrix $\hat{T}$ obtained from $\tilde{T}$ by deleting the first row and column. Consider the eigenvalues $\tilde{\lambda}_i$ of $\tilde{T}$ and $\hat{\lambda}_i$ of $\hat{T}$. Since degeneracies are not expected from an essentially random matrix, we accept each *multiple* eigenvalue of $\tilde{T}$ as a correct simple eigenvalue of $\mathrm{i}\mathcal{M}$. If a simple eigenvalue of $\tilde{T}$ is equal to some simple eigenvalue of $\hat{T}$, we identify it as spurious. (The numerical criterion of equality here is that the difference should be less than about $\tilde{N} \times$ machine precision $\times$ maximum eigenvalue.) We find that taking $\tilde{N} \approx 2N$ is enough (for lattices up to 8^4) to obtain all (exactly N) eigenvalues of our original $N \times N$ matrix $\mathrm{i}\mathcal{M}$. For a clear discussion of *why* all this should work see ref. [21]. For a recent textbook treatment of the Lanczos algorithm see ref. [22]. We now turn to the results of these numerical calculations.

We shall begin by demonstrating that the chiral symmetry of our action in eq. (7) is spontaneously broken at $\beta = 5.7$. (The fact that the 0^{++} and 2^{++} glueballs already show continuum scaling at this β [23, 24] indicates that the lattice spacing is small enough not to seriously distort the relevant continuum gluonic fluctuations. One reaches similar conclusions [24] by examining the gluonic condensate.) In fig. 1 we plot the calculated $\langle\bar{\psi}\psi(m)\rangle$ for $4^3 \times 8$ (averaged over 6 gauge field configurations), for $6^3 \times 8$ (1 configuration) and for 8^4 lattices (averaged over 4 configurations). We also show $\langle\bar{\psi}\psi\rangle$ at three mass values for a $10^3 \times 16$ lattice. These values come from a hadron spectrum calculation [14], using the conjugate gradient algorithm, and are obtained from 112 rows ($\times$ 3 colours) of the inverse. To indicate the statistical fluctuations between individual configurations and to give an idea of the error we furthermore plot $\langle\bar{\psi}\psi\rangle$ for the 4 configurations on the 8^4 lattice. Since we are only interested in $\langle\bar{\psi}\psi\rangle$ for quark masses smaller than $O(\Lambda_{\mathrm{mom}})$, we present results in the range $ma \leqslant 0.1$.

We observe that a $4^3 \times 8$ lattice shows no significant signal of spontaneous chiral symmetry breaking. As we increase the lattice size, we see a clear envelope developing, and this envelope has a non-zero intercept at zero quark mass. Comparing our 8^4 and $10^3 \times 16$

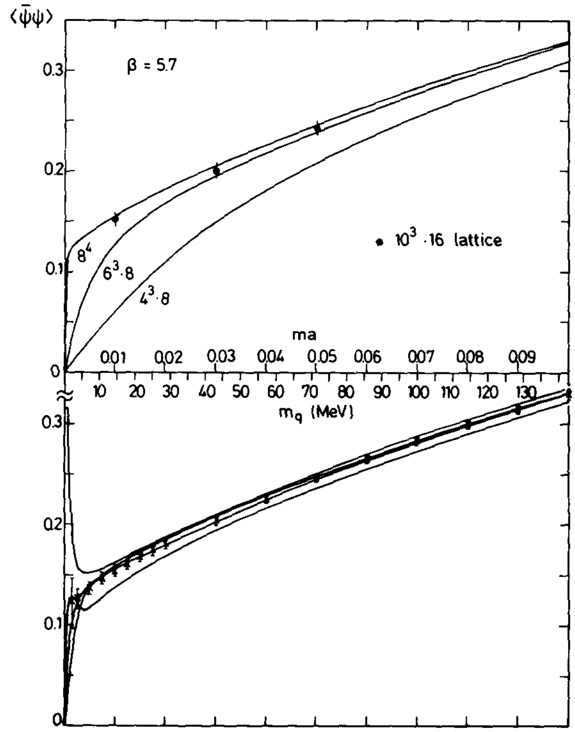

Fig. 1. $\langle\bar{\psi}\psi\rangle$ as a function of ma (and the renormalization group invariant quark mass $m_q = \alpha_{\mathrm{mom}}^{-4/11}$ for $\Lambda_{\mathrm{mom}} = 200$ MeV) obtained on the $4^3 \times 8$, $6^3 \times 8$ and 8^4 lattice at $\beta = 5.7$, and for 4 individual gauge field configurations on the 8^4 lattice. The solid circles come from the hadron spectrum calculation on the $10^3 \times 16$ lattice in ref. [14]. The crosses represent the average of the 4 gauge field configurations.

results we see that, for this physics, an 8^4 lattice is effectively of infinite volume down to $ma \approx 0.01$ at least. The break-away to zero occurs at a quark mass

$$ma = O(0.002) \ll O(\Lambda_{\mathrm{mom}} a), \tag{10}$$

where it is obviously a kinematic, not a dynamic, effect.

Having demonstrated spontaneous chiral symmetry breaking at $\beta = 5.7$, we now need to demonstrate that this is indeed a *continuum* effect. To do so we calculate $\langle\bar{\psi}\psi(m)\rangle$ for values of β from 0.01 to 5.9. For $\beta \geqslant 5.5$ we show results using 8^4 lattices, while for $\beta \leqslant 5.5$ we show results from $4^3 \times 8$ lattices (the physical size of the lattice increases with decreasing β). Our results are plotted in fig. 2 for $ma \leqslant 0.1$. Note that we see directly that a $4^3 \times 8$ lattice at $\beta = 5.5$

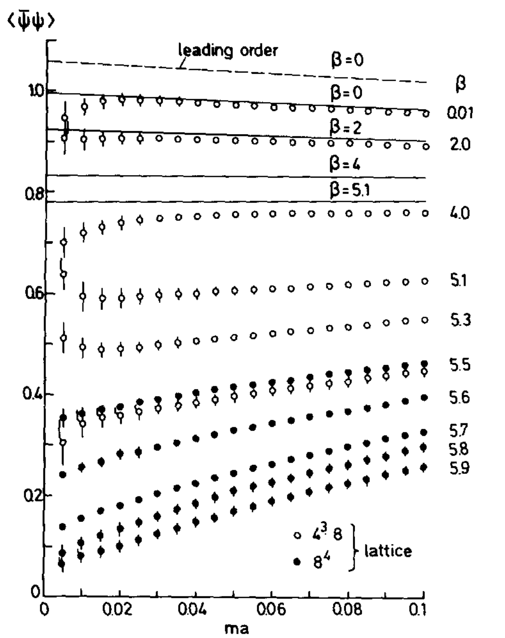

Fig. 2. $\langle\bar{\psi}\psi\rangle$ plotted at discrete points of ma for various values of β. The dashed line corresponds to the leading-order strong-coupling result ($d = \infty$). The solid lines include the O($1/d$) corrections.

is already large enough. We plot at discrete points so as to be able to show error bars (these come from fluctuations between different configurations; the errors on the numerical calculation would not be visible).

We observe that we have a (roughly) linear dependence on ma for $ma < 0.1$. We obtain $\langle\bar{\psi}\psi(0)\rangle$ by extrapolating this linear dependence to $ma = 0$. The extrapolation introduces no significant changes, and we could get almost the same results by using our measured values at, say, $ma = 0.01$. Our values of $\langle\bar{\psi}\psi(0)\rangle$ are plotted in fig. 3a. We can see the strong-coupling behaviour of $\langle\bar{\psi}\psi\rangle$ at low β, a transition region between $\beta = 4$ and 5.1, and very clear continuum (asymptotic freedom) behaviour for $\beta > 5.1$.

Our measured (dimensionless) $\langle\bar{\psi}\psi\rangle$ can be expressed in terms of the continuum (dimensionful) renormalization group invariant $\langle\bar{\psi}\psi\rangle_{\mathrm{inv}}$ by

$$\langle\bar{\psi}\psi\rangle = 2\alpha_{\mathrm{mom}}^{-4/11} a^3 \langle\bar{\psi}\psi\rangle_{\mathrm{inv}}, \quad \alpha_{\mathrm{mom}} = g_{\mathrm{mom}}^2/4\pi \tag{11}$$

(the normalization uses 4 flavours). We plot our extracted $\langle\bar{\psi}\psi\rangle_{\mathrm{inv}}^{1/3}$ (in MeV units; see below) as a func-

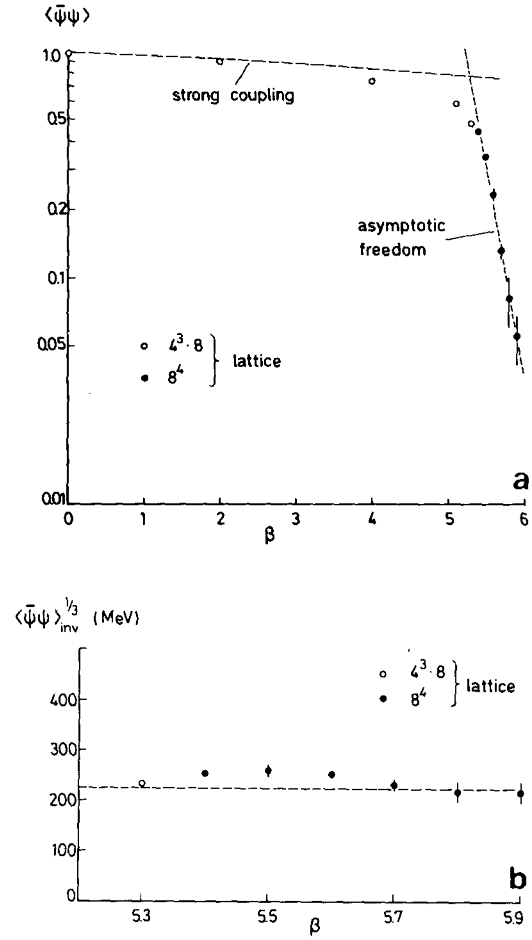

Fig. 3. (a) The intercept $\langle\bar{\psi}\psi(0)\rangle$ for various values of β together with the O($1/d$) strong-coupling and scaling (asymptotic freedom) curves. (b) The renormalization group invariant $\langle\bar{\psi}\psi\rangle_{\mathrm{inv}}^{1/3}$ for $5.3 \leqslant \beta \leqslant 5.9$. The dashed line represents the experimental value (see ref. [11]) of $\langle\bar{u}u\rangle^{1/3} = 225$ (± 25) MeV. Our scale is set by $\Lambda_{\mathrm{mom}} = 200$ MeV.

tion of β in fig. 3b. In obtaining $\langle\bar{\psi}\psi\rangle_{\mathrm{inv}}$ we have employed the perturbative relation

$$a(\beta) = (83.5/\Lambda_{\mathrm{mom}}) \exp(-\tfrac{4}{33}\pi^2\beta)(\tfrac{8}{33}\pi^2\beta)^{51/121}, \tag{12}$$

so the constancy (against β) of our results are to be judged in relation to the variation by a factor of 2.5 of $a(\beta)$ in (12) over the same range. We clearly see a good signal of continuum behaviour. In fact the significance of the scaling found here is as good as that of the 0^{++} glueball [23].

If we now set our scale in MeV units by $\Lambda_{mom} = 200$ MeV, as we have done in fig. 3b, we see that we have good numerical agreement with the experimental value for $\langle \bar{u}u \rangle$. One obtains roughly this scale for Λ_{mom} by using the measured [14] ρ mass as input. A scale of $\Lambda_{mom} = 200$ MeV is also consistent with calculations of the gluon condensate [24] and with the best measurements of the string tension [25].

Having provided strong evidence for the continuum breaking of chiral invariance, we briefly return to the strong-coupling regime. It is clear that we have also demonstrated spontaneous chiral symmetry breaking for $d = 4$ and small β. If we now compare with the small β, large d calculations of ref. [7], we see, in fig. 2, that the $d = \infty$ results (dashed line) do *not* agree with our measured values. However, if we include $O(1/d)$ corrections [7] and set $d = 4$, the agreement becomes excellent (solid line). If we go away from $\beta = 0$ we see reasonable agreement up to $\beta = 2.0$, but the strong-coupling series begins to deviate substantially by $\beta = 4.0$ and bears no relation to the measured values for $\beta > 5.0$ as we enter the region of continuum physics.

We return now to the question of what one can learn about $\langle \bar{\psi}\psi(0) \rangle$ from $\langle \bar{\psi}\psi(m) \rangle$ at large, rather than small, m. In fig. 4 we show our measurements of $\langle \bar{\psi}\psi(m) \rangle$ for 8^4 and $4^3 \times 8$ lattices at $\beta = 5.7$ up to $ma = 1.0$. We see that the large difference between 8^4 and $4^3 \times 8$ lattices at *small m* disappears at *larger m*. Indeed it is clear that a calculation with errors $\gtrsim 5\%$, and confined to $ma \geqslant 0.01$, could not distinguish between the $4^3 \times 8$ and 8^4 lattices, which indeed contain very different chiral dynamics. A more serious problem comes with lattice perturbatice pieces, which are very small at small ma, but increase rapidly at larger ma. We plot in fig. 4 the lowest-order perturbative contribution. The extraction of a physical, although ambiguous, $\langle \bar{\psi}\psi \rangle$ can perhaps be obtained by subtracting the perturbative pieces. If we subtract the lowest-order piece, we obtain the dashed–dotted line which extrapolates very differently from the unsubtracted values! This is of course only illustrative: for $ma \geqslant 0.1$ it is clear that one has to calculate at least one order further to check that higher-order perturbative corrections are small. (This is in progress.) Nonetheless it is amusing to observe that almost any extrapolation will, after we take the third root to obtain numbers in MeV units, come to within O(30%) of the value we find with a large lattice. It would appear that although a large-mass extrapolation of the type performed in refs. [9,10] cannot tell you whether chiral symmetry is spontaneously broken or not, if it *is* broken then the value obtained will not be too far from the correct value for $\langle \bar{\psi}\psi \rangle^{1/3}$.

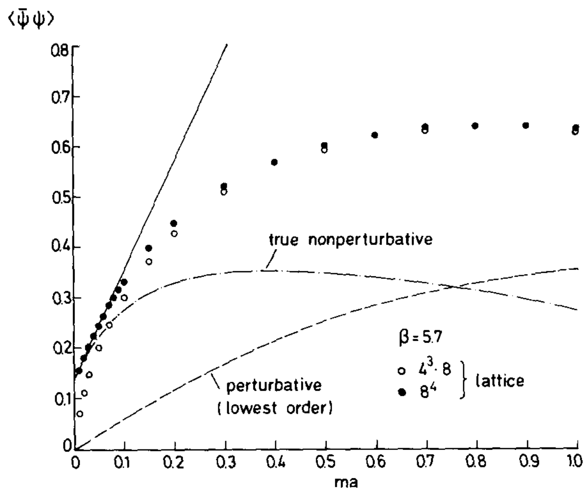

Fig. 4. $\langle \bar{\psi}\psi \rangle$ on the 8^4 and $4^3 \times 8$ lattice for masses up to $ma = 1$. The dashed curve is the lowest-order perturbative contribution to $\langle \bar{\psi}\psi \rangle$ on 8^4. The dashed–dotted curve represents the "true" non-perturbative contribution. The solid line indicates our extrapolation to $\langle \bar{\psi}\psi(0) \rangle$ relying on small quark masses.

The above calculations have all been performed in the quenched approximation. We can consider the first correction in an expansion in the number of flavours, n_f,

$$\langle \bar{\psi}\psi \rangle = \langle \bar{\psi}\psi \rangle_Q \left(1 + n_f \frac{1}{\langle \bar{\psi}\psi \rangle_Q} \left. \frac{d\langle \bar{\psi}\psi \rangle}{dn_f} \right|_Q + O(n_f^2) \right), \tag{13}$$

where Q denotes the quenched ($n_f = 0$ up to an overall factor) value. The first-order correction is

$$\frac{1}{\langle \bar{\psi}\psi \rangle_Q} \left. \frac{d\langle \bar{\psi}\psi \rangle}{dn_f} \right|_Q = \frac{1}{4\langle \bar{\psi}\psi \rangle_Q} \langle (\bar{\psi}\psi - \langle \bar{\psi}\psi \rangle) \times [\ln\det(\mathcal{M} + 2ma) - \langle \ln\det(\mathcal{M} + 2ma) \rangle] \rangle. \tag{14}$$

Our measurements of this quantity are not very accurate (we do not have many configurations for the average) but reveal the expected feature that this correction is *negative* and decreases rapidly for increasing quark masses. (It also is small in the strong-coupling region.) This emphasizes the fact that if one inserts only massive quark loops into the vacuum, this is not going to provide much progress in going beyond the quenched approximation. One has to update with *light* quarks to get at the physics.

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