LATTICE QCD WITH LIGHT QUARK MASSES: DOES CHIRAL SYMMETRY GET BROKEN SPONTANEOUSLY?

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We present a first direct calculation of the properties of QCD for the small quark masses of phenomenological interest without extrapolations. We describe methods specially adapted to invert the fermion matrix at small quark masses. We use these methods to calculate $\langle\bar{\psi}\psi\rangle$ directly on presently used lattice sizes with different boundary conditions. As is to be expected for a finite system, we do not observe spontaneous chiral symmetry breaking. By comparing the results obtained on lattices of different size we see, however, indications that are consistent with eventual spontaneous chiral symmetry breaking in the infinite volume limit. Our calculations underline the importance of using antiperiodic boundary conditions for fermions.

Lattice regularised [1] quantum chromodynamics, together with the Monte Carlo method [2] for generating the vacuum, invites a first principles calculation of the low energy properties of QCD. For such a calculation to be relevant for continuum physics at least the following criteria should be met: (i) an action with the correct (classical) continuum limit should be used; (ii) the action and boundary conditions should preserve positivity [3], so that calculations of correlation functions on finite lattices, at finite lattice spacing, should make sense; (iii) physical values of the bare quark masses should be used; (iv) the $(L_s a_s)^3 \cdot L_t a_t$ lattice should be large enough to accommodate the physics of interest, the lattice spacing should not be too coarse, and the temperature should not be too high. Calculations within the pure gauge theory, e.g. of the glueball mass spectrum [4], do indeed meet these standards.

Calculations with fermions, on the other hand, have made little progress since the first attempts [5] at the hadron mass spectrum, and, like those first efforts, usually satisfy none of our above criteria. Specifically: (i) fermions are not included dynamically in the action – the quenched approximation; (ii) fermions are usually given periodic rather than the correct antiperiodic boundary conditions, which are necessary for positivity; (iii) calculations for light quarks have not been performed for physically realistic values of the masses – convergence problems with the Gauss–Seidel and hopping parameter methods mean that the actual calculations are made for quark masses of hundreds of MeV, and then light quark physics is obtained by means of extrapolations of unknown reliability; (iv) typically the lattice is smaller than the hadron whose mass is being calculated.

In this paper we report on the first results of a program to remedy these defects. Specifically, we shall describe and apply methods for calculating directly with light quark masses. This will enable us to see what is *really* predicted by QCD, on the lattice we work with, without the biases imposed by the extrapolation procedures in the quark mass. We shall also employ the correct boundary conditions for positivity. The impact of not doing so will become apparent. In addition the methods we use enable us to go beyond the quenched approximation because they calculate the fermion determinant for us. In the calculation of this paper we shall, however, not pursue this last point beyond some remarks.

The specific problem we address in this paper is the spontaneous breakdown of chiral symmetry. We shall calculate the condensate $\langle\bar{\psi}\psi\rangle$ down to zero bare quark mass in an attempt to elucidate whether lattice QCD indicates such a spontaneous breakdown or not. Since a finite lattice, being a system with a finite number of degrees of freedom, is not expected to manifest strict spontaneous symmetry breakdown, what one must do is to calculate for different lattice sizes so as to obtain an indication of the infinite volume limit.

The lattice. We work with SU(3) gauge field configurations on $4^3\cdot 8$ and $6^3\cdot 8$ lattices at $\beta=5.7$ ($\beta\equiv 6/g^2$). Using a string tension of $(400\ \mathrm{MeV})^2$ (one gets a similar scale by measuring [‡1] $\langle\alpha_s F_{\mu\nu}F_{\mu\nu}\rangle$ and comparing to the value expected from QCD sum rules [8]) the parameters of our lattices are shown in table 1. The value of β has been chosen with the experience of the glueball spectrum calculations [4] in mind: at this β the glueball is about $2a$ across so that the lattice spacing should be small enough to carry the characteristic nonperturbative fluctuations of the gluon field. Since we expect hadrons with quarks to be about 1 fm across, the physics of such hadrons should, in most respects, be reproducible with such a lattice spacing. The volume of these lattices is less satisfactory; they are large enough for the typical physics of the pure gauge theory, but are smaller than the two pion Compton wavelengths across that is presumably a minimal size for good pion physics. The temperature is adequately low, although it will modify any physics on a scale $\lesssim O$ (100 MeV). We shall use the correct boundary conditions for positivity – antiperiodic for fermions, periodic for the gauge field – except when stated.

[‡1] For recent calculations in SU(3) see ref. [6] and SU(2) see ref. [7].

Table 1
Parameters of the lattices used.

Lattice	Lattice spacing (fm)	Spatial lattice size (fm)	Lattice temperature (MeV)
$4^3\cdot 8$	0.275	1.10	91
$6^3\cdot 8$	0.275	1.65	91

The action. The euclidean lattice QCD action S may be written in terms of gluonic and fermionic pieces as

$$S\equiv S_G+S_F\ , \qquad (1)$$

where

$$S_G=\frac{\beta}{6}\sum_{n,\mu,\nu\neq\mu}\mathrm{tr}(U_{n,\mu}U_{n+\mu,\nu}U^\dagger_{n+\nu,\mu}U^\dagger_{n,\nu})\ , \qquad (2)$$

$$S_F\equiv-\bar{\psi}\,[M(U)+2ma]\,\psi$$
$$=-\sum_{n,\mu}\bar{\psi}_n\gamma_\mu(U_{n,\mu}\psi_{n+\mu}-U^\dagger_{n-\mu,\mu}\psi_{n-\mu})$$
$$-2ma\sum_n\bar{\psi}_n\psi_n\ . \qquad (3)$$

S_G is the standard Wilson action [1]. The fermion action we use is the Kogut–Susskind type [9]. This has the explicit advantage of being chirally symmetric in the massless case which makes it appropriate for our purposes. Here m is the bare quark mass. The matrix M is an $N\times N$ sparse complex matrix where $N=12\,L_s^3L_t$. For the purposes of doing fermion physics the basic technical problem is to calculate the inverse matrix $[M(U)+2ma]^{-1}$ and (if one wants to do better than the quenched approximation) the determinant $\det(M(U)+2ma)$. The huge size of such a matrix leads to problems with memory storage and rounding errors that is a major difficulty with large lattices.

$\langle\bar{\psi}\psi\rangle$. The condensate $\langle\bar{\psi}\psi\rangle$ is the quark propagator at zero spacing (averaged over gauge fields)

$$\langle\bar{\psi}\,\psi(m)\rangle = (3/N)\,\langle \mathrm{tr}(M + 2ma)^{-1}\rangle\,. \tag{4}$$

The statement of spontaneous chiral symmetry breaking is (the order of limits is important)

$$\lim_{m\to 0}\ \lim_{\text{volume}\to\infty}\ \langle\bar{\psi}\,\psi(m)\rangle = \text{constant} \neq 0\,. \tag{5}$$

We can decompose the antihermitean matrix M into

$$M = \Gamma\,\mathcal{M}\,\Gamma^{+}\,, \tag{6}$$

where Γ is a unitary block diagonal matrix containing all the γ factors [10]. Clearly $\mathrm{tr}(M) = 4\,\mathrm{tr}(\mathcal{M})$. Let λ_i, $i = 1, ..., N/4$ 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

$$\langle\bar{\psi}\,\psi(m)\rangle = \frac{12}{N}\left\langle\sum_{i=1}^{N/4}\frac{2ma}{\lambda_i^2 + (2ma)^2}\right\rangle$$
$$\xrightarrow[\text{volume}\to\infty]{} 3\left\langle\int_{-\infty}^{+\infty}\mathrm{d}\lambda\,\frac{2ma\rho(\lambda)}{\lambda^2 + (2ma)^2}\right\rangle\,, \tag{7}$$

for a normalised spectral density $\rho(\lambda)$, and hence

$$\lim_{m\to 0}\ \lim_{\text{volume}\to\infty}\ \langle\bar{\psi}\,\psi(m)\rangle = 3\pi\rho(0)\,. \tag{8}$$

Hence it is the volume dependence of the eigenvalues of M close to zero that determines whether chiral symmetry breaks spontaneously or not. These are the long distance fluctuations of the fermion fields. Hence it will not be important for us to take account of lattice weak coupling subtraction to $\langle\bar{\psi}\,\psi\rangle$ in this particular calculation.

We now describe three methods that will calculate the eigenvalue spectrum, determinant, and inverse. Details of their practical application, including some indispensable tricks for suppressing accumulating round-off errors and for speeding up convergence (in the third method) will be published elsewhere [11].

Lanczos method [12] [‡2]. The Lanczos method will reduce a hermitian matrix, H, to tridiagonal form. One can then diagonalise with a standard library routine for diagonalising tridiagonal matrices. Having done this once for the zero quark mass case, we can then use (7) to obtain $\langle\bar{\psi}\,\psi(m)\rangle$ for all m. The actual algorithm proceeds by constructing for an $N \times N$ matrix N orthonormal vectors $\{v_i\}$ as follows:

$$v_{i+1} = (b_{i+1})^{-1}\,[(H - a_i)v_i - b_i v_{i-1}]\,,$$

$$a_i = v_i^{\dagger} H v_i\,,$$

$$b_{i+1} = |(H - a_i)v_i - b_i v_{i-1}|\,. \tag{9}$$

It is clear from the first relation that applying the unitary matrix $V = (v_0, ..., v_{N-1})$ to H will produce a matrix $T = VHV^{\dagger}$ which is tridiagonal with diagonal elements $a_0, ..., a_{N-1}$ and off-diagonal elements $b_1, ..., b_{N-1}$. Moreover, T and H have the same eigenvalues because the transformation relating them is unitary.

The product of the eigenvalues gives us the determinant, which, used as a weighting factor on the gauge field configurations, will incorporate the vacuum fermion dynamics neglected in the quenched approximation. It is also obvious that one can reverse the above procedure so as to go from the inverted diagonal matrix to H^{-1}.

Exact inverse (simplex method [15]). Let A be a square matrix and let δA be a matrix with just one column non-zero:

$$\delta A_{ij} = a_i \delta_{jr}\,. \tag{10}$$

Then

$$(A + \delta A)^{-1} = (1 + A^{-1}\delta A)^{-1} A^{-1} \equiv TA^{-1}\,,$$

$$T_{ij} = \delta_{ij} - \delta_{jr}(A^{-1}a)_i\,[1 + (A^{-1}a)_r]^{-1}\,. \tag{11}$$

So we can start with the unit matrix and gradually fill in column by column to obtain the inverse of an arbitrary matrix, M. It will not work, however, if M has any zeroes on the diagonal. This means that the quark mass must be non-zero. Since the method works well down to very small masses this is not a serious restriction. The advantage of this particular inversion method is its numerical stability (resistance to round-off errors). The main defect is that it requires the inverse to be stored at every state, which is not a problem on a $4^3 \cdot 8$ lattice but becomes prohibitive for much larger lattices.

Conjugate gradient method [16]. This method will solve

$$Ax = b \tag{12}$$

[‡2] For nuclear physics applications see ref. [13]. For condensed matter applications see ref. [14].

for a given $N \times N$ matrix A and vector $\boldsymbol{b}$. The solution proceeds iteratively and is guaranteed (barring round-off errors) to give the exact solution within N steps. To obtain the inverse we solve the N such equations where the $\boldsymbol{b}$ are the columns of the unit matrix. The method requires A to be positive definite. Since our fermion matrix is not, we present the more general version of the algorithm which solves

$$A^\dagger A\boldsymbol{x} = A^\dagger \boldsymbol{b} . \tag{13}$$

To solve (13) we obtain a sequence of vectors $\boldsymbol{x}_i$ which converge to $\boldsymbol{x}$. The algorithm proceeds as follows. Choose some initial vector $\boldsymbol{x}_0$. Then

$$\boldsymbol{x}_{i+1} = \boldsymbol{x}_i + \alpha_i \boldsymbol{p}_i , \tag{14}$$

where

$$\boldsymbol{p}_0 = A^\dagger \boldsymbol{r}_0 , \quad \boldsymbol{r}_0 = \boldsymbol{b} - A\boldsymbol{x}_0 ,$$

$$\boldsymbol{p}_{i+1} = A^\dagger \boldsymbol{r}_{i+1} + \beta_i \boldsymbol{p}_i , \quad \boldsymbol{r}_{i+1} = \boldsymbol{r}_i - \alpha_i A\boldsymbol{p}_i ,$$

$$\alpha_i = |A^\dagger \boldsymbol{r}_i|^2/|A\boldsymbol{p}_i|^2 , \quad \beta_i = |A^\dagger \boldsymbol{r}_{i+1}|^2/|A^\dagger \boldsymbol{r}_i|^2 . \tag{15}$$

We have found this method to be far more efficient for small quark masses than the Gauss–Seidel or Neumann iterative schemes. By comparing with the exact inverse (previous section) on a $4^3 \cdot 8$ lattice we see that even with 5 MeV quarks the method is well converged for all elements within $\simeq 100$ iterations. Unlike the exact inverse, however, this method is practical for larger lattices [11].

Relevance of the quenched approximation. We will work in the quenched approximation because it makes the calculation more tractable. What will our results have to do with the full dynamical theory? It is sometimes argued that the success of the simplest quark spectroscopy for hadrons implies that the quenched approximation must be good. This argument is, however, spurious: it might just imply that gauge fields fall mainly into two classes, one of which suppresses fermion loops, while the other is suppressed *by* fermion loops. If one neglects fermion loops altogether, this latter class of gauge fields will be suppressed no longer and could easily alter the physics. One can make up examples of this involving (continuum) configurations with instantons.

The constructive remark we wish to make comes from the following observation: a small eigenvalue of the fermion matrix will, in the quenched approximation, lead to a large contribution to $\langle\bar\psi\psi\rangle$ [as is clear from (7)], while in the full theory this effect will be reduced by the presence of the same small eigenvalue in the numerator from the determinant. This suggests that spontaneous symmetry breakdown occurs more readily in the quenched than in the full theory:

$$|\langle\bar\psi\psi\rangle|_{\text{quenched}} \geqslant |\langle\bar\psi\psi\rangle|_{\text{QCD}} . \tag{16}$$

So if QCD breaks chiral symmetry spontaneously, this will be visible in the quenched approximation. We now turn to our results on $\langle\bar\psi\psi\rangle$.

Results. Our results are based on measurements performed upon two $4^3 \cdot 8$ lattice gauge field configurations and one $6^3 \cdot 8$ configuration. Since we calculate $\bar\psi\psi$ at every site of each lattice, we have in fact made thousands of measurements of this quantity, and our statistical errors are very small. We are able to obtain reliable results on very few lattice configurations because one finds that the fermion physics varies very little for different gauge field configurations (see below). We remark that the two $4^3 \cdot 8$ configurations are completely independent. They were generated from independent starting configurations and were then iterated through some 4000 configurations using the SU(3) heat bath algorithm.

Using the Lanczos algorithm we have calculated the complete eigenvalue spectrum $\rho(\lambda)$ of each $4^3 \cdot 8$ configuration. The similarity of the two spectra is remarkable. Is this perhaps just an effect of the quenched approximation? To answer this we have calculated the ratio of the determinants for the two configurations as a function of the bare quark mass which turns out to be of O(1). So we conclude that the similarity will persist even if we include fermion vacuum fluctuations.

In fig. 1a we plot $\langle\bar\psi\psi(m)\rangle$, averaged over the two $4^3 \cdot 8$ configurations, as obtained from the above eigenvalue spectrum (Lanczos), the exact inverse method and the conjugate gradient method. Note that in all three cases we get identical results which prove the accuracy of our methods. For comparison reasons we also have plotted the results of the more popular pseudo-fermion Monte Carlo method [17] of inverting matrices, for which we have written a heat bath algorithm [11]. It is apparent that this last method is less efficient than the others (while it needs the same amount of computer time). The two individual configurations showed only tiny differences at

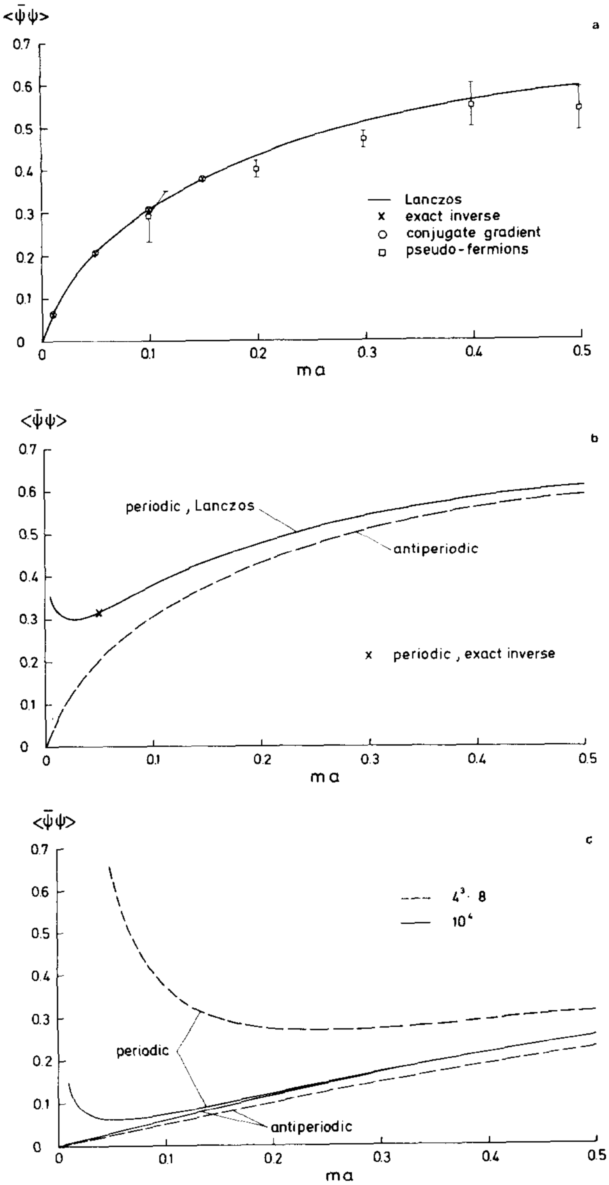

Fig. 1. (a) $\langle\bar{\psi}\psi\rangle$ on $4^3 \cdot 8$ for antiperiodic boundary conditions averaged over configurations 1 and 2. (b) $\langle\bar{\psi}\psi\rangle$ on $4^3 \cdot 8$, periodic versus antiperiodic boundary conditions. (c) $\langle\bar{\psi}\psi\rangle$ for free theory, periodic versus antiperiodic boundary conditions and volume dependence.

small masses ($\lesssim 5\%$) which underlines that the fermion physics indeed varies very little for different gauge field configurations.

We observe that, as expected for a finite lattice, $\langle\bar{\psi}\psi(m)\rangle_{m\to 0} \to 0$. More to the point, we can see no obvious break in the curve that might mark the onset, at lower masses, of finite size effects (and which might motivate an infinite volume extrapolation). The lesson is that the physics of a single small lattice provides no unprejudiced guidance as to the infinite volume limit of $\langle\bar{\psi}\psi\rangle$ at zero mass. The only reliable approach is to obtain the volume dependence directly by working on lattices of differing sizes.

Before proceeding to that, it is interesting to redo the above calculations with the (incorrect) periodic fermion boundary conditions which have been extensively used in the recent literature. In fig. 1b we compare $\langle\bar{\psi}\psi(m)\rangle$ for the two types of boundary condition. The change is drastic. It is clear that imposing periodicity on the fermion fields increases the number of small eigenvalues. In particular, the smallest eigenvalue is a factor of ten smaller than in the antiperiodic case ($\lambda_{min} = 0.007$ versus $\lambda_{min} = 0.07$) so that although $\langle\bar{\psi}\psi\rangle$ does tend to zero at zero quark mass it does so at such small masses that the turnover is not visible on the scale of the figure.

To understand what is happening we repeat these calculations for the free fermion theory (all link elements are unit matrices). In fig. 1c we plot $\langle\bar{\psi}\psi(m)\rangle$ for both boundary conditions. The relative behaviour of the two curves is similar to that of the interacting case but even more pronounced. Here, however, it is easy to understand the difference. The minimum momentum on a periodic lattice is zero, but is non-zero on an antiperiodic lattice:

$$(p_\mu)_{min} = 0 \quad \text{periodic}\,,$$
$$= \pi/L_s a \quad \text{antiperiodic}\,, \qquad (17)$$

and this translates, via (7), into

$$\lim_{m\to 0} \langle\bar{\psi}\psi(m)\rangle = \infty \quad \text{periodic}\,,$$
$$= 0 \quad \text{antiperiodic}\,. \qquad (18)$$

In $\langle\bar{\psi}\psi\rangle$ this zero eigenvalue contributes with a coefficient of $O(1/N_s)$, where N_s is the number of sites in the lattice. Hence the difference between the two sets of boundary conditions disappears in the large volume limit (compare the $4^3 \cdot 8$ and 10^4 lattice curves in fig. 1c) and

$$\lim_{m\to 0} \lim_{N_s\to\infty} \langle\bar{\psi}\psi(m)\rangle = 0\,, \qquad (19)$$

so that (fortunately) chiral symmetry is not spontaneously broken in the free field theory.

It is very plausible that it is the same effect, smeared out by the presence of interactions, that produces the difference between the curves in fig. 1b. So we expect that

$$\langle\bar{\psi}\psi\rangle_{\text{periodic}} \xrightarrow[\text{volume}\to\infty]{} \langle\bar{\psi}\psi\rangle_{\text{antiperiodic}}\,, \tag{20}$$

which indeed is consistent with our later results.

The correct way to proceed at this point is to perform the calculation for several lattices of increasing volume, and to see if an envelope develops for the $\langle\bar{\psi}\psi(m)\rangle$ curves which naturally extrapolates to a non-zero value at zero mass. One then repeats the calculation at several values of β to check for renormalisation group behaviour.

To take the first step in this program we have repeated our measurements on a $6^3 \cdot 8$ lattice, which has a volume of $\approx$3.5 times that of the $4^3 \cdot 8$ lattice. In fig. 2a we plot $\langle\bar{\psi}\psi(m)\rangle$ for a single $6^3 \cdot 8$ gauge field configuration, together with the average for the two $4^3 \cdot 8$ configurations. The difference is in a direction consistent with eventual spontaneous symmetry breaking. In fig. 2b we compare the small eigenvalue spectrum of the $4^3 \cdot 8$ and $6^3 \cdot 8$ configurations. We observe that the $6^3 \cdot 8$ density extends to lower eigenvalues, while scaling roughly for larger eigenvalues. This is of course precisely the trend required for eventual spontaneous chiral symmetry breaking.

Let us now return to (20). We have repeated our calculation on the $6^3 \cdot 8$ lattice for periodic boundary conditions. The result is plotted in fig. 2c which shows that in the interacting theory as well the difference between the two sets of boundary conditions gradually disappears in the large volume limit, though it might take quite a big lattice until the two curves meet for physical quark masses. The practical observation here is that the case with periodic fermion boundary conditions shows much stronger finite size effects and hence, for this reason also, is dangerous to use.

Final remarks. We observe that presently used small lattices do not reproduce the desired chiral symmetry – and hence pion – properties of QCD. Calculations with Wilson fermions, which do not contain the quark mass explicitly, use that value of the hopping parameter, K, which reproduces the experimental ρ/π ratio. For the small lattices used, this forces the calculation into an unphysical region of mass parameters and may very well destabilise the calculated spectrum. We prefer to use an action where the quark mass is a variable, and to be realistic about how well we can deal with the pion.

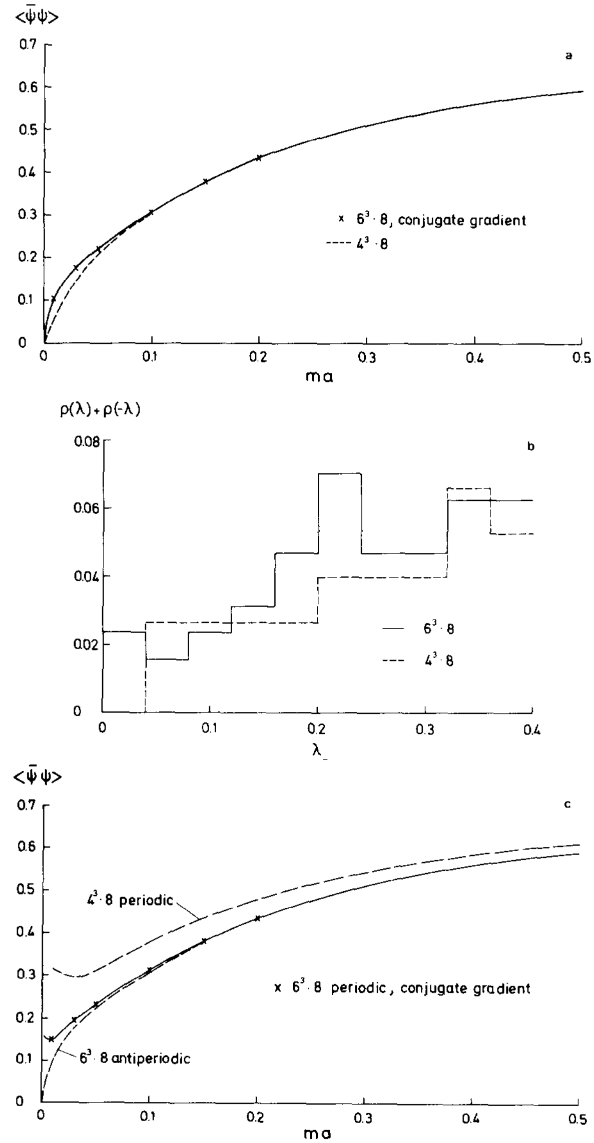

Fig. 2. (a) $\langle\bar{\psi}\psi\rangle$ for antiperiodic boundary conditions, $6^3 \cdot 8$ versus $4^3 \cdot 8$. (b) Eigenvalue spectrum at small λ for antiperiodic boundary conditions, $6^8 \cdot 8$ versus $4^3 \cdot 8$. (c) $\langle\bar{\psi}\psi\rangle$ on $6^3 \cdot 8$, periodic versus antiperiodic boundary conditions and volume dependence.

In a forthcoming paper we complement the present discussion with a similarly realistic calculation of the hadron spectrum on a large lattice, using the methods described herein. We shall also use our measurements of the determinant to go beyond the quenched approximation.

We have presented the algorithms for our methods of calculating at physically realistic quark mass in sufficient detail so as to make them useful for the reader who wishes to perform lattice QCD calculations without ad hoc extrapolations.

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