Simulating lattice fermions by microcanonically averaging out the nonlocal dependence of the fermionic action

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We attempt to increase the efficiency of simulations of dynamical fermions on the lattice by calculating the fermionic determinant just once for all the values of the theory's gauge coupling and flavor number. Our proposal is based on the determination of an effective fermionic action by the calculation of the fermionic determinant averaged over configurations at fixed gauge energy. The feasibility of our method is justified by the observed volume dependence of the fluctuations of the logarithm of the determinant. The algorithm we have used in order to calculate the fermionic determinant, based on the determination of all the eigenvalues of the fermionic matrix at zero mass, also enables us to obtain results at any fermion mass, with a single fermionic simulation. We test the method by simulating compact lattice QED, finding good agreement with other standard calculations. New results on the phase transition of compact QED with massless fermions on 6^4 and 8^4 lattices are also presented.

I. INTRODUCTION

The last few years have seen a great refinement in the quality of numerical results obtained by lattice-field-theory calculations. Improvements in computer performance, statistics, numerical techniques, and theoretical methods, all converged to a clearer understanding of Abelian and non-Abelian field theories, provided that a certain simplification was imposed; namely, that of ignoring either the effects of fermions (pure gauge theory) or the effects of sea fermions (quenched field theory). In the above framework we now have consistent results for reasonably large lattices and nonperturbative values of the inverse gauge field couplings β. A problem arises when the effect of sea fermions is included in the form of the fermionic determinant of the theory. The action then becomes nonlocal and its simulation requires exceptional computing resources by today's standards.

The confrontation of this problem has been the object of considerable research efforts in the last few years, which followed two main directions: (1) the construction of custom-made computers which are more or less dedicated to lattice field theory (see Ref. 1 and references therein) and (2) the development of faster algorithms (see Ref. 2 and references therein). The results of algorithm development have been positive in that the earlier proposals involved computational costs of $O(V^2)$,[3,4] whereas now we have at our disposal algorithms with a theoretical cost of almost $O(V)$, such as the hybrid algorithm[5] or hybrid Monte Carlo[6] algorithm.

Impressive as this progress may sound, we are still far from resolving the problem. The costs quoted above are theoretical order-of-magnitude estimates of the dependence of the calculation on the lattice volume V. In realistic calculations, the cost is augmented by several other factors. One is critical slowing down, for which some remedies have been proposed such as Fourier acceleration[7] and lower-upper decomposition of the fermion matrix.[8] Another problem is the number of parameters that characterize a field theory. These are normally the fermion mass m, the inverse gauge coupling β, and the number of flavors N_f. In order to tackle a typical lattice problem, the calculation must be repeated for, say, M mass values, B gauge couplings, and sometimes for F different numbers of flavors. Thus, the real cost of the computation is $C_1 C_2 V^p$, where C_1 is a factor that depends on the algorithm and the theory's parameters, p is the volume dependence already discussed above (both C_1 and p include critical slowing down effects) and $C_2 = M \times B \times F$ is the repetition factor (i.e., the total number of the theory's parameters for which we have to repeat the calculation). The considerable progress we have sketched above involves a reduction of C_1 and p by the development of fast algorithms and acceleration techniques.

The object of this paper, which is a more extensive and detailed version of a previous publication,[9] is to propose a method to reduce C_2 which will give, in addition, good results for C_1 also in that critical slowing down is controlled. In other words, we seek to find ways of not having to repeat the numerical simulation for different values of at least one of the theory's parameters.

At this point we wish to stress that, in exploring such possibilities, we have implemented exact diagonalization algorithms which are at least $O(V^2)$. We are fully aware that this is a weakness that has to be dealt with as we move to larger volumes, but, at least for the physics explored so far, our method turned out to be much faster than the fast algorithms.

We have carried out two attempts. The first consists of expressing the determinant as a power series of the mass. Then the partition function and any observables (we shall mainly consider $\langle\bar{\psi}\psi\rangle$) may be expressed as a function of a power series in m, the coefficients of which are quenched averages and depend solely on β and the eigenvalues of the massless fermion matrix. Thus, the simulation is performed once for all masses and the repetition factor is $C_2=B\times F$. This method, although very promising in theory, turns out to be a disaster in the physically interesting cases. In particular, near the critical points of the theory, the importance sampling of the pure gauge action misses the neighborhood of the configuration space that contributes most and the results in the critical region are wrong.

The second method consists of reexpressing the theory in terms of an "averaged" determinant which is a function of the system's energy and the mass (all other dependences are averaged out). This "averaged" determinant is then calculated numerically for a wide energy range, either at a fixed mass or by means of the determination of all the zero-mass eigenvalues of the fermionic matrix. Since the determinant does not depend on β, this calculation, which is the costliest, is performed only once in the second case or once for each mass in the first case.

We then use this result in a standard simulation of the reexpressed theory; the determinant is now a known function of the energy and the pure gauge part is not costly to simulate. The repetition factor is essentially reduced to $C_2=1$ or $C_2=M$. The number of flavors enters trivially in this formulation and does not increase the computational cost significantly. This method has given results in agreement with more traditional approaches.

In order to test our proposals, we have used our methods in order to study the compact unquenched U(1) lattice theory and, in particular, its chiral phase transition already studied with the pseudofermion method by Azcoiti *et al.*,[10] and in more detail by Dagotto and Kogut[11,12] (DK). DK have used both deterministic and stochastic algorithms and comparison of their results to ours will give evidence of the accuracy and efficiency of the method we propose.

The paper is divided into five sections. Sections II and III are a presentation of the two methods we propose for the inclusion of dynamical fermions in the theory. We also speculate on whether these are going to work in practice, and discuss their advantages and disadvantages. In Sec. II we present the results obtained with the first method (henceforth termed naive) on the chiral condensate. On the face of discrepancy between our results and those of Ref. 11, we discuss in Sec. III the reasons for which the naive method fails. In Sec. IV we present our results obtained with the second method on the chiral condensate, the plaquette energy, and the specific heat for the case $N_f=4$ and $m=0.1$, $m=0.0$. These are found in excellent agreement with the results of Refs. 11 and 12 in the $m=0.1$ case. Section IV also contains results on the same physical observables for different number of flavors. We have performed all the above simulations on 6^4 lattices, and present some results for the 8^4 case. Finally, Sec. V contains our conclusions.

II. THE NAIVE METHOD

We consider, for simplicity, the partition function of the Abelian case; what follows can be easily generalized to any unitary gauge group:

$$\begin{aligned} Z&=\int[d\bar{\psi}][d\psi][dU]e^{+S_f}e^{\beta S}\\ &=\int[dU]\det\Delta(U,m)e^{\beta S}\ , \end{aligned} \tag{2.1}$$

where S_f is the Kogut-Susskind fermionic action,

$$\begin{aligned} S_f=&m\sum_x\bar{\psi}(x)\psi(x)\\ &+\tfrac{1}{2}\sum_{x,\mu}\eta_\mu(x)\bar{\psi}(x)[U_\mu(x)\psi(x+\mu)\\ &-U_\mu^*(x-\mu)\psi(x-\mu)]\ ,\\ \eta_\mu(x)=&(-1)^{x_1+\cdots+x_{\mu-1}}\ , \end{aligned} \tag{2.2}$$

and S is the pure-gauge Wilson action,

$$S=\sum_{\rm pl}\mathrm{Re}U_{\rm pl}\ . \tag{2.3}$$

$\Delta(U,m)$ is the lattice Dirac operator whose determinant appears when we integrate out the fermionic Grassmann variables.

The form of Z suggests its calculation by Monte Carlo (MC) methods by measuring the average of $\det\Delta(U,m)$ in pure-gauge configurations generated according to the pure-gauge probability distribution $[dU]e^{\beta S}$. We will refer to this method as the "naive" one: we will show in the following that, although in the strong- and weak-coupling regimes it gives correct results, it is bound to give wrong results in the physically interesting intermediate-coupling region.

The method consists in computing the partition function Z at some fixed value of the bare coupling constant β; thermodynamic functions such as the chiral condensate $\langle\bar{\psi}\psi\rangle$ and the specific heat $C_m=d/(dm)\langle\bar{\psi}\psi\rangle$ are then obtained as derivatives of $\ln Z$. To this effect we can define

$$\overline{Z}=\frac{\int[dU]\det\Delta(U,m)e^{\beta S}}{\int[dU]e^{\beta S}}=\langle\det\Delta(U,m)\rangle_{\rm PG}\ . \tag{2.4}$$

It is obvious from expression (2.4) that the logarithmic derivatives of $\overline{Z}$ with respect to m are just the same as those of Z. Then our program is to compute numerically the vacuum expectation value of the fermionic determinant with the probability distribution of the pure-gauge theory and subsequently to obtain the chiral condensate and specific heat by differentiating $\overline{Z}$.

In order to have a better understanding of what we are

really computing when we calculate expression (2.4), let us recall the properties of the lattice Dirac operator. The fermionic determinant is a gauge-invariant operator which only has even powers of m because of the symmetries of the Δ matrix. The gauge-invariance properties of $\det\Delta$ allow us to construct, in a simple way, the coefficients of the polynomial given by expression (2.4).[13,14] Indeed, we can write

$$\langle \det\Delta(U,m)\rangle_{\mathrm{PG}} = m^V + a_1 m^{V-2} + \cdots + a_{V/2-1} m^2 + a_{V/2} , \quad (2.5)$$

where a_1 is proportional to the pure-gauge vacuum expectation value of the sum of all gauge-invariant loops of perimeter 2; that is to say, the number of lattice links. In general, the coefficient a_i will be proportional to the vacuum expectation value of the sum of all combinations of gauge-invariant loops with total perimeter $2i$ which do not touch (otherwise their contribution to the determinant is zero). The sign of these sums is always positive if we take the Kogut-Susskind phases in the correct way. We note, in passing, that similar expansions of the determinant have been used, for instance, in quantum chromodynamics (QCD) finite-density simulations.[15]

Thus, the numerical evaluation of expression (2.4) amounts to computing the vacuum expectation values of all loops of a perimeter less than or equal to the lattice volume V. It is clear that the computation of a_i will suffer, near the transition point, from large statistical errors for large values of i, since in this case we are dealing with large loops.

The $\beta=0$ case can, in principle, be solved analytically[14] since the vacuum expectation values of loops of the nonzero area is zero. Then we get

$$a_i(\beta)|_{\beta=0} = \left(\tfrac{1}{2}\right)^{2i} \text{ number of combinations of } i \text{ disconnected links on the lattice .}$$

In the following we describe in more detail how we perform the numerical computation of (2.4). We generate equilibrium configurations at some fixed value of β with the probability distribution of the pure-gauge theory, separated by 1000 MC gauge sweeps. We compute for these configurations all the eigenvalues of the fermionic matrix Δ at $m=0$. All the coefficients of the fermionic determinant are then, in principle, known and, in fact, they can be computed iteratively from the eigenvalues; averaging them over the configurations, we get the numerical value of expression (2.4).

The first numerical results we report concern the $\beta=0$ case. This particular value of β is interesting because we can compare with analytic calculations. In fact, as we mentioned before, the $\beta=0$ case can be reduced to the combinatorial problem of finding the number of disconnected link configurations we can construct in a hypercubic lattice of volume V. This problem can be easily solved in the smallest lattice (2^4). In Table I we compare the rigorous results for the coefficients of the partition function (2^4 lattice) to the numerical results obtained applying the "naive" method to the evaluation of expression (2.4). The agreement is excellent. In Fig. 1 we plot our results for the chiral condensate at $\beta=0$ and 2^4, 4^4, 6^4, and 8^4 lattices. The top (straight) line in Fig. 1 is an analytic prediction.[16,10] The agreement between the analytic and numerical calculations is good and gets better for lower values of the fermion mass, at larger lattice volumes.

We have further compared our results in the deep strong-coupling region with those obtained in Ref. 17 with the pseudofermion (PF) method. The authors of Ref. 17 measured the fluctuations of the trace of the inverse fermionic matrix by the PF method and found a peak around $m=0.11$ for this quantity in the confining phase, the height of the peak being independent of the lattice size. We have done the same calculation using our method and we have found that, in the 2^4 lattice, there is a peak around $m=0.1$ in the strong-coupling phase but it moves quickly to the left and its height increases rapidly with increasing lattice size.

In Fig. 2 we compare the results for the normalized fluctuations of the trace of the inverse fermionic matrix obtained with the pseudofermion method[17] with those obtained with our method (solid line in the figure); the peak in this quantity is localized around $m=0.002$, $\beta=0.1$ in the 4^4 lattice in contrast with the value ($m=0.11$) obtained with the PF algorithm. This disagreement can probably be attributed to convergence problems of the pseudofermion method at small masses.

We have also done a simulation in the large-β region checking that the chiral condensate approximates the free case when β increases. Having checked that this method is in good agreement with the analytical predictions in the $\beta\to 0$ as well as $\beta\to\infty$ limits, we have performed simulations at several values of β in order to compare with existing standard calculations. In Fig. 3 we plot our results for the chiral condensate as a function of β at two representative values of the fermionic mass ($m=0.05$ and 0.1) for a 6^4 lattice. At these intermediate couplings, our results start differing from those in the literature: for instance, the critical value β_c for the chiral transition seems to be independent from the fermion mass and approaches the critical value of the quenched theory

TABLE I. Coefficients of the partition function $\overline{Z}$ at $\beta=0$ in the 2^4 lattice.

i	a_i rigorous	a_i Monte Carlo algorithm
1	16	16.03(6)
2	100	100.4(8)
3	312	314(4)
4	516	521(8)
5	444	450(10)
6	182	185(5)
7	29	30(1)
8	1.0625	1.08(11)

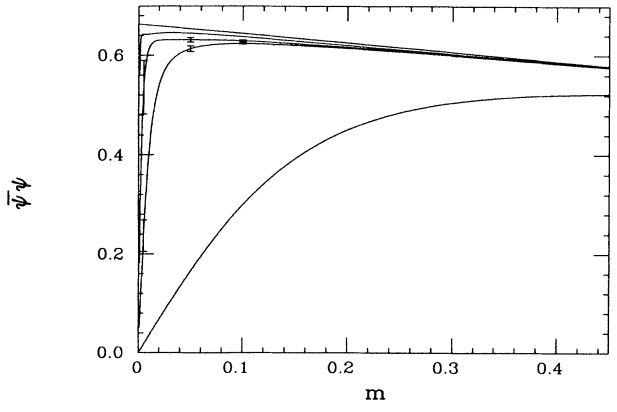

FIG. 1. Results for $\langle\bar{\psi}\psi\rangle$ at $\beta=0$ for 2^4 (exact), 4^4 (467 meas.), 6^4 (584 meas.), and 8^4 (8 meas.) lattices: the top (straight) line is the analytic prediction of Ref. 16.

β_c^Q when the lattice size increases. The independence of β_c from the fermionic mass has also been observed by plotting the specific heat C_m as a function of m and checking that this quantity shows a single maximum at $m=0$. These results are in disagreement with those of Dagotto and Kogut in the sense that our β_c in the 6^4 lattice at $m=0.1$ is $\beta_c=0.993(3)$ to be compared to the values $\beta_c=0.890$ (stochastic method) and $\beta_c=0.873$ (deterministic method) reported in Ref. 11.

In conclusion, the situation of the method exposed above is the following.

(i) In the weak- and strong-coupling limits, the numerical results show a good agreement with analytical predictions.

(ii) At intermediate values of the coupling constant we find significant differences between our results on the chiral condensate and those obtained with the use of standard methods. The possible origin of these discrepancies will be discussed in the next paragraph.

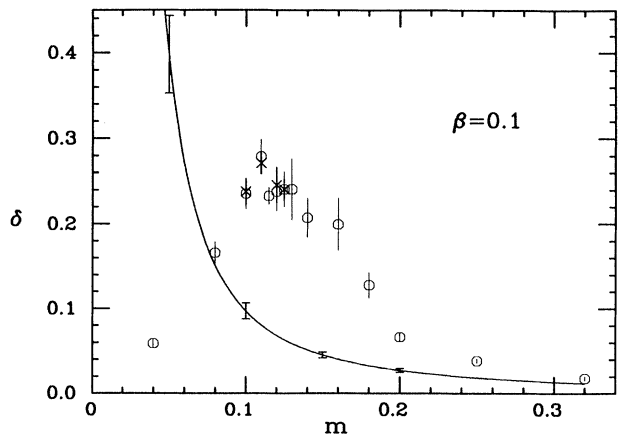

FIG. 2. $(1/V)[\langle(\mathrm{Tr}\Delta^{-1})^2\rangle-\langle\mathrm{Tr}\Delta^{-1}\rangle^2]$ vs m at $\beta=0.1$ and one flavor. The solid line reports our results for a 4^4 lattice. The circled (crossed) points are the results of Ref. 17 obtained with the PF algorithm in 4^4 (8^4) lattices, respectively.

III. DESCRIPTION OF OUR PROPOSAL

In the previous section we have presented a detailed exposition of a way for including dynamical fermions, based on the computation of the mean value of the fermionic determinant averaged over gauge configurations generated with the pure-gauge probability distribution. As was pointed out, proceeding in this way one can introduce a strong bias in the determination of the full partition function because of the very large fluctuations of the fermionic determinant, especially near the transition point.

In this section, we propose a (possibly) better method which is a highly modified version of the previous one. Our new proposal[9] tries to overcome the problem of the large fluctuations of the fermionic determinant, which are directly connected with the importance sampling problem. It consists of the determination of an effective fermionic action as a function of the plaquette energy and fermion mass which can subsequently be used to perform numerical simulations of an equivalent pure-gauge theory, measuring the various physical quantities for every value of the coupling constant β and/or for arbitrary number of flavors.

To illustrate the method, let us consider the partition function of compact quantum electrodynamics (QED).

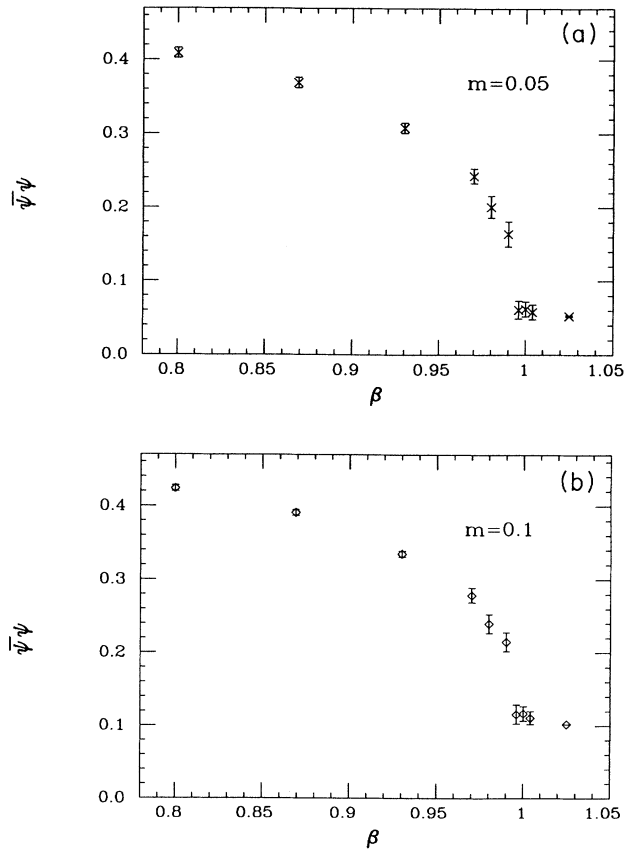

FIG. 3. $\langle\bar{\psi}\psi\rangle$ vs β for a 6^4 lattice at (a) $m=0.05$ and (b) 0.10.

From the discussion in the previous paragraph, the determinant of the lattice Dirac operator can be written as

$$\det\Delta(m,U)=\det\Delta(m,S(U),S_i(U)) , \tag{3.1}$$

where $S(U)$ is the pure gauge action and $S_i(U)$ is the collection of all other gauge-invariant operators necessary to build up the coefficients $a_n(U)$ of the fermionic determinant with $n>2$. Using relation (3.1), the partition function (2.1) can be written as

$$\begin{aligned} Z&=\int [dU]\delta(S(U)-E)\left[\prod_i \delta(S_i(U)-E_i)\right] \\ &\quad\times e^{\beta E}\det\Delta(m,E,E_i)dE\prod_i dE_i \\ &=\int \left[\prod_i dE_i\right] dE\, N(E,E_i)e^{\beta E}\det\Delta(m,E,E_i) \end{aligned} \tag{3.2}$$

with

$$N(E,E_i)=\int [dU]\delta(S(U)-E)\prod_i \delta(S_i(U)-E_i)$$

the density of states of fixed "energies" E,E_i. Defining then the average value of the fermionic determinant at fixed energy E

$$\overline{\det\Delta}(m,E)=\frac{\int \left[\prod_i dE_i\right] N(E,E_i)\det\Delta(m,E,E_i)}{\int \left[\prod_i dE_i\right] N(E,E_i)} , \tag{3.3}$$

one gets, for the partition function,

$$Z=\int dE\, N(E)e^{\beta E}\overline{\det\Delta}(m,E)=\int [dU]e^{-S_{\text{eff}}} , \tag{3.4}$$

where $N(E)$ is the density of states at energy E:

$$\begin{aligned} N(E)&=\int \left[\prod_i dE_i\right] N(E,E_i) \\ &=\int [dU]\delta(S(U)-E) . \end{aligned} \tag{3.5}$$

Equations (3.4) and (3.5) define an effective action

$$S_{\text{eff}}=-\beta S(U)-\ln\overline{\det\Delta}(m,S(U)) . \tag{3.6}$$

The method we propose consists in determining $\ln\overline{\det\Delta}(m,E)$ numerically, as a function of the energy E, and then in performing a numerical simulation of the equivalent pure-gauge model (3.6) in order to measure thermodynamical quantities. The first step consists in the generation of gauge configurations at fixed energy E with a microcanonical process and in the determination of the average fermionic determinant over the different configurations generated. By repeating the procedure for different values of E, one finally gets an expression for $\ln\overline{\det\Delta}(m,E)$ by means of an interpolation of the points obtained.

Since the numerical determination of the expression (3.3) is the crucial step of our method, some discussion about the feasibility of this computation is in order. The nonlocal character of the fermionic determinant implies that, computing the fermionic determinant on configurations generated with the pure-gauge probability distribution at a fixed β, one has large fluctuations that make its computation, from a finite sample of points, very difficult. On the other hand, by fixing the energy of the configurations over which the determinant is computed, a large part of the fluctuations disappear. This can be explained by considering that all the coefficients of the fermionic determinant contain a term proportional to the pure-gauge action with, in general, large coefficients; moreover, fixing the energy prevents the system, near the phase transition, from fluctuating between different vacua, reducing the fluctuations of larger loops. The remaining fluctuations are associated with changes in the gauge configuration that leave the average energy per plaquette (but not more complicated loops) constant.

In these circumstances the quantity of importance is the amount of computer time needed to measure $\ln\overline{\det\Delta}(m,E)$ with the precision necessary for the method to lead to reasonable results. The answer to this question is, in general, far from trivial; however, a simple analysis of the feasibility of the method can be carried out under some general assumptions. Figure 4 shows the probability distribution of the logarithm of the fermionic determinant at $m=0.1$ and $E/(6V)=0.5103$ for a 4^4 lattice. As can be seen, the histogram can be very well approximated by a Gaussian (solid line).

Based on this result, let us consider a toy model in which the probability distribution $P_E(x)$ of the logarithm of the fermionic determinant at energy E is described by a Gaussian function

$$P_E(x)=Ce^{-\alpha(x-x_0)^2} , \tag{3.7}$$

where C is a normalization constant and α and x_0 are parameters which depend on the volume V, the energy E, and fermion mass m. From the above distribution, one can obtain, through an elementary calculation,

$$\ln\overline{\det\Delta}(m,E)=x_0+\frac{1}{4\alpha} . \tag{3.8}$$

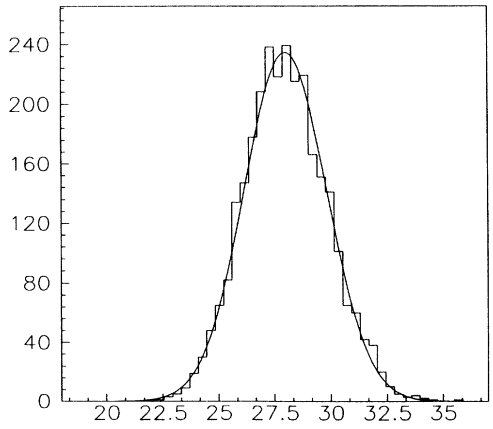

FIG. 4. Probability distribution of the logarithm of the fermionic determinant at fixed energy for a 4^4 lattice; superimposed (solid line) a Gaussian distribution.

Since x_0 is the average value of the logarithm of the determinant at energy E, $x_0 = \ln \det \Delta(m,E)$, it will, in general, be a linear function of the volume V, thus giving a contribution to the effective action (3.6) of the same order as the pure-gauge term. The crucial point is the dependence of α, i.e. of the width of the Gaussian (3.7) on V. Let us assume that $\alpha \to 0$ as $V^{-\nu}$ when $V \to \infty$. There are three possibilities.

(i) $\nu > 1$. Then $1/4\alpha$ diverges as V^{ν} and in the thermodynamical limit this will be the dominant contribution to the effective action (3.6).

(ii) $\nu = 1$. Then $1/4\alpha$ is comparable to x_0 as well as to the pure-gauge term.

(iii) $\nu < 1$. Then the contribution of $1/4\alpha$ disappears in the thermodynamical limit.

Case (i) will certainly be surprising, since it will imply that, in the thermodynamical limit, the physical results do not depend on the gauge coupling constant. Case (ii) is the most probable from a statistical point of view, but even (iii) is not absurd, since it implies that the fluctuations of the logarithm of the determinant are damped as a consequence of the fixing of the energy of the configurations.

In Fig. 5 we show the behavior of the fluctuations of the logarithm of the fermionic determinant for $m = 0.1$ [Fig. 5(a)] and $m = 0.0$ [Fig. 5(b)] as a function of $E/6V$ in 4^4, 6^4, and 8^4 lattices. The weak dependences of the fluctuations on the volume which one observes, even at $m = 0$, seem to favor the behavior described in (iii); in which case, the contribution of $1/4\alpha$ to the effective action is a pure volume effect, in the sense that it will disappear in the large-volume limit. This result provides a justification of the feasibility of the numerical computation of $\ln \det \Delta(m,E)$. The interpretation of the results shown in Fig. 5 in the light of the Gaussian model, though not providing a rigorous proof, suggests that the method proposed can be applied, with reasonable amount of computer time, to realistic models and larger lattices.

Before going on, let us discuss in the light of our numerical results for the effective fermionic action, the feasibility of the method reported in the previous paragraph. Figure 6 shows the numerical results obtained for $\ln \det \Delta(m,E)$ in 6^4 lattices as a function of the normalized plaquette energy at typical values of the fermion mass ($m = 0.01$ and 0.0). The details of the numerical simulation can be found in the next paragraph.

From the results plotted in Fig. 6, it follows that the effective fermionic action is a smooth function of the plaquette energy for $E < 0.5$ and for $E > 0.68$, and shows an inflection in the intermediate energy region which is deeper when the fermion mass decreases. From this discussion it follows that, in the strong- and weak-coupling regimes, the effect of dynamical fermions can be described in a first approximation as a renormalization of the coupling constant β, the shift in β being just the slope of the curve of Fig. 6 in the relevant energy interval. However, when we approach the critical point from the confining or Coulomb phases, the intermediate-energy region becomes the relevant one and just in this region, the slope of the curve of Fig. 6 changes rapidly. This effect becomes stronger for decreasing fermion mass. Then we

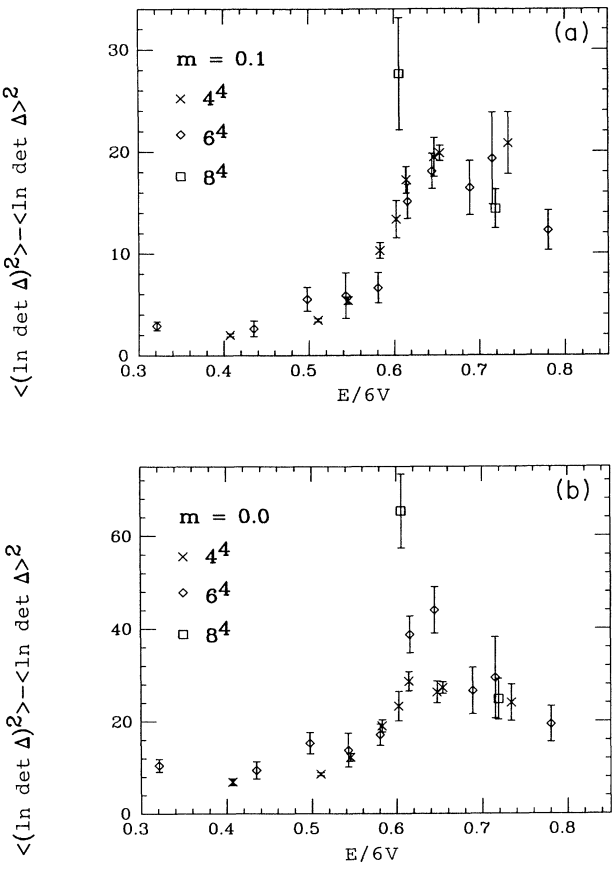

FIG. 5. Fluctuations of the logarithm of the fermionic determinant at fixed energy as a function of the normalized energy, for 4^4, 6^4, and 8^4 lattices. (a) $m = 0.1$ and (b) $m = 0.0$.

expect that the naive method developed in Sec. II will give good results, as it was checked, in the strong- and weak-coupling regions, but it can be affected by strong systematic errors near the phase-transition point.

To illustrate these concepts in a clearer way, we plot in Fig. 7 the mean plaquette probability distribution at three

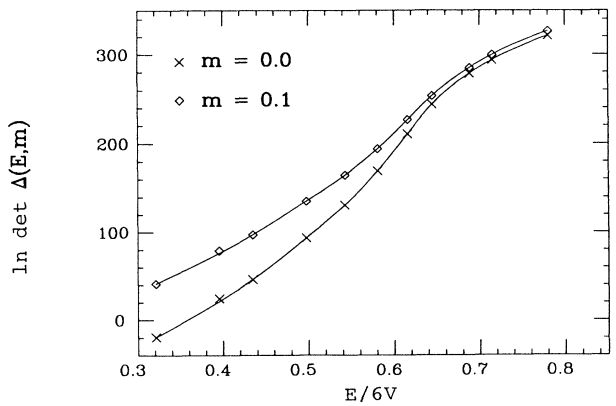

FIG. 6. Numerical results for the effective fermionic action for a 6^4 lattice vs the normalized plaquette energy at $m = 0.1$ and 0.0. Statistical errors are not larger than the points.

β values both in the quenched and unquenched cases. At $\beta=0.7$ [Fig. 7(a)], the distributions have an overlap region showing that the fermionic determinant shifts slightly the probability distribution function. This shift is expected to be smaller when β decreases since the slope of the curves in Fig. 6 seems to be a decreasing function of the energy E (a similar argument also applies in the large-β region). However, in the intermediate-β region the situation changes drastically as can be seen in Figs. 7(b) and 7(c), where essentially no overlap between the two distributions is observed at $\beta=0.885$ and 0.95. Therefore, and in the light of these results, we can understand the success of the "naive" method in the strong- and weak-coupling regimes as well as its failure in the intermediate-coupling region.

IV. NUMERICAL RESULTS

We now discuss the numerical results, and give some details on the simulations. As stated above, our simulation is divided into two parts: first, we compute the average determinant as a function of the energy, by means of a microcanonical procedure; second, the average determinant gives rise to an effective action which is used in a canonical simulation.

We have used a standard overrelaxation procedure[18] to implement the microcanonical simulation; energy values have been chosen in such a way as to uniformly sample the energy interval relevant to the canonical simulation. For the 6^4 (8^4) lattice, the determinant is computed for configurations separated by 500 (1000) overrelaxation iterations, in order to guarantee the complete decorrelation between successive configurations. In measuring the fermionic determinant, we used the complete U(1) group, while in the canonical simulation, the group used is the discrete subgroup $Z(256)$. The continuous group has been implemented in the exact microcanonical algorithm, which is, in general, inapplicable to discrete subgroups. The determinant has been computed by exactly diagonalizing the fermionic matrix at zero mass on the chosen configuration. The diagonalization is performed either by means of a standard library routine (6^4), or using a modified Lanczos algorithm ($6^4, 8^4$). In both cases we keep all the eigenvalues of all the configurations used.

This method has the obvious advantage of allowing the computation of the average determinant and of its derivatives with respect to the mass for every value of the fermion mass: it is only necessary to perform the microcanonical simulation once in order to perform the ensuing canonical simulation for every value of gauge coupling constant, number of flavors and fermion mass. The disadvantage of this method is the increase in computer time with respect to the time needed to compute the average determinant at fixed mass; this is compensated by the accuracy with which the determinant is measured. Having all the eigenvalues at our disposal, it is possible to check to which accuracy the relation

$$-\sum_{i=1}^{V/2}\lambda_i^2=V \tag{4.1}$$

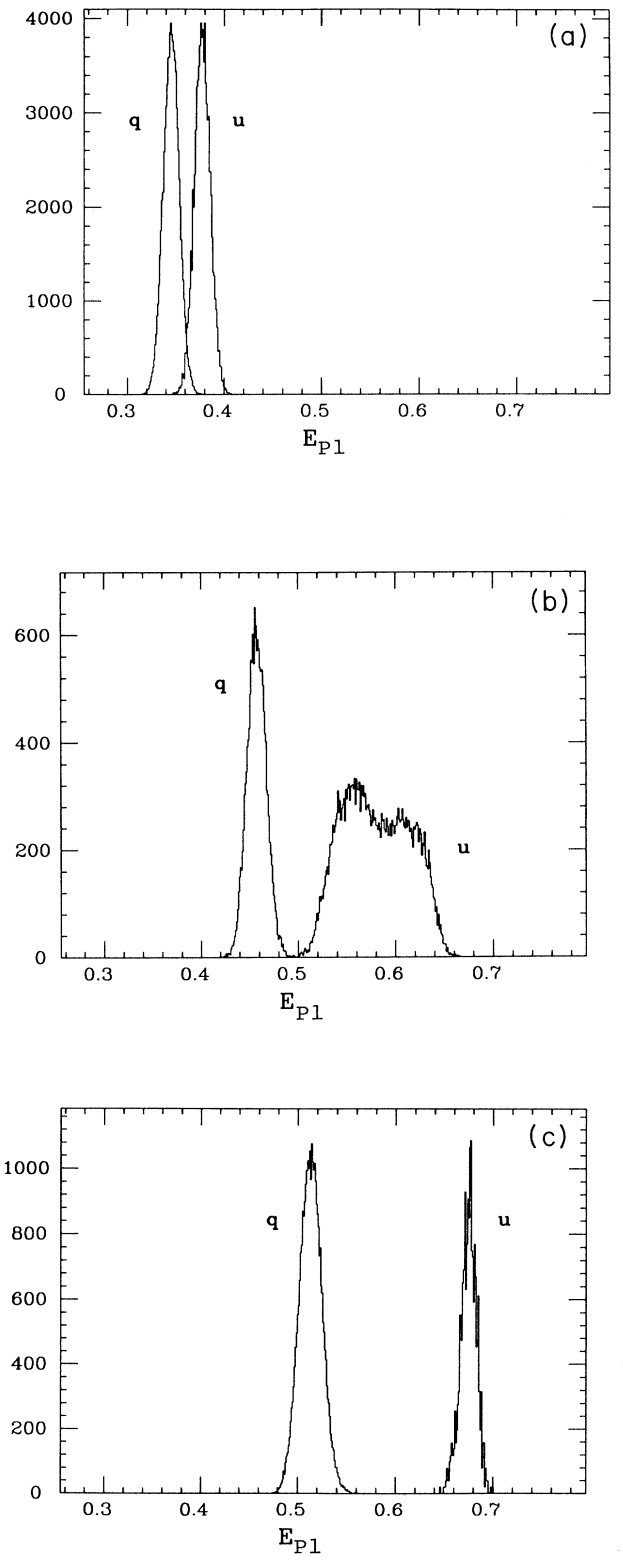

FIG. 7. Histogram of the mean plaquette energy for the quenched (q) against the unquenched (u) case at (a) $\beta=0.7$, (b) $\beta=0.885$, and (c) $\beta=0.95$ for 6^4 lattices. The fermion mass in the unquenched case is $m=0.1$.

is satisfied. All results from both algorithms are in excellent agreement with Eq. (4.1). A further check on the precision of the algorithms has been performed by comparing the eigenvalues obtained from both algorithms on the zero-mass matrix; also in this case, the agreement is excellent.

Having the eigenvalues for each configuration, it is possible to compute the determinant as

$$\det\Delta(m)=\prod_{i=1}^{V/2}(-\lambda_i^2+m^2) \tag{4.2}$$

from which we compute the effective fermionic action for the canonical simulation (see Fig. 6). In the determination of the effective action as well as in the canonical simulations, statistical errors have been computed in a standard way by means of the jackknife method.

As for the chiral condensate, it can be written as

$$\langle\bar{\psi}\psi\rangle=\frac{1}{V}\frac{\partial \ln Z}{\partial m}$$

$$=\frac{1}{V}\frac{\int dE\, N(E)e^{\beta E}\partial/(\partial m)\overline{\det}\Delta(E,m)}{\int dE\, N(E)e^{\beta E}\overline{\det}\Delta(E,m)}, \tag{4.3}$$

i.e.,

$$\langle\bar{\psi}\psi\rangle$$

$$=\frac{1}{V}\frac{\int dE\, N(E)e^{\beta E}\overline{\det}\Delta(E,m)\partial/(\partial m)\ln\overline{\det}\Delta(E,m)}{\int dE\, N(E)e^{\beta E}\overline{\det}\Delta(E,m)}. \tag{4.4}$$

It is thus directly calculable using the effective action and fermion matrix eigenvalues already obtained.

Let us now describe the canonical simulations: it is important to control the reliability of the interpolation procedure necessary to compute the effective action for every energy from the finite number of points on which the average determinant has been measured. In the simulations which will be presented in the following, we have used a standard polynomial interpolation routine which allows the reconstruction of the effective fermionic action with a little CPU time overhead. To check that we do not introduce systematic errors in the canonical simulations with this particular choice of interpolating function, we have also performed simulations using different interpolation schemes, or varying the order of the interpolating polynomial. We have further checked whether the statistical errors of the effective fermionic action introduce systematic errors in the canonical simulations. To test this we have shifted the value of the effective fermionic action within the range of the statistical errors. All these tests led to results in agreement within statistical errors. This implies that systematic errors are well under control.

The observables we measured are the plaquette energy, the specific heat, and the chiral condensate. In order to determine the height of the peak in the specific heat and the critical value of the coupling constant, we have performed an analysis similar to the one developed for the quenched case.[19,20] In the numerical simulations we have used a modified overrelaxation procedure to take into account the use of a discrete U(1) subgroup.[20] In the canonical simulation, in fact, the use of a discrete subgroup does not spoil the overrelaxation procedure, which does not need to be exactly microcanonical, since it is used for a few sweeps (1–5) between Metropolis ones; the acceptance of this modified procedure is, in any case, very high (99%).

We will now describe the results obtained in the following cases: (1) 6^4 lattice with $n_f=4$, (2) 6^4 lattice with both $n_f=1$ and 16, and (3) 8^4 lattice with $n_f=4$.

(1) For the 6^4 lattice, the effective action has been determined in the energy range 0.32–0.78; 11 values of the energy have been considered, and for each value between 100 and 500 configurations have been diagonalized with the method described above. The number of configurations has been chosen in such a way as to keep approximately constant the relative error on the effective action. In the canonical simulations, the statistics used away from the transition region is 200 thermalizations (starting from an equilibrium configuration of the preceding β value) and 800 measurements, while in the critical region we have reached 1000 thermalizations and 36 000 measurements, with three overrelaxation cycles between Metropolis ones. The results of the longest run have been used for the computation of the specific heat at the critical coupling.

In Fig. 8(a) we present the measured behavior of the plaquette energy for two mass values ($m=0.0$ and 0.1). The latter case is used for comparison with the results of different methods.[11] In Fig. 8(b) we present the values of the chiral condensate at $m=0.1$, as a function of β. The position of the phase transition is clear, as well as the progressive shift of the critical coupling to lower values with decreasing fermion mass; our results at $m=0.1$ are in excellent agreement with those of Ref. 11, obtained with standard methods.

From the analysis of the peak of the specific heat we can accurately measure the critical values: $\beta_c=0.8854(3)$ at $m=0.1$ and $\beta_c=0.8540(5)$ at $m=0$; the height of the maximum of the specific heat is $h_c=8.9(2)$ at $m=0.1$ and $h_c=8.2(3)$ at $m=0$ to be compared with the value $h_c=7.57(13)$ of the quenched case. From the behavior of h_c as a function of the mass, we can observe that, as noted in Ref. 11, the introduction of light fermions tends to produce a stronger transition.

(2) As a consequence of the properties of the fermionic action and of the fact that the determinant is known for all the configurations generated in the microcanonical simulation, it is possible to simulate any flavor number, without a significant increase in CPU time, since only the simulations in the effective theory are to be repeated. We have thus performed simulations in a 6^4 lattice and $n_f=1$

and 16, checking with existing data.

In Figs. 9(a) and 9(b) and 10(a) and 10(b) we present the results for $n_f=1$ and 16, respectively, measuring $E_{\rm pl}$ and $\langle\bar{\psi}\psi\rangle$. From these figures it is evident that both the shift in β_c and the sharpness of the transition (evidenced by the wide hysteresis cycle in the $n_f=16$ case) increase with the number of flavors. In the $n_f=1$ case there is no real hysteresis, probably due to the fact that the statistics used allowed the system to reach equilibrium. However, the transition is well characterized by the huge variation of the average values and the increase of the statistical errors, which signals violent fluctuations of the system.

Again, our results in the one-flavor case are compatible with those obtained by a stochastic method in Ref. 11. However, in the 16-flavor case, we have obtained results slightly different from those of Ref. 11 in the sense that our critical coupling seems to be somewhat larger. This is not very surprising since systematic errors increase significantly with the number of flavors both in our method and that of DK.

(3) Finally, we present some results obtained in the 8^4 lattice; the statistics used for the determination of the effective action is, in this case, much lower than before (4 configurations for each of the 12 energy values in the range 0.40–0.73). However, in light of the discussion on the behavior of the fluctuations of the logarithm of the determinant as a function of the volume (see Sec. III), it is not inconceivable that these results are significant.

In Figs. 11(a) and 11(b) we present the results for the plaquette energy and the chiral condensate; the statistics for the canonical simulation of the effective theory amount to a few thousands of iterations away from the critical region, increasing to 172 500 iterations (with overrelaxation) around the critical point. Using the data of two long runs in the vicinity of the critical value we can derive the specific heat at $m=0.1$ and 0.0. At $m=0.1$ and $\beta=0.8935$ we performed 30 000 iterations with overrelaxation; the critical coupling is $\beta_c=0.8937(2)$ and the height of the maximum of the specific heat is $h_c=24.5(6)$. The histogram of the distribution of the plaquette energy is shown in Fig. 12(a); the two-peak structure is evident. The system has fluctuated 30 times between the two va-

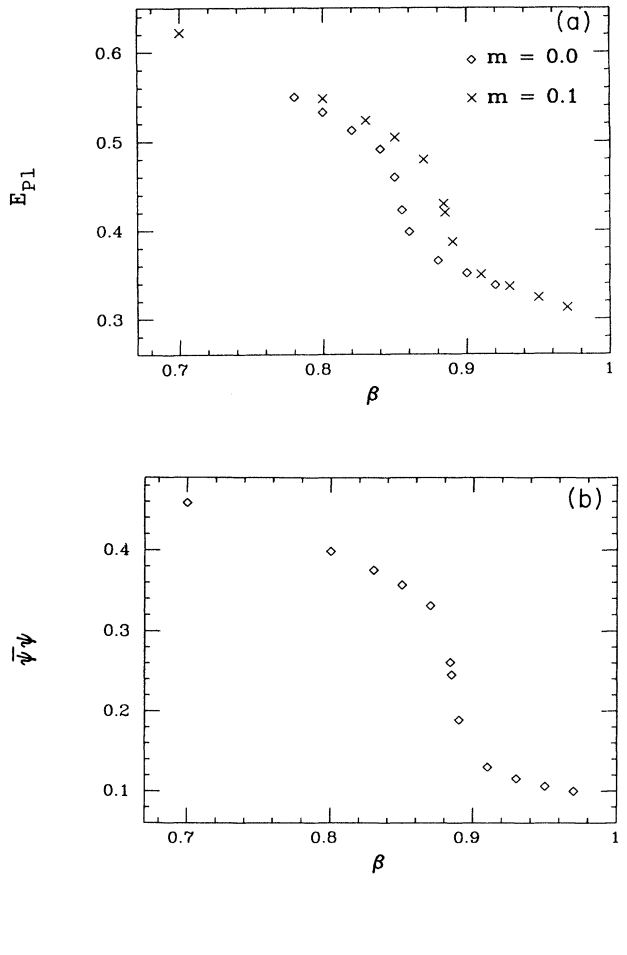

FIG. 8. Numerical results for the mean plaquette energy (a) at $m=0.01$ and 0.0 and for the chiral condensate (b) at $m=0.1$ vs β for a 6^4 lattice ($N_f=4$). Statistical errors are not larger than the points.

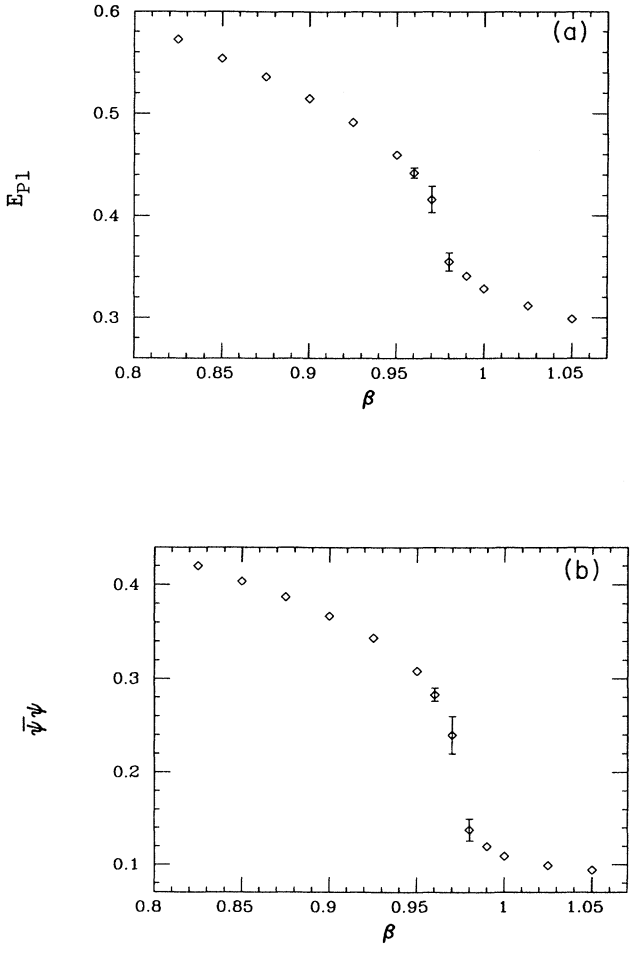

FIG. 9. Same as Fig. 8 but for $N_f=1$ and $m=0.1$.

cua. Again, these results are in good agreement with those of Ref. 12. At $m=0$ and $\beta=0.864$ we have data from a run of 172 500 iterations, with overrelaxation; the system stayed during 30 000 iterations in the Coulomb phase and then jumped to the confining phase remaining there even after 140 000 iterations [see Fig. 12(b)]. Therefore, we cannot give an accurate value of the critical coupling, which is in any case in the very proximity of $\beta=0.864$.

The value of the peak of the specific heat is $h_c=48.9(5)$. This can be compared with the quenched case, which is $h_c=13.73(26)$ (Ref. 20); comparing these numbers with those of the 6^4 lattice, we note that the transition tends to become stronger at low masses, although we cannot give reasonable values for the critical exponents. In fact, the effects of scaling violations due to the finite size are still important in these lattices. The results at $m=0$, however, point in the direction of a strong first-order transition.

V. CONCLUSIONS

In this paper we have discussed some possibilities of speeding up Monte Carlo computations with dynamical fermions. The general idea is to factorize out the computation of the fermionic determinant, which is the most costly in terms of CPU, so as to avoid repeating it for every value of the parameters of the theory. Thermodynamical quantities such as specific heat, chiral condensate, etc., are then recovered as appropriate derivatives of the action.

A first attempt, amounting essentially to computing the quenched average of the determinant, turned out to miss the region of important configurations when the system approaches the phase transition. The second approach turns out to be much more promising. We computed the average determinant at fixed (total) energy. The logarithm of the mean value of the fermionic determinant is then inserted as an effective term in the action,

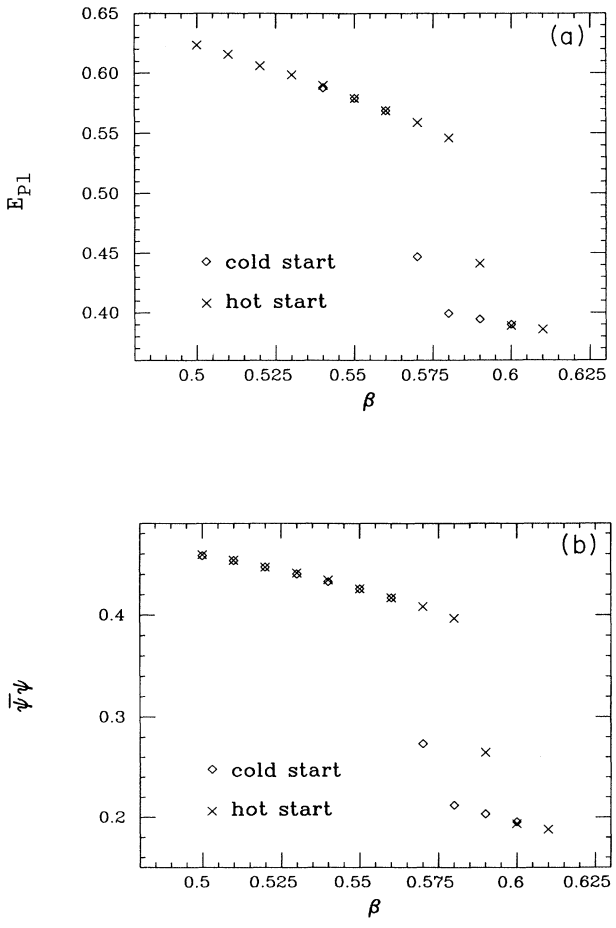

FIG. 10. Same as Fig. 9 but for $N_f=16$.

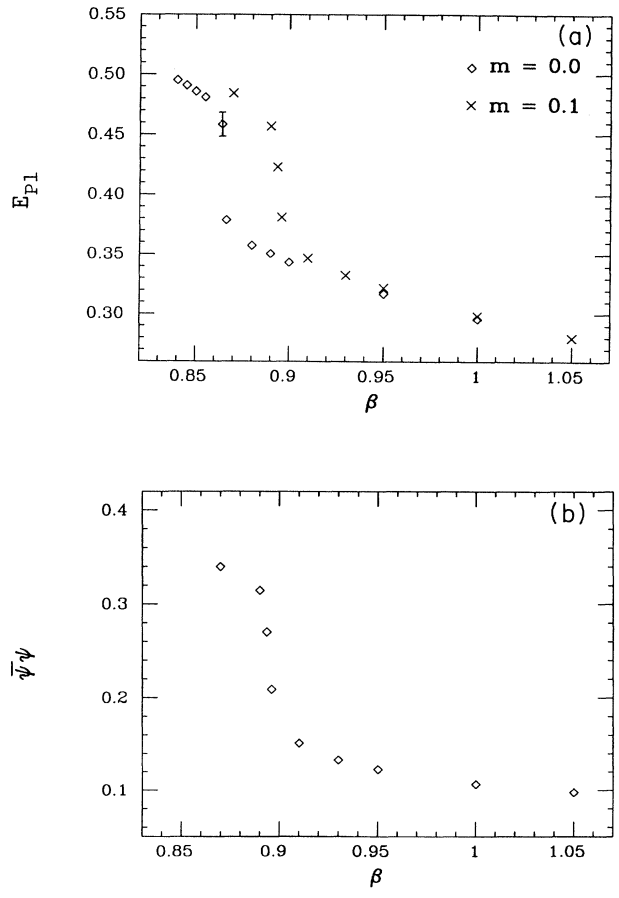

FIG. 11. Numerical results for the mean plaquette energy (a) at $m=0.1$ and 0.0 and for the chiral condensate (b) at $m=0.1$ vs β for a 8^4 lattice ($N_f=4$). Statistical errors are not larger than the points.

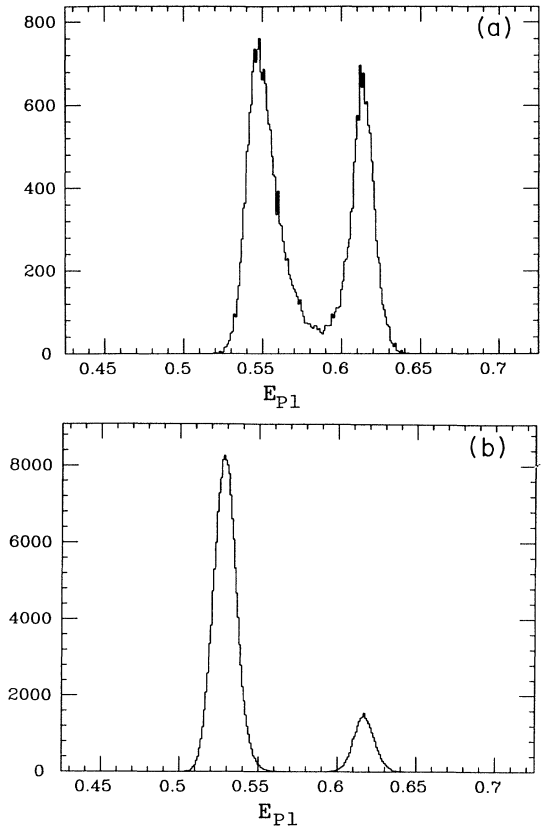

FIG. 12. Probability distribution of the mean plaquette energy for 8^4 lattices at (a) $\beta=0.8935$, $m=0.1$ and (b) $\beta=0.864$, $m=0.0$.

which is used in a standard pure-gauge simulation. We have used this method in an investigation of compact QED, although, in principle, it can be used for other gauge groups.

We have checked that, at least in the lattices examined (i.e., up to 8^4), the fluctuations of the logarithm of the determinant at fixed energy increase very slowly with the volume. The fact that these fluctuations increase slowly with the volume (i.e., the normalized fluctuations decrease), if taken at face value, justifies the feasibility of our method even for larger lattices. The results obtained are extremely encouraging. We obtain results in good agreement with those in the literature, using a relatively small amount of computer time (700 CPU h for the microcanonical simulations) in a scalar computer (Vax 8650).

Furthermore, the method proposed here (at least in conjunction with an algorithm which computes exactly the determinant) allows us to perform computations at small values of the fermionic mass, in particular, at $m=0$. Moreover, whenever it is possible to exactly compute the eigenvalues of the fermionic matrix, the mass dependence becomes trivial and can be factored out. The results we present are obtained in this way. Another relevant feature of our method is that correlations between consecutive configurations can be very well controlled since, in the microcanonical procedure, the cost of computer time in the overrelaxation algorithm is negligible.

We presented some intuitive arguments to explain why computing the fermionic determinant at fixed energy reduces its fluctuations. It is, however, fair to say that we lack a more rigorous proof of the feasibility of the method.

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