New algorithm for the numerical simulation of fermions

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A new algorithm for the numerical simulation of lattice field theories with fermion degrees of freedom is presented. Changes are proposed on a set of lattice sites or links using an approximate, local updating algorithm. The entire set of changes is then accepted or rejected according to a prescription that makes the algorithm exact. An efficient method of measuring the fermion Green's functions during the simulation is also presented. The algorithm is expected to be useful in studying a variety of lattice-field-theory problems in three space and one time dimensions.

I. INTRODUCTION

Numerical techniques are presently being used to study a wide variety of problems in quantum field theory. One of the major challenges in this area is to develop efficient algorithms for the simulation of systems with fermion degrees of freedom. In this paper we present a new algorithm for this purpose. We believe that it has considerable potential for the simulation of lattice field theories in three-space and one-time dimensions.

We are primarily interested in lattice-field-theory problems that arise in condensed-matter and high-energy physics. Ordinarily in these areas the action is either quadratic in the fermion fields or can be made so by the introduction of one or more auxiliary boson fields. One can therefore integrate out the fermion fields to obtain a nonlocal effective action for the bosonic degrees of freedom. As is well known, one cannot use standard Monte Carlo methods to study this effective action, since each step in the Markoff chain requires the solution of a set of linear equations of dimension at least equal to the number of fermion degrees of freedom. Thus to update the boson fields individually at each lattice site or link is prohibitively expensive in computer time. Attention has focused instead on approaches such as the pseudofermion method,[1] the microcanonical ensemble,[2] and the Langevin equation[3] in which one updates many degrees of freedom in a single step. Our algorithm also involves the simultaneous updating of many degrees of freedom. We first propose changes in each member of a set of variables according to an approximate local algorithm. We then accept or reject the entire proposed set of changes in a Metropolis step that ensures that the algorithm is exact. It is only in the final acceptance-rejection step that one must pay the computational price associated with the nonlocality of the effective action.

In Sec. II we describe the algorithm in detail. We also present an efficient method for measuring fermion Green's functions during the course of the simulation. This method is applicable to most fermion algorithms presently in use. In Sec. III we present numerical results obtained by applying our algorithm to the spinless Hubbard model in one space and one time dimension. Although this model has a simple structure, we believe that it provides a significant test of fermion algorithms because the fermion matrix has a wide range in its eigenvector spectrum even for small systems. Finally we discuss the application of the method to large systems in three space and one time dimensions.

II. THE ALGORITHM

We take the path integral for the partition function to have the form

$$Z=\int \delta A\,\delta\psi\,\delta\bar{\psi}\,e^{-[S_B(A)+\bar{\psi}M(A)\psi]}$$
$$=\int \delta A\,e^{-S_B(A)}\det M(A)\ . \tag{1}$$

Here A is a boson or gauge field, $\bar{\psi}$ and ψ are Grassman variables representing the fermion field, $S_B(A)$ the pure bosonic part of the Euclidean action, and $M(A)$ the fermion matrix which includes both the fermion kinetic energy and interaction with the A field. D, the dimension of M, is of course equal to the total number of fermion degrees of freedom. M is ordinarily a very sparse matrix.

We shall assume throughout this paper that M is positive definite. In many applications in condensed matter physics it is also real. We shall start by considering this case, and then discuss the modifications that are necessary when it is complex. For M real the determinant can be represented by a Gaussian integral over a real c-number field.[4] The partition function then takes the form

$$Z=\int \delta A\,\delta\Phi\,e^{-[S_B(A)+\Phi O^{-1}\Phi]}$$
$$=\int \delta A\,\delta\Phi\,e^{-S_{\rm eff}(A,\Phi)}\ , \tag{2}$$

where $O=M(A)^TM(A)$.

In carrying out the simulation we wish to generate configurations of the A and Φ fields such that the probability of finding a particular configuration is proportional to $\exp(-S_{\rm eff})$. We shall alternatively update all components of A and all components of Φ. Let us being by considering the updating of the Φ field. Although M is a sparse matrix, M^{-1} is not. As a result, the Metropolis algorithm will not be useful for this procedure. Instead we use a

generalized Langevin equation. Given a field configuration Φ, we choose a new one, Φ', through the relation[3]

$$\Phi'-\Phi=-\frac{c}{2}(\Phi'+\Phi)+\sqrt{2c}M^{T}R \ . \tag{3}$$

Here $R=(R_1,R_2,\ldots,R_D)$ is a vector of Gaussian random numbers, so the probability density for finding a particular value of R is $\pi^{-D/2}\exp(-R^2)$. c is a constant which determines the step size of Φ. If we make use of Eq. (3), the probability density for obtaining a field configuration Φ' starting from the configuration Φ is

$$P_{\Phi\to\Phi'}=\left[\frac{\sqrt{2c}\,\pi}{1+c/2}\right]^{-D/2}\det M^{-1}\exp[-(1/2c)\tilde{\Phi}O^{-1}\tilde{\Phi}] \ , \tag{4}$$

where $\tilde{\Phi}=(\Phi'-\Phi)+(c/2)(\Phi'+\Phi)$. Detailed balance is satisfied exactly since

$$\frac{P_{\Phi\to\Phi'}}{P_{\Phi'\to\Phi}}=e^{-(\Phi'O^{-1}\Phi'-\Phi O^{-1}\Phi)} \ . \tag{5}$$

Notice that Eq. (5) holds for all values of c. A particularly appealing choice is $c=2$ for which $\Phi'=M^{T}R$, and is thus independent of Φ.[5]

Let us now turn to the problem of updating the boson field, A. If we make a change $A\to A'$, then $O\to O'=O+\Delta O$. The change in the effective action is given by

$$\Delta S_{\rm eff}=\Delta S_B(A)-\Phi O'^{-1}\Delta O\, O^{-1}\Phi \ . \tag{6}$$

Thus, in order to evaluate $\Delta S_{\rm eff}$ we must calculate $O^{-1}\Phi$ and $O'^{-1}\Phi$. Each of these calculations requires the solution of a set of D linear equations. We propose to solve these equations by conjugate gradient or other iterative methods. Clearly we cannot afford to update one component of A at a time. On the other hand if we propose random changes in a significant number of components of A at once, the probability of accepting a set of changes is likely to be unacceptably small. In order to deal with this dilemma we divide the updating process into two parts. First we propose changes in all, or a significant fraction, of the components of A using an approximate transition probability, $P_{A\to A'}$. $P_{A\to A'}$ will be chosen so that the algorithm for suggesting changes in the individual components of A is a local one. In order to ensure that detailed balance is satisfied exactly we accept the entire set of proposed changes with a probability $Q_{A'}$, which is chosen so that

$$\frac{P_{A\to A'}Q_{A'}}{P_{A'\to A}Q_A}=e^{-\Delta S_{\rm eff}} \ . \tag{7}$$

If, for example, we use the Metropolis algorithm for Q, then we would write

$$Q_{A'}=\theta(\rho-1)+\rho\theta(1-\rho) \tag{8}$$

with

$$\rho=e^{-\Delta S_{\rm eff}}\frac{P_{A'\to A}}{P_{A\to A'}} \ . \tag{9}$$

With a good choice for the approximate probability, ρ will be sharply peaked about one, giving an acceptance probability close to one. The important questions are whether one can find suitable approximate transition probabilities, and how sharply ρ must be peaked to have a useful algorithm.

We have examined a variety of choices for the approximate transition probabilities. The simplest was motivated by the pseudofermion algorithm. In the pseudofermion method one makes a full sweep of the lattice ignoring changes in O^{-1} resulting from changes in the components of A. This suggests that one use the Metropolis algorithm to determine $P_{A\to A'}$, approximating the change in the effective action by Eq. (6) with $\Phi O'^{-1}$ replaced by ΦO^{-1}. Before making a sweep of the lattice we must calculate $O^{-1}\Phi$, which we propose to do by the conjugate gradient method. Then changes in each element of A are suggested by a completely local process. After A' has been determined, we must calculate $O'^{-1}\Phi$ in order to obtain the exact value of $\Delta S_{\rm eff}$ and the reverse transition probability $P_{A'\to A}$ which are needed to determine ρ.

This simple pseudofermion approach can be improved significantly in the following manner. If one begins by randomly suggesting changes in each component of the A field, one obtains an intermediate field configuration, A'', and its corresponding fermion matrix O''. One can then define $P_{A\to A'}$ to be the product of the probabilities for accepting each change using Eq. (6) with O'^{-1} replaced by O''^{-1}. In order to calculate the reverse transition probability, one needs the intermediate state A''' encountered in going from A' to A. We define it by taking $A_i'''=A_i$ for those i for which a change was accepted, and $A_i'''=A_i''$ for those i for which it was rejected. This algorithm requires one extra conjugate gradient calculation for each of these transition probabilities, but we have found that, at least for the model discussed in Sec. III, these extra calculations are more than made up for by the ability to make larger field changes, while keeping a reasonable final acceptance probability, leading to a significant decrease in the number of sweeps needed to obtain independent configurations. As we shall see, it is necessary to operate with rather large local acceptance probabilities. This means that the vector $O''^{-1}\Phi$ is a significantly better approximation to $O'^{-1}\Phi$ than is $O^{-1}\Phi$. Of course in the limit $A''\to A'$, ρ becomes one. We expect this improved pseudofermion algorithm to be particularly useful when the correlation length is short, since it correctly takes into account the proposed *on-site changes*.

We have also explored an approximate transition probability based on the Langevin equation. In its simplest form the Langevin equation gives for the updating of the A field

$$A'=A-\tfrac{1}{2}\epsilon\nabla S_{\rm eff}+\sqrt{2\epsilon}R \ . \tag{10}$$

Equation (10) is a vector equation of dimension, D_A, equal to the number of degrees of freedom of the A field. $\nabla_i=\partial/\partial A_i$ and $R=(R_1,R_2,\ldots,R_{D_A})$ is a vector of Gaussian random numbers distributed as $\pi^{-(D_A/2)}\exp(-R^2)$. The transition probability for going from the configuration A' to A is then given by

$$P(A'\rightarrow A)=\pi^{-D_A/2}\exp[-(A'-A+\tfrac{1}{2}\epsilon\nabla S_{\rm eff})^2/2\epsilon]\ . \tag{11}$$

This approach requires one conjugate gradient calculation to update each new set of A fields, so the number of arithmetic operations per sweep of the lattice is comparable to the simple pseudofermion method. However, the Langevin equation typically has a significantly shorter autocorrelation time because it leads the system to more probable distributions, thus producing a larger final acceptance probability.

The Langevin approach can be improved in the same manner as described above for the pseudofermion algorithm. In this case the intermediate field configuration A'' is generated by the Langevin equation, Eq. (10), and then used to determine $O''^{-1}\Phi$. Then one proceeds with an acceptance-rejection step for each of the proposed local changes to obtain A', determines the reverse transition probability, and makes a final decision as to whether to accept the configuration A'. We will refer to this as the combined algorithm.

After one has obtained equilibrium distributions of the A fields, it is ordinarily a time consuming task to measure the fermion Green's function. For example, it takes one conjugate gradient calculation to obtain each row of M^{-1}. One can run a separate Monte Carlo calculation to obtain the Green's function as in the traditional pseudofermion method, but this ordinarily gives noisy estimates at large distances. Our algorithm suggests a new approach to this problem. In the course of our calculation we must compute the quantity $O^{-1}\Phi=M^{-1}R$. Thus no significant extra computation is needed to obtain

$$\langle M_{ij}^{-1}\rangle=2\langle(O^{-1}\Phi)_i R_j\rangle\ . \tag{12}$$

The average in Eq. (12) is over configurations of the A field and over random number vectors R. We obtain an independent measurement every time that we update the Φ field. Note that we obtain a measurement of all components of the Green's function. If one wishes to measure the expectation value of a product of Green's functions, it is necessary to cast an additional vector of random numbers and perform an additional conjugate gradient calculation for each additional Green's function in the product. Nevertheless the cost is small compared to the updating time as well as to conventional approaches. This measurement method can obviously be used with any fermion algorithm.

The eigenvalue spectrum of the matrix $O=M(A)^TM(A)$ strongly affects both the number of conjugate gradient sweeps required in the computation of $O^{-1}\Phi$ and the distribution of the final acceptance factor ρ. We have found that preconditioning O to decrease the spread in its eigenvalues can significantly improve the calculation. One can write

$$\begin{aligned}\det M&=\det M_0 \det M_0^{-1}M\\&=\det M_0\int\delta\Phi\, e^{-\Phi\tilde{O}^{-1}\Phi}\end{aligned} \tag{13}$$

with $\tilde{O}=(M_0^{-1}M)^T(M_0^{-1}M)$. Two particularly simple choices for M_0 that we have explored are obtained by dropping the kinetic or potential energy terms in the Hamiltonian. In general they are expected to be useful in the strong and weak coupling limits, respectively, but for the model discussed in Sec. III we found that they both gave considerable improvement over a wide range of couplings. In the weak coupling approximation M_0 is ordinarily independent of the bosonic variables, and only the conjugate gradient calculation is improved by the conditioning. In the strong coupling approximation one can hope to calculate $\det M_0$ analytically and include it in the bosonic part of the action. In this case both the conjugate gradient calculation and the distribution of ρ benefit. Preconditioning is of particular importance at low temperatures. Here an interesting possibility is to take M_0 to be M with $\Delta\tau$ replaced by $\Delta\tau/2$. $\det M_0$ cannot be evaluated analytically in this case, so it is necessary to introduce a second auxiliary field analogous to Φ. Although this approach requires additional conjugate gradient calculations, preliminary studies indicate that it may well lead to significant savings in total computer time. We hope to return to this point on a later occasion.

Up to now we have assumed that the matrix elements of the fermion determinant, M, are real. That is not the case in lattice gauge theory. However, all of our results remain valid if we simply allow Φ to become a complex vector and replace M^T by $M^\dagger$. R now becomes a complex vector with the real and imaginary parts of each component being Gaussian random numbers. For example, Eq. (2) becomes

$$\begin{aligned}Z&=\int\delta A\,\delta\Phi\,\delta\Phi^* e^{-[S_B(A)+\Phi^*O^{-1}\Phi]}\\&=\int\delta A(\det O)e^{-S_B(A)}\ .\end{aligned} \tag{14}$$

with $O=M^\dagger M$. In lattice gauge theory $\det M=\det M^\dagger$, so the price we have paid for the introduction of the complex field, Φ, is a doubling of the fermion species. However, this doubling can be avoided for staggered fermions.[6]

III. NUMERICAL RESULTS

To explore the algorithm described in Sec. II, we have studied a model of fermions in one-space and one-time dimensions interacting through nearest-neighbor Coulomb interactions. The Hamiltonian is given by

$$H=\sum_{i=1}^{N}[-t(c_i^\dagger c_{i+1}+c_{i+1}^\dagger c_i)+V(n_i-\tfrac{1}{2})(n_{i+1}-\tfrac{1}{2})]\ . \tag{15}$$

Here $c_i^\dagger$ and c_i are the creation and annihilation operators of the fermions, $n_i=c_i^\dagger c_i$, and N is the number of spatial lattice sites. For $0\le V/2t\le 1$, the ground state of the model is gapless and the correlation functions exhibit power-law correlations determined by $V/2t$. This model has been extensively studied by bosonization techniques as well as by various stochastic methods. Thus it provides a natural testing ground for new numerical approaches. We are interested in studying the model at finite temperatures, so the average value of an operator Q will be given by

$$\langle Q \rangle = \frac{\mathrm{tr} Q e^{-\beta H}}{\mathrm{tr} e^{-\beta H}} . \tag{16}$$

As usual we use periodic boundary conditions in space and antiperiodic boundary conditions in imaginary time.

In integrating out the fermion degrees of freedom we follow the approach of Ref. 7. We first divide the imaginary time interval $0 \leq \tau \leq \beta$ into L intervals each having a width $\Delta\tau$, so the partition function can be written in the form

$$Z = \mathrm{tr} e^{-\beta H} = \mathrm{tr}(e^{-\Delta\tau H})^L . \tag{17}$$

We then introduce a Hubbard-Stratonovich variable, $A_i(\tau_l)$, for each pair of lattice points, $(i,i+1)$, on each time slice, τ_l, using the identity

$$e^{-\Delta\tau V(n_i - 1/2)(n_{i+1} - 1/2)} = \sqrt{\Delta\tau/\pi}\, e^{-\Delta\tau V/4} \times \int_{-\infty}^{+\infty} dA_i(\tau_l) e^{-\Delta\tau[A_i(\tau_l)^2 + (2V)^{1/2} A_i(\tau_l)(n_i - n_{i+1})]} . \tag{18}$$

In applying Eq. (18) to the factors of $\exp(-\beta H)$ in Eq. (17) we must temporarily separate the hopping and Coulomb terms in the Hamiltonian. This process is only good to order $\Delta\tau^2$, so this variable will be kept small. In the results reported here we have taken $t = V = 1.0$ and $\Delta\tau = 0.25$, although we have also studied the strong-coupling regime. All results are for a lattice with 32 spatial sites and eight time slices.

With the introduction of the Hubbard-Stratonovich field A, the partition function has the form of Eq. (1) with the bosonic part of the action, S_B, quadratic in A. We can therefore make use of the algorithms discussed in Sec. II. In updating the Φ field we generally set $c = 2$ in Eq. (3) so it reduces to $\Phi' = M^T R$, and successive Φ field configurations are independent of each other.

Let us begin by considering the improved pseudofermion algorithm. Changes in the A field are proposed through the relation

$$A_i'' = A_i + \delta(r_i - \tfrac{1}{2}) , \tag{19}$$

where r_i is a random number uniformly distributed in the interval (0,1), and δ is a constant that sets the scale for changes in A. In Fig. 1 we show the distribution in the acceptance factor, ρ, resulting from the simultaneous updating of all 256 Hubbard-Stratonovich variables on our 32×8 lattice. Data is shown for $\delta = 1.0$, 1.5, 2.0, and 3.0. Naturally for small δ, ρ is sharply peaked about one. However as δ in increases the peak broadens and eventually shifts to the origin indicating the decreased likelihood of acceptance. In Fig. 2 we show the correlation time, T, measured in lattice sweeps between independent field configurations. For small δ, T is large since the Hubbard-Stratonovich variables are being changed little from sweep to sweep. For large δ, T is also large since the global acceptance factor is small and the set of changes is frequency rejected. This latter situation corresponds to Fig. 1(d).

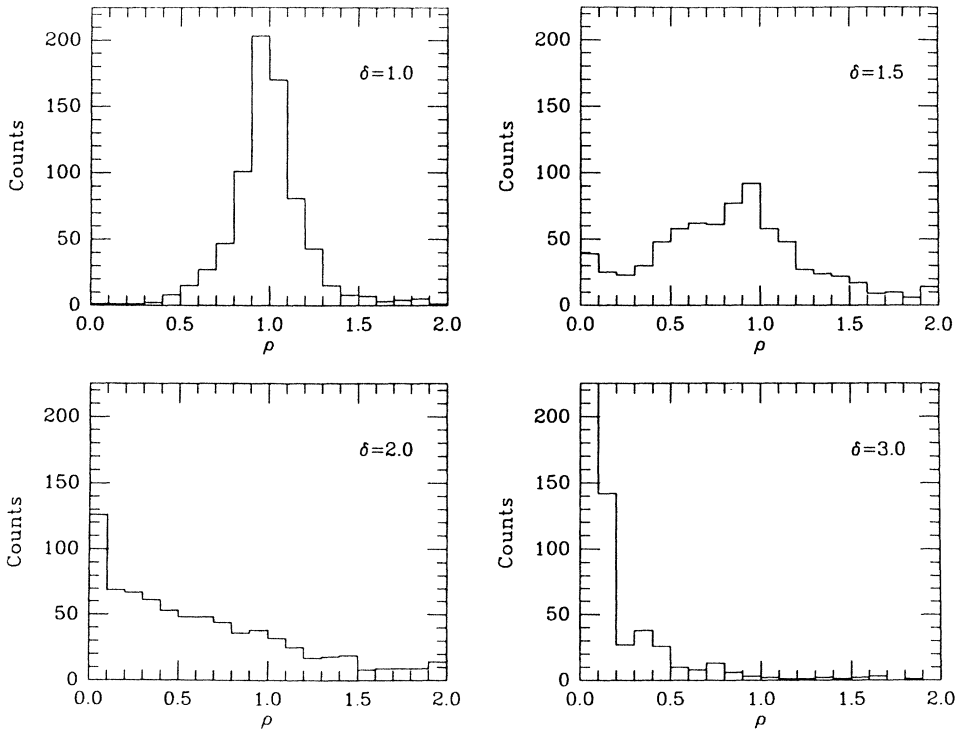

FIG. 1. Distribution of the acceptance factor, ρ, resulting from the simultaneous updating of all 256 Hubbard-Stratonovich variables on a 32×8 lattice using the improved pseudofermion algorithm. Data are shown for the step size $\delta = 1.0$, 1.5, 2.0, and 3.0. For $\delta = 3.0$ the first bin goes off the graph by a factor of 2.

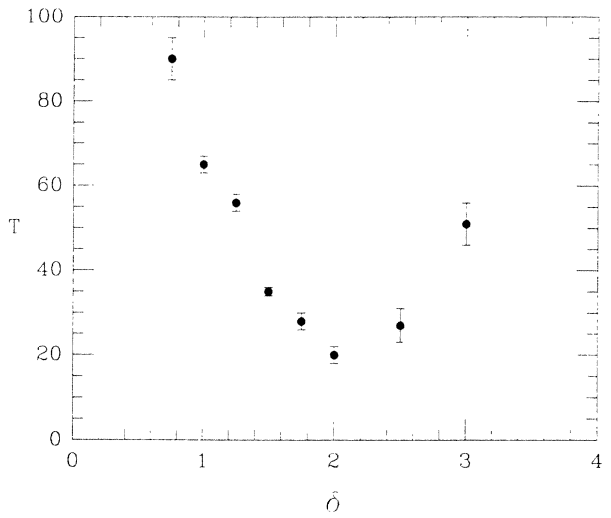

FIG. 2. The correlation time, T, between independent field configurations as a function of the step size δ. T is measured in lattice sweeps. The data are from the improved pseudofermion algorithm on a 32×8 lattice.

There exists an optimal step size, $\delta_{\rm opt}$, which gives a minimum correlation time, $T_{\rm min}$. As one might expect, $\delta_{\rm opt}$ corresponds to a global acceptance probability of order one-half. This means that we explore phase space most rapidly when ρ has roughly the distribution of Fig. 1(c).

For the pseudofermion, improved pseudofermion, Langevin, and combined algorithms discussed in Sec. II, $T_{\rm min}$ is 95, 20, 26, and 15 sweeps, respectively. In choosing between algorithms one must take into account the time per sweep as well as the value of $T_{\rm min}$. Thus for this model the Langevin approach is preferred over the improved pseudofermion algorithm since it has approximately the same value of $T_{\rm min}$ but requires half the number of conjugate gradient calculations to implement. The Langevin and combined algorithms take approximately the same amount of computer time to generate independent configurations, giving a slight advantage to the Langevin approach because of its simplicity. In general, we expect the choice of algorithm to be model and even parameter dependent. The important point is that with our exact algorithms we can simultaneously update a substantial number of sites with step sizes large enough to produce reasonably small correlation times.

In Table I we give results for the equal time fermion Green's function

$$G(l)=\langle c_{i+l}c_i^{\dagger}\rangle \tag{20}$$

obtained using Eq. (12). As always we work on a 32×8 lattice with $V=t=1.0$. The "exact" results quoted in this table were obtained from the well-tested algorithm of Ref. 6. The data were collected from 3,750 sweeps through the lattice, so the noise is gratifyingly low. This is due in part to the fact that Eq. (12) gives an unbiased estimate of each element of M^{-1}, so the right-hand side of Eq. (20) can be averaged over the lattice sites, i. In addition, we obtain a measurement of $G(l)$ each time that the Φ field is updated at no significant cost in computer time. Even if the A field is slowly varying, we obtain an independent contribution to the average over the vector of random numbers, R, from each sweep.

TABLE I. The fermion Green's function $G(l)$ on a 32×8 lattice for $V=t=1$. The Monte Carlo results, $G(l)_{\rm MC}$, where obtained with the algorithm based on the Langevin equation using 3,750 sweeps of the lattice. The exact results, $G(l)_E$, were obtained with the algorithm of Ref. 6. The numbers in parentheses are statistical errors in the last two decimal places quoted.

l	$G(l)_{\rm MC}$	$G(l)_E$
0	0.5001(19)	0.5000
1	−0.2896(28)	−0.2891
2	0.0008(17)	0.0000
3	0.0584(22)	0.0580
4	0.0006(18)	0.0000
5	−0.0171(21)	−0.0152
6	−0.0002(23)	0.0000
7	0.0056(15)	0.0042
8	−0.0010(31)	0.0000
9	−0.0010(26)	−0.0012
10	−0.0003(19)	0.0000
11	0.0004(21)	0.0003

Another illustration of the fermion measurement procedure is given in Table II where we present results for the density-density correlation function

$$\begin{aligned} C(l)&=\langle (n_{i+l}-\tfrac{1}{2})(n_i-\tfrac{1}{2})\rangle \\ &=-0.25+0.5\delta_{l,0}+\langle M^{-1}_{i+l,i+l}M^{-1}_{i,i}\rangle \\ &\quad -\langle M^{-1}_{i,i+l}M^{-1}_{i+l,i}\rangle \ . \end{aligned} \tag{21}$$

Since this correlation function involves the average of a product of two matrix elements of M^{-1}, we must introduce an extra vector of random numbers and perform one extra conjugate gradient calculations as was discussed in Sec. II. Once again we obtain excellent results from only 2,000 sweeps through the lattice. The results presented in both Tables I and II are from the Langevin algorithm, but similar accuracy was obtained with both the improved pseudofermion and combined algorithms. This correlation function could also be obtained from a measurement of the Green's function of the A field, but the noise would

TABLE II. The correlation function $C(l)$ on a 32×8 lattices with $V=t=1$. The Monte Carlo results, $C(l)_{\rm MC}$ were obtained with the algorithm based on the Langevin equation using 2,000 sweeps of the lattice. The exact results $C(l)_E$, were obtained using the algorithm of Ref. 6. The numbers in parentheses are statistical errors in the last two decimal places quoted.

l	$C(l)_{\rm MC}$	$C(l)_E$
0	0.2500(10)	0.2500
1	−0.1164(14)	−0.1152
2	0.0233(21)	0.0270
3	−0.0149(18)	−0.0139
4	0.0052(16)	0.0043
5	−0.0015(08)	−0.0018
6	0.0001(08)	0.0004

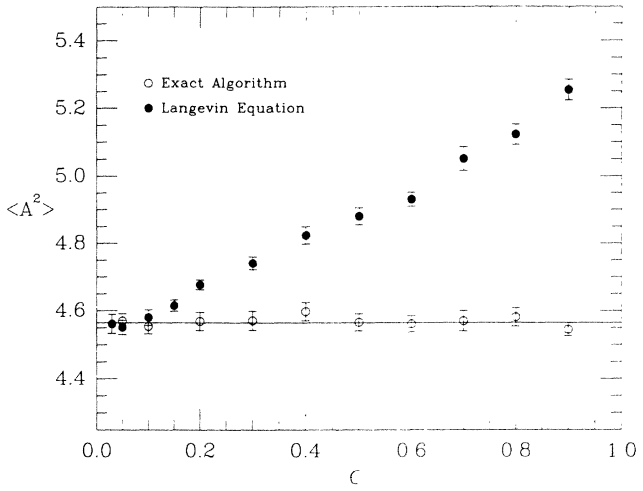

FIG. 3. $\langle A^2 \rangle$ as a function of the step size ϵ. The straight line is the exact result, the open circles are Monte Carlo data obtained from our exact algorithm based on the Langevin equation. The filled circles are data taken without the standard Langevin algorithm.

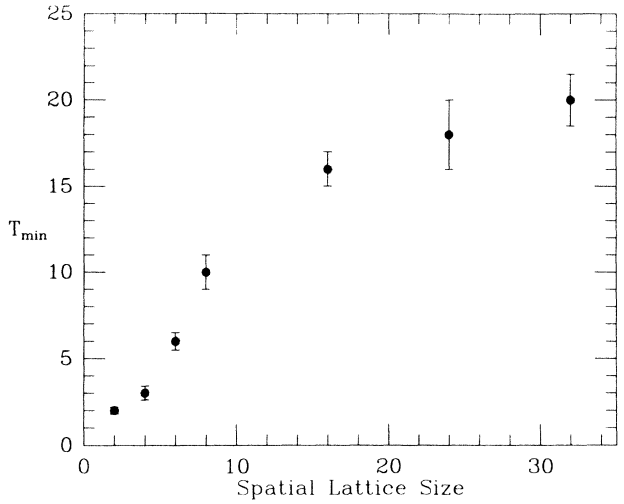

FIG. 4. The minimum correlation time, $T_{\min}$ as a function of spatial lattice size for the algorithm based on the Langevin equation.

be considerably greater.

In Fig. 3 we plot data for $\langle A^2 \rangle$ obtained from the Langevin algorithm as a function of the step size, ϵ. The straight line is the exact result, and the open circles Monte Carlo results using our algorithm. The filled circles are data taken without the final acceptance-rejection step, that is using the standard Langevin algorithm. It is clear that in this case one would not want to use the standard Langevin algorithm with $\epsilon \geq 0.1$, whereas in our exact algorithm $T_{\min}$ occurs at $\epsilon = 0.3$. Thus, in this case the exact algorithm has a distinct advantage. However, we should emphasize again that the relative merits of the algorithms is likely to depend on the model, the lattice size, and even the particular range of parameters being studied.

It is important to understand how $T_{\min}$ varies as a function of the number of degrees of freedom being updated, N. In the absence of long-range correlations, one expects that the maximum step size allowable in the standard pseudofermion or Langevin algorithms will be roughly independent of lattice size. In our exact algorithms we expect $T_{\min}$ to increase as $N^{1/2}$ under these circumstances. This expectation is born out in Fig. 4 where we plot $T_{\min}$ as a function of spatial lattice size for the algorithm based on the Langevin equation. Of course the coefficient of $N^{1/2}$ and in principle the power of N can be decreased by improving the approximate transition probability.

The calculations reported in this paper were carried out on a VAX 11/750, so it was not practical to explore the behavior of $T_{\min}$ on large lattices in three-space and one-time dimensions. While it may not be possible to update all of the degrees of freedom of the A field simultaneously on such lattices, one can also imagine updating a fraction of the lattice at a time. The improved pseudofermion algorithm in particular will be enhanced by updating near neighbors in different passes. Even if the approximate algorithms prove more efficient on large lattices, we believe that it will be useful to have a reasonably efficient exact algorithm for use on intermediate sized lattices. Data such as that shown in Fig. 3 can be used to determine the maximum step size allowable in the approximate algorithms for the desired accuracy. The final acceptance-rejection step can then be removed to collect high statistics data on large lattices.

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