Comparative study of numerical techniques for the simulation of a one-dimensional spinless fermion system

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A comparative study of the efficiency of different algorithms (Metropolis, Langevin, and Hybrid) for the simulation of a one-dimensional spinless fermion model with a half-filled band is presented. The Metropolis updating of the fields is performed with an algorithm introduced by Blankenbecler, Scalapino, and Sugar. The density-density correlation function, the order parameter, and the autocorrelation are calculated. A study of the dependence of the systematic errors on the temperature and the step size for the Langevin and hybrid algorithms is presented. The relation between the accuracy and the speed of the algorithms is studied.

I. INTRODUCTION

At present, some of the most challenging problems in computer simulation techniques are those involving dynamical fermions. The progress of different fields in physics, like condensed matter, and the ultimate test in quantum chromodynamics (QCD), the direct computation of properties of hadronic matter including the effects of dynamical quark loops, depends on the development of an efficient algorithm to simulate systems with fermionic degrees of freedom.

In the path-integral formulation of field theories,[1] fermions are represented by anticommuting variables, not accessible to direct numerical simulation. Thus, they must be replaced by some appropriate boson functional in the action.[2] If the action is quadratic in the fermionic fields, $\psi,\bar{\psi}$, the fermion integral can be done analytically and we find[2,3]

$$\langle O\rangle=\frac{\int[d\phi][d\bar{\psi}\,d\psi]O(\phi)\exp[-S_B(\phi)-\bar{\psi}M(\phi)\psi]}{\int[d\phi][d\psi\,d\psi]\exp[-S_B(\phi)-\psi M(\phi)\psi]}$$
$$=\frac{\int[d\phi]O(\phi)\det M(\phi)\exp[-S_B(\phi)]}{\int[d\phi]\det M(\phi)\exp[-S_B(\phi)]}\,. \quad (1)$$

We can regard this expression as a configurational average, calculated in the canonical ensemble of classical statistical mechanics, where the probability of finding the system in some particular configuration $[\phi]$, is given by the Boltzmann factor $\exp(S_B-\mathrm{tr}\ln M)$.

Unfortunately, for a system described by a nonlocal action of the type described in Eq. (1), the computer time needed to update one single link of the lattice, with the Metropolis algorithm,[4] grows with the cube of the lattice volume. This makes the study of even small systems highly costly.

In the last years there has been an incredible amount of effort directed to the development of efficient techniques to perform the numerical simulation of systems with nonlocal actions. A great part of this effort has been oriented towards designing more practical ways to include the fermion determinant in the Metropolis algorithm. For example, pseudofermion techniques[5] that write the determinant in terms of bosonic fields and perform an auxiliary Metropolis, run to update the pseudofields. Another example is the algorithm developed by Blankenbecler, Scalapino, and Sugar (BSS)[6] that gives an exact calculation of the change in the fermion determinant in terms of the Green's function, this algorithm requires N^{2d} steps per link instead of the LN^{3d} that would require the direct calculation of the fermion determinant. L is the number of temporal sites and N is the number of spatial sites in each one of the d spatial dimensions.

On the other hand, several groups have been exploring alternative ways to calculate averages of the form (1) without relying on the Metropolis algorithm. The main purpose is to develop a global updating procedure where the determinant does not need to be computed so often as in the Metropolis updating. In this category fall the so-called dynamical techniques: microcanonical,[7] Langevin,[8,9] and their combination, the so-called hybrid algorithms.[10,11]

The basic idea behind these dynamical methods is to introduce an extra degree of freedom, a fake time, and describe the evolution of the system by a set of differential equations in such a way that, for large times, the system will reach equilibrium. Configurational averages of the type (1) are replaced by time averages on the dynamical trajectories.[12] The most attractive feature of these techniques is that the computer time required to perform a complete sweep through the lattice grows linearly with the volume. All these methods have shortcomings. Algorithms based on the solution of differential equations involve systematic errors due to the finite step size introduced to find their numerical solution. If in order to get correct physical results, it is necessary to choose time steps that are too small, the evolution of the system will slow down considerably and, in the long run, these methods can be more expensive than the exact updating. Then, the question is, which technique will give the best compromise between the accuracy

and the speed?

In order to shed some light on this controversial topic, the simulation of fermionic systems, we are going to present a comparative study of some of the most promising techniques developed in this field: the Langevin, the hybrid, and the exact updating algorithm developed by BSS.

We believe that the behavior of these techniques can be clarified by studies of simple models. We are going to perform our comparison on a pure fermion system, the one-dimensional (1D) spinless fermion model with a half-filled band.[13] This is a reasonably well-known model, simple enough that it can be extensively simulated but with enough structure to be interesting. This system has a phase transition when the temperature is zero,[14] a crucial characteristic because, by decreasing the temperature, we are going to be able to study the behavior of the algorithms near critical points.

We calculate the density-density correlation function, the order parameter, and the autocorrelation function of sequences of measurements obtained with the different algorithms. From these results we perform a systematic study of the errors and the relative efficiency of the techniques. In Sec. II we are going to describe the 1D spinless fermion model and explain how the fermionic degrees of freedom can be eliminated by the introduction of a Hubbard-Stratonovich transformation.[15]

II. THE 1D SPINLESS FERMION MODEL

The Hamiltonian of the 1D spinless fermion system with a half-filled band is[13]

$$H=-t\sum_i (c_i^\dagger c_{i+1}+c_{i+1}^\dagger c_i) + u\sum_i (n_i-\tfrac{1}{2})(n_{i+1}-\tfrac{1}{2})=H_0+H_1 , \tag{2}$$

where $n_i=c_i^\dagger c_i$ is the number operator of fermions at site i, t is the single-fermion transfer integral between sites, and u is the strength of the nearest-neighbor repulsion. In order to eliminate the quartic term (H_1) we apply a Hubbard-Stratonovich (HS) transformation.[15] This transformation allows the mapping of an interacting fermion system to a system of noninteracting fermions coupled to a fluctuating external field. With a path-integral formulation in mind, we divide the imaginary time interval into L equal subintervals of width $\Delta\tau$, such that $L\Delta\tau=\beta$ (Trotter expansion), where β is the inverse of the temperature. The partition function for the system can be written as

$$\begin{aligned} Z&=\mathrm{Tr}\, e^{-\beta(H_0+H_1)} \\ &=\mathrm{Tr}\prod_{l=1}^{L} e^{-\Delta\tau_l(H_0+H_1)} \\ &=\mathrm{Tr}\prod_{l=1}^{L} e^{-\Delta\tau_l H_0}e^{-\Delta\tau_l H_1}+O(\Delta\tau^2[H_0,H_1]) . \end{aligned} \tag{3}$$

Using the well-known relation for the occupation number

$$n_l n_{l+1}=-\tfrac{1}{2}(n_l-n_{l-1})^2+\tfrac{1}{2}(n_l+n_{l+1}) , \tag{4}$$

and applying the HS transformation, the interacting part of the Hamiltonian can be written as

$$\exp\left[\int_0^\beta d\tau\left[\frac{u}{2}(n_i-n_{i-1})\right]^2\right]=(2\pi\Delta\tau)^{NL/2}\int_{-\infty}^{\infty}\prod_i dx_{i,i+1}\exp\left[-\int_0^\beta d\tau\left[\frac{x_{i,i+1}^2}{2}+\sqrt{u}\,x_{i,i+1}(n_i-n_{i+1})\right]\right] , \tag{5}$$

where $x_{i,i+1}$ is the HS bosonic field associated with the link $i\rightarrow i+1$. After performing the trace over the fermionic degrees of freedom, the partition function takes the form

$$\begin{aligned} Z&=(2\pi\Delta\tau)^{NL/2} \\ &\times\int_{-\infty}^{\infty}\prod_i dx_{i,i+1}\exp[-S_B(x)] \\ &\times\det\left[1+T\exp\left[-\int_0^\beta d\tau\, h(\tau)\right]\right] , \end{aligned} \tag{6}$$

where

$$S_B(x)=\int_0^\beta d\tau\sum_i \tfrac{1}{2}x_{i,i+1}^2 \tag{7}$$

is the bosonic part of the action, T means time ordering, the $h(\tau)$ is an $N\times N$ matrix, where N is the number of spatial sites of the system. The elements of $h(\tau)$ for the time slice l are,

$$\begin{aligned} h(\tau_l)_{ij}&=-t(\delta_{i,j-1}+\delta_{i,j+1}) \\ &+\sqrt{u}\,[x_{i,i+1}(\tau_l)+x_{i,i-1}(\tau_l)]\delta_{i,j} . \end{aligned} \tag{8}$$

Introducing an $N\times N$ matrix at each time interval

$$B_l=\exp[-\Delta\tau h(\tau_l)] , \tag{9}$$

we can write

$$\begin{aligned} Z&=(2\pi\Delta\tau)^{NL/2}\int_{-\infty}^{\infty}\prod_{i=1}^{N} dx_{i,i+1}e^{-S_B(x)} \\ &\times\det(1+B_L B_{L-1}\cdots B_1) . \end{aligned} \tag{10}$$

Also, there is a discrete version of the HS transformation[16] where the interaction is eliminated by a spin-type variable. It has been shown[17] that this transformation is more efficient than the continuous one. However, for the purpose of performing simulations with algorithms that involve differential equations as the Langevin and the hybrid, we are limited to the standard HS transformation that involves continuous variables. In the next sections we are going to describe the algorithms employed to simulate this system.

III. THE EXACT UPDATING

The Metropolis algorithm[4] requires the calculation of the change in the action corresponding to each field change. Field configurations are generated by sweeping through the lattice and making a random change in the field variable at each link. A change is accepted or rejected in a way that assures that once the equilibrium has been reached, the probability of a particular field configuration is proportional to $\exp(-S)$ where S is the action of the system. A straightforward application of this procedure for systems with nonlocal action of the type described by Eq. (1) requires a computer time that grows as LN^{3d}, where L is the number of temporal sites and N is the number of lattice points in each one of the d spatial dimensions. This can be extremely costly even for small systems.

In our calculations we employ an improved Metropolis algorithm developed by BSS.[6] In this algorithm the change in the effective action is written in terms of the Green's function with a considerable reduction of computer time. The equal-time Green's function at the time slice l, defined as

$$g_l(i,j)=\langle c_l^*(i)c_l(j)\rangle \ , \tag{11}$$

can be written in term of the B's matrices as

$$g_l(i,j)=(1+B_{l-1}B_{l-2}\cdots B_1B_L\cdots B_l)^{-1}(i,j) \ . \tag{12}$$

In order to start the simulation we choose some initial field configuration and compute the initial Green's function g_1, accordingly we sweep through the lattice one time slice at a time, making changes in the fields, and then we follow the prescription given by BSS to recompute the action. Going from one time slice to the next, we use the relation

$$g_{l+1}=B_l g_l B_l^{-1} \ . \tag{13}$$

IV. THE LANGEVIN ALGORITHM

In this section and in the next one, we are going to present alternative ways of performing numerical simulations that are believed to be particularly suitable for systems with fermionic degrees of freedom. The basic idea behind these techniques is that the mean value of operators

$$\langle O\rangle=\frac{\int d\phi\, O(\phi)e^{-S(\phi)}}{\int d\phi e^{-S(\phi)}} \ , \tag{14}$$

that are ordinarily calculated with a Metropolis algorithm, can be obtained by solving a set of differential equations instead. If we assume that the system has an extra degree of freedom, a fake time t, we can write a differential equation for the evolution of the fields such that, at large times, they will be distributed with the Boltzmann weight. Now configurational averages defined by (14) can be replaced by time averages[12]

$$\langle O\rangle=\bar{O}=\lim_{T\to\infty}\frac{1}{T}\int_0^T dt\, O(\phi(t)) \ . \tag{15}$$

The simplest equation that can be written that gives the desired equilibrium for large times is the so-called Langevin equation[18]

$$\frac{\partial\phi(x,t)}{\partial t}=-\frac{\partial S}{\partial\phi(x,t)}+\eta(x,t) \ , \tag{16}$$

where $\eta(x,t)$ is a random function that satisfies

$$\langle\eta(x,t)\rangle=0 \ , \tag{17}$$

$$\langle\eta(x,t)\eta(x',t')\rangle=2\delta(x-x')\delta(t-t') \ . \tag{18}$$

The presence of the noise term guarantees that, for sufficiently large times, the field configurations will be distributed with probability density $e^{-S(\phi)}$.

After performing the integration over the fermionic fields, the effective action for the 1D spinless fermion model takes the form

$$e^{-S}=e^{-S_B}\det M=e^{-S_B}\det(1+B_LB_{L-1}\cdots B_1) \ , \tag{19}$$

where S_B and B_l are given by Eqs. (7) and (9), respectively.

Adding an extra degree of freedom, a fake time t, the discrete version of the Langevin equation for this system can be written as

$$x_l(i,t_{n+1})-x_l(i,t_n)=-\epsilon\left[\frac{\partial S_B}{\partial x_l(i,t_n)}-\mathrm{tr}\frac{1}{M}\frac{\partial M}{\partial x_l(i,t_n)}\right]+\sqrt{\epsilon}\eta_l(i,t_n);\ \epsilon=t_{n+1}-t_n \ , \tag{20}$$

now the variable x depends on the site i, the β time slice l, and the Langevin time t. Now, let us show how the term

$$\mathrm{tr}\frac{1}{M}\frac{\partial M}{\partial x_l(i,t_n)}$$

can be expressed in a very convenient way using the formulation described in the last section by the introduction of the Green's function.

Using the cyclic properties of the trace, we can write

$$\begin{aligned}\frac{1}{M}\frac{\partial M}{\partial x_l(i,t_n)}&=\frac{1}{1+B_{l-1}\cdots B_1B_L\cdots B_l}\times\frac{\partial(1+B_{l-1}\cdots B_1B_L\cdots B_l)}{\partial x_l(i,t_n)}\\&=\frac{B_{l-1}\cdots B_1B_L\cdots B_{l+1}B_l}{1+B_{l-1}\cdots B_1B_L\cdots B_l}\frac{1}{B_l}\frac{\partial B_l}{\partial x_l(i,t_n)}\end{aligned} \tag{21}$$

and by introducing the Green's function at the temperature time slice l,

$$g_l=(1+B_{l-1}\cdots B_1B_L\cdots B_l)^{-1} \ , \tag{22}$$

we can write (21) as

$$\frac{1}{M}\frac{\partial M}{\partial x_l(i,t_n)}=(1-g_l)\frac{\partial\ln B_l}{\partial x_l(i,t_n)} \ , \tag{23}$$

and from the definition of B_l we can calculate the term

$$\left[\frac{\partial \ln B_l}{\partial x_l(i,t_n)}\right]_{jk} = -\Delta\tau\sqrt{u}\,\delta_{jk}(\delta_{i,j}-\delta_{i,j+1}) \ . \tag{24}$$

Then, the trace that appears in Eq. (20) can be written as

$$\mathrm{tr}\frac{1}{M}\frac{\partial M}{\partial x_l(i,t_n)} = \Delta\tau\sqrt{u}\,[g_l(i,i)-g_l(i+1,i+1)] \ . \tag{25}$$

Finally, in terms of the Green's function, the discrete Langevin equation takes the form

$$x_l(i,t_{n+1})-x_l(i,t_n) = -\epsilon\Delta\tau\{x_l(i,t_n)-\sqrt{u}\,[g_l(i,i)-g_l(i+1,i+1)]\}+\sqrt{\epsilon}\eta_l(i,t_n) \ , \tag{26}$$

where the first term on the right-hand side comes from taking the derivative of the bosonic action.

At this point, we should make clear our definition of step size. For a system like the 1D spinless fermion model, with a partition function of the form $Z=\mathrm{tr}\prod_l e^{-\Delta\tau H_l}$, a Langevin equation for each field can be defined at each temperature time slice as

$$x(t+1)=x(t)-\Delta\frac{\partial H}{\partial x(t)}+\sqrt{\Delta}\eta'(t) \ , \tag{27}$$

where $\langle\eta'^2\rangle=2/\Delta\tau$, the kinetic energy per degree of freedom. Equations (16) and (27) are equivalent if we make the identification $\Delta_L=\epsilon\Delta\tau$. Then, from now on, when we refer to the step size in the Langevin algorithm, we mean Δ_L. After updating all the fields at the temperature time slice l, we go to the next one, using the relation (13).

A crucial difference between this algorithm and the one described in the preceding section, is that the Langevin method involves a parallel updating. All the sites and all the temperature time slices are updated simultaneously for a given step. The costly process of recomputing the Green's function is performed once per complete update, compared with the Metropolis algorithm, where it must be recomputed after each individual updating.

V. THE HYBRID ALGORITHM

As we already mentioned, there are alternative ways of performing configurational averages of the type (1) without relying on the Metropolis algorithm. The Langevin technique described in the last section is a possible choice. Another obvious choice is to write the equations that describe the classical evolution of the system with constant energy, and replace the configurational averages by time averages over the dynamical trajectories. This is the so-called microcanonical method.[7]

In this section we are going to describe an algorithm that can be considered as an interpolation between the Langevin and the microcanonical algorithms. As we will see, this hybrid method seems to combine the best features of both techniques.

The hybrid algorithm works in the following way. First, an extra degree of freedom, a fake time t, and then a new set of coordinates, the conjugate momenta to the fields, are introduced. The system evolves most of the time with the classical equations of motion (the microcanonical algorithm), and occasionally the momenta are refreshed. This means that all the momenta are replaced by new ones taken from a Gaussian random distribution, normalized in such a way that the average kinetic energy is correct. In this way the system evolves most of the time with the fast algorithm, while the occasional refreshing of the momenta introduces the randomness that will assure ergodicity.[10]

It is easy to see that the Boltzmann distribution is an invariant distribution of the system. The microcanonical steps simply evolve the system along a trajectory of constant H. The refreshing step is designed so that it obviously preserves the distribution.

In the microcanonical approach, the system is given dynamics by writing

$$\dot{\phi}=p \quad \dot{p}=\frac{\partial S}{\partial\phi} \ . \tag{28}$$

Applying a leapfrog algorithm to discretize the above equations, we get

$$\phi(t_{n+1})=\phi(t_n)+\epsilon_H p(t_n)-\tfrac{1}{2}\epsilon_H^2\frac{\partial S}{\partial\phi(t_n)} \ ,$$

$$\epsilon_H=t_{n+1}-t_n \ , \tag{29}$$

where $p(t_n)$ is defined as

$$p(t_n)=\frac{\phi(t_{n+1})-\phi(t_{n-1})}{2\epsilon_H} \ . \tag{30}$$

We can think of the hybrid method in the following way. Starting with Eq. (29), we take each step as a microcanonical step with probability $\epsilon_H q$, or as a Langevin step with probability $(1-\epsilon_H q)$. This is done by selecting

$$p(t_n)=\begin{cases}\dfrac{\phi(t_{n+1})-\phi(t_{n-1})}{2\epsilon_H} & \text{probability } q\epsilon_H, \\ \zeta(t_n) & \text{probability } (1-q\epsilon_H) \ ,\end{cases} \tag{31}$$

where $\zeta(t_n)$ is a Gaussian random term, normalized such that

$$\langle\zeta(t_n)\zeta(t_m)\rangle=\beta^{-1}\delta(t_n-t_m) \ . \tag{32}$$

In the limit $q=0$ (never refreshing), the microcanonical algorithm is recovered. On the contrary, if $q\epsilon_H=1$ (refreshing after each step), we get the Langevin equation with the identification $\epsilon_L=\frac{1}{2}\epsilon_H^2$.

After performing the integration over the fermionic fields, we add an extra degree of freedom, a fake time t. Introducing a new set of variables $p_l(i,t)$, conjugate to the fields $x_l(i,t)$, the discrete system of equations to solve can be written as

$$p_l(i,n-\tfrac{1}{2})=p_l(i,n-\tfrac{3}{2})-\epsilon\left[\frac{\partial S_B}{\partial x_l(i,n-1)}-\mathrm{tr}\frac{1\partial M}{M\partial x_l(i,n-1)}\right],$$
$$x_l(i,n)=x_l(i,n-1)-\epsilon p_l(i,n-\tfrac{1}{2}),\quad \epsilon=t_n-t_{n-1}, \tag{33}$$

where S_B and M have been defined previously.

Taking the expressions (7) and (25), we can write the above system as

$$p_l(i,n-\tfrac{1}{2})=p_l(i,n-\tfrac{3}{2})-\epsilon\Delta\tau\{x_l(i,n-1)-\sqrt{u}\,[g_{l,n-1}(i,i)-g_{l,n-1}(i+1,i+1)]\},$$
$$x_l(i,n)=x_l(i,n-1)+\epsilon p_l(i,n-\tfrac{1}{2}). \tag{34}$$

We ran this algorithm for a predetermined number of steps before refreshing. For the step immediately after the refreshing, the above system of equations must be replaced by

$$p_l(i,n+\tfrac{1}{2})=\zeta(i,n)-\frac{\epsilon\Delta\tau}{2}\{x_l(i,n)-\sqrt{u}\,[g_{l,n}(i,i)-g_{l,n}(i+1,i+1)]\},$$
$$x_l(i,n+1)=x_l(i,n)+\epsilon p_l(i,n+\tfrac{1}{2}). \tag{35}$$

Defining the step size as $\Delta_H=\epsilon_H\sqrt{\Delta\tau}$, it is easy to see that our discretized hybrid algorithm involves an error of order Δ_H^2.

From here on, the procedure is identical to the one already described for the Langevin algorithm. It is interesting to notice that the Langevin algorithm is just the hybrid algorithm with refreshing done at each step, provided we make the identification $\epsilon_L=\epsilon_H^2/2$.

VI. NUMERICAL CALCULATIONS AND RESULTS

We work in a lattice with eight spatial sites and a Trotter expansion parameter $\Delta\tau=0.1$. We verified that a smaller value of $\Delta\tau$ only slows the algorithm without giving any appreciable change in the physical quantities. Since we are going to perform a study of the systematic errors associated with the discretization of the Langevin and hybrid algorithms, we do not want to introduce additional sources of errors so we use an exact algorithm to invert the matrices. In general, to study higher-dimensional systems in bigger lattices, QCD, for example, the computer cost must be kept to a reasonable limit by employing an approximate method to invert the matrices. Conjugate gradient, Gauss-Seidel, and pseudofermions are some of the most common choices.

First we calculate a physical quantity, the density-density correlation function. These results will let us verify that all the programs are working properly and most importantly, perform a study of the errors due to the finite step size introduced in the Langevin and hybrid methods. Also, with the purpose to assess the speed of the different algorithms in the generation of statistically independent configurations, we calculate the order parameter and the autocorrelation function.

A. The density-density correlation function

The density-density correlation function at a distance j is defined by

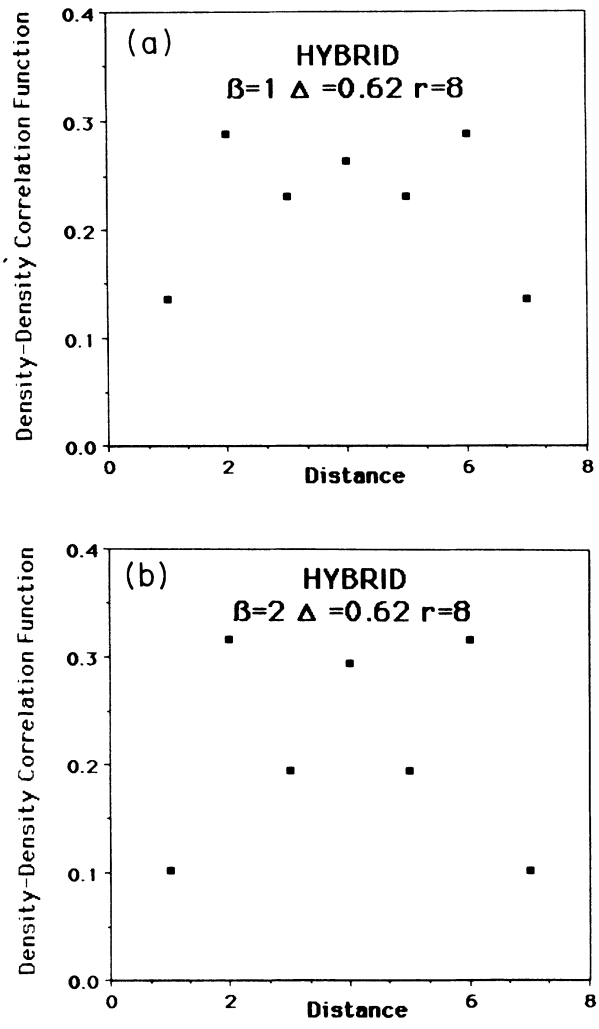

FIG. 1. (a) and (b) Density-density correlation as a function of the distance for $\beta=1$ and 2.

TABLE I. Coefficient $A(i)$ in Eq. (39) for the systematic error in the density-density correlation function at a distance i, calculated with the Langevin algorithm.

	$A(1)$	$A(2)$	$A(3)$	$A(4)$
$\beta=1$	0.0105±0.0006	0.0175±0.0007	0.0110±0.0009	0.0072±0.0009
$\beta=2$	0.0238±0.0009	0.0378±0.002	0.0361±0.002	0.0368±0.002
$\beta=3$	0.28±0.4	0.65±0.7	0.59±0.8	0.77±0.9

$$d(j)=\langle n(i)n(i+j)\rangle \ , \tag{36}$$

where $n(i)$ is the occupation number at the site i and can be obtained from the Green's function

$$n(i)=1-g(i,i) \ . \tag{37}$$

The density-density correlation function gives an insight into how the particles are distributed in the lattice and serves as a measure of the relative strength of the two components of the Hamiltonian. At high temperatures, the hopping term must predominate and the particles must tend to be uniformly distributed in the sites. At low temperatures the repulsion term tends to dominate, leading to occupation on alternative sites, i.e., an alternating $d(j)$. As an illustration, Figs. 1(a) and 1(b) show the density-density correlation function for different values of the temperature.

Since the Metropolis algorithm is an exact updating method, the errors presented in its results are only of statistical nature. On the other hand, the errors in the quantities calculated with the Langevin and the hybrid algorithms are not only due to statistical effects, but also to systematic errors introduced by the finite step size. These errors are going to be analyzed in detail in the next section.

B. Systematic errors

The systematic errors are calculated by subtracting the value of the density-density correlation function $d(i)$ obtained with the Langevin or the hybrid algorithm from the value obtained with the Metropolis algorithm, i.e.,

$$\Delta d(i)=d(i)-d_M(i) \ . \tag{38}$$

Since we use a first-order discretization algorithm to solve the Langevin equation, its systematic errors must be proportional to the step size, i.e.,

$$[\Delta d(i)]_L=A_L(i)\Delta_L=A_L(i)\epsilon_L\Delta\tau \ . \tag{39}$$

On the other hand, since we are using a second-order discretization scheme to solve the system of equations associated with the hybrid method, we expect that its systematic error goes as

$$[\Delta d(i)]_H=A_H(i)\Delta_H^2=A_H(i)\epsilon_H^2\Delta\tau \ . \tag{40}$$

The values of the coefficients $A(i)$, are shown in Tables I and II.

We must mention that we made a slight modification to the algorithm described in Sec. V. During the microcanonical part of the algorithm, the system should evolve with constant energy. However, the numerical method involves a discrete time step and energy conservation is violated at some high order of the time step. We try to minimize this effect by rescaling the momenta after each microcanonical step such that

$$p_i'=\left[\frac{\langle E_k\rangle}{\frac{1}{2}\sum_i p_i^2}\right]^{1/2} p_i \ , \tag{41}$$

where $\langle E_k\rangle$ is the average kinetic energy of the system, equal to one-half the number of degrees of freedom,

$$\langle E_k\rangle=\tfrac{1}{2}LN \tag{42}$$

with N the number of spatial sites and L the number of time slices associated with the Trotter expansion $L=\beta/\Delta\tau$. This modification helps to preserve energy conservation on the average and lets us keep the stability of the system for large values of the step size and, in particular, for large intervals between refreshing.

C. Autocorrelation function

To establish the efficiency of the algorithms in the generation of statistically independent configurations, we are going to study the behavior of the autocorrelation function. In order to calculate the autocorrelation function we need to compute the order parameter of the system which is defined as

$$O=\frac{1}{N}\sum_{i=1}^{N}(-1)^i(n_i-\tfrac{1}{2}) \ , \tag{43}$$

where N is the number of spatial sites.

Due to the particle-hole symmetry, otherwise equivalent configurations can differ in the sign of the order parameter. For the purpose of calculating the auto-

TABLE II. Coefficient $A(i)$ in Eq. (40) for the systematic error in the density-density correlation function at a distance i, calculated with the hybrid algorithm.

	$A(1)$	$A(2)$	$A(3)$	$A(4)$
$\beta=1$	0.0028±0.0005	0.0023±0.0005	0.0016±0.0009	0.0027±0.0007
$\beta=2$	0.0018±0.0005	0.0032±0.0007	0.0020±0.001	0.0027±0.001
$\beta=3$	1.48±0.5	2.1±0.7	2.2±1	2.0±1

correlation, we are only interested in distinguishing between configurations which differ in the absolute value of the order parameter. The autocorrelation function after M sweeps is defined as

$$C(M)=\frac{\langle O'(m)O'(m+M)\rangle-\langle O'(m)\rangle^2}{\langle O'^2(m)\rangle-\langle O'(m)\rangle^2}\ , \tag{44}$$

where

$$\langle O'(m)O'(m+M)\rangle=\frac{1}{M-S}\sum_{m=1}^{M-S}O'(m)O'(m+M) \tag{45}$$

with S the total number of sweeps and $O'(m)=\mathrm{abs}[O(m)]$.

For Markov processes like the microcanonical and the Langevin, the fluctuations of the probability around the equilibrium distribution decay exponentially with the time, such that the autocorrelation function behaves as

$$C(t)=C_0e^{-\gamma t}\ . \tag{46}$$

In order to calculate the inverse correlation time γ, we do the following. First we calculate the autocorrelation function according to Eq. (44) and then we define an inverse correlation time γ_m for the mth interval as

$$\gamma_m=-\ln C(t_{m+1})+\ln C(t_m)\ . \tag{47}$$

We get the value of γ by averaging the γ_m over the range where they are approximately constant. The values of γ calculated in this way for the Metropolis and the Langevin techniques are shown in Table III.

For the hybrid method, the situation is somewhat different. This method has an extra parameter, the refreshing frequency, that can be tuned in order to optimize the algorithm. The best value of the refreshing frequency will be the one for which the autocorrelation time takes its minimum value. To find this value, we run the algorithm with a fixed value of the time-step size $\epsilon\sqrt{\Delta\tau}$ and different values of the refreshing interval $r\epsilon\sqrt{\Delta\tau}$, and see how the autocorrelation behaves.

We found that the autocorrelation time has a maximum in the Langevin limit $r=0$ (refreshing after each step), and decreases as we increase r, until a point when the autocorrelation function starts to show strong periodic fluctuations. Since each microcanonical step requires the values of the fields at the two previous steps, the sequence of the configurations generated by this algorithm does not constitute a Markov chain, then we do not know *a priori* the theoretical behavior of the autocorrelation function for the hybrid method. However, the sequence obtained by taking into account only configurations separated by a refreshing interval constitute a Markov chain because each configuration can be obtained from the precedent by following the recipe given by the algorithm.

TABLE III. Inverse correlation time γ.

	Metropolis	Langevin	Hybrid
$\beta=1$	0.24±0.02	0.56±0.03	0.68
$\beta=2$	0.19±0.03	0.49±0.02	0.459±0.02
$\beta=3$	0.21±0.04		
$\beta=4$	0.17±0.03		

The autocorrelation function at a distance M (between sweeps), calculated by taking in account configurations obtained just after the refreshing step, is

$$C^{ar}(M)=C_0e^{-\gamma\sqrt{\Delta\tau}\epsilon M}=C_0e^{-\gamma\sqrt{\Delta\tau}\epsilon rN}\ . \tag{48}$$

From here the procedure to calculate γ is identical to the one already described. Table III also shows the results for the inverse correlation time calculated for the hybrid algorithm.

A complete sweep through the lattice with the Metropolis algorithm takes twice the time that it takes with the Langevin and the hybrid. These last two algorithms take approximately the same time.

VII. DISCUSSION OF RESULTS

So far we have shown the results obtained for the different test we consider necessary to perform in order to evaluate the relative efficiency of the algorithms. In this section we are going to analyze the results and try to find out which technique gives the best compromise between accuracy and speed.

As we already mentioned, the only source of error of our Metropolis algorithm comes from the finite size of the samples. Since the statistical error is inversely proportional to the square root of the number of statistically independent sweeps $\sigma\sim N^{-1}$, to change the accuracy of a measurement from x_0 to x, i.e., by a factor $\alpha=x_0/x$, the number of sweeps must change as $N=N_0\alpha^2$. Considering that the computer time is proportional to the number of sweeps, the time needed for the Metropolis algorithm to change the accuracy by a factor α goes as

$$T_M=T_{0M}\alpha^2\ , \tag{49}$$

where T_{0M} is the computer time that takes to obtain an accuracy of x_0.

The situation is different for the Langevin and the hybrid methods. The degree of accuracy of these algorithms depends on statistical and systematic errors. As a rule, in a simulation we want to keep these two errors of the same order. As in the Metropolis algorithm, to reduce the statistical error by a factor of α, the number of sweeps must increase by a factor of α^2, but now in order to decrease the systematic error by the same amount without changing the statistical error, the number of sweeps must increase by an extra factor of α for the first-order Langevin equation, or by a factor of $\alpha^{1/2}$ for the hybrid method, since it involves a second-order discretization scheme. Then, in order to change the overall error by a factor of α, the computer time must change as

$$T_L=T_{0L}\alpha^3,\quad T_H=T_{0H}\alpha^{5/2}\ , \tag{50}$$

where T_{0L} (T_{0H}) is the computer time that it takes to produce results with an error of x_{0L} (x_{0H}) with the Langevin (hybrid) algorithm.

TABLE IV. Values of the time step size for which the algorithms are equivalent to the Metropolis. Calculated with Eq. (53).

	Langevin	Hybrid
$\beta=1$	$\Delta_0^L=0.22\pm0.02$	$\Delta_0^H=0.172\pm0.02$
$\beta=2$	$\Delta_0^L=0.20\pm0.03$	$\Delta_0^H=0.21\pm0.01$

If there is some error for which two of the techniques are equivalent (take the same computer time), the ratio between the computer time that it will take the techniques to change this error by a factor of α can be expressed as

$$\frac{T_L}{T_M}=\frac{T_0\alpha^3}{T_0\alpha^2}=\alpha \quad \text{(Langevin-Metropolis)},$$

$$\frac{T_H}{T_M}=\frac{T_0'\alpha^{5/2}}{T_0'\alpha^2}=\alpha^{1/2} \quad \text{(hybrid-Metropolis)}, \tag{51}$$

$$\frac{T_L}{T_H}=\frac{T_0''\alpha^2}{T_0''\alpha^{5/2}}=\alpha^{1/2} \quad \text{(Langevin-hybrid)}.$$

Now, taking into account the difference in the computer time employed by these algorithms to perform a single sweep through the lattice, they will generate statistically independent configurations in the same computer time if

$$\frac{1}{\gamma_L\epsilon_L\Delta\tau}=\frac{1}{\gamma_M}\frac{t_M}{t_L} \quad \text{(Langevin-Metropolis)},$$

$$\frac{1}{\gamma_H\epsilon_H\sqrt{\Delta\tau}}=\frac{1}{\gamma_M}\frac{t_M}{t_H} \quad \text{(hybrid-Metropolis)}, \tag{52}$$

$$\frac{1}{\gamma_L\epsilon_L\Delta\tau}=\frac{t_H}{\gamma_H\epsilon_H\sqrt{\Delta\tau}t_L} \quad \text{(hybrid-Langevin)},$$

i.e., the correlation time in units of lattice sweeps for one algorithm must be equal to the correlation time of the other algorithm, multiplied by the ratio between the respective computer times per sweep.

The above relations are satisfied if

$$\Delta_L^M=\epsilon_L\Delta\tau=\frac{\gamma_M}{\gamma_L}\frac{t_L}{t_M} \quad \text{(Langevin-Metropolis)},$$

$$\Delta_H^M=\epsilon_H\sqrt{\Delta\tau}=\frac{\gamma_M}{\gamma_H}\frac{t_H}{t_M} \quad \text{(hybrid-Metropolis)}, \tag{53}$$

$$\frac{\Delta_H^L}{\Delta_L^H}=\frac{\epsilon_H}{\epsilon_L'}\frac{\Delta\tau}{\sqrt{\Delta\tau}}=\frac{\gamma_L t_H}{\gamma_H t_L} \quad \text{(hybrid-Langevin)}.$$

These values are shown in Table IV. By substituting the values for the step size given in Table IV in Eqs. (38) and (39), we can calculate the percentage of error at which the algorithms are equivalent. This percentages are shown in Table V. For errors above these quantities, the Langevin and hybrid are faster than the Metropolis. To calculate the relative amount of computer time that will take to change these errors by a factor of α, we must use relations (51).

The results of this comparison are summarized in Figs. 2(a) and 2(b) where we plot the computer time in terms of

TABLE V. Percentage of error in the density-density correlation function $d(1)$, calculated with the step sizes given in Table IV. This is the error that must be accepted before the algorithms start to become faster than the Metropolis.

	Langevin (%)	Hybrid (%)
$\beta=1$	$x(1)=1.7\pm0.2$	$x(1)=0.06\pm0.02$
	$x(2)=1.3\pm0.2$	$x(2)=0.02\pm0.007$
	$x(3)=1.0\pm0.1$	$x(3)=0.02\pm0.01$
	$x(4)=0.58\pm0.07$	$x(4)=0.03\pm0.01$
$\beta=2$	$x(1)=4.7\pm0.8$	$x(1)=0.08\pm0.02$
	$x(2)=2.4\pm0.4$	$x(2)=0.05\pm0.01$
	$x(3)=3.7\pm0.6$	$x(3)=0.05\pm0.02$
	$x(4)=2.5\pm0.4$	$x(4)=0.04\pm0.02$

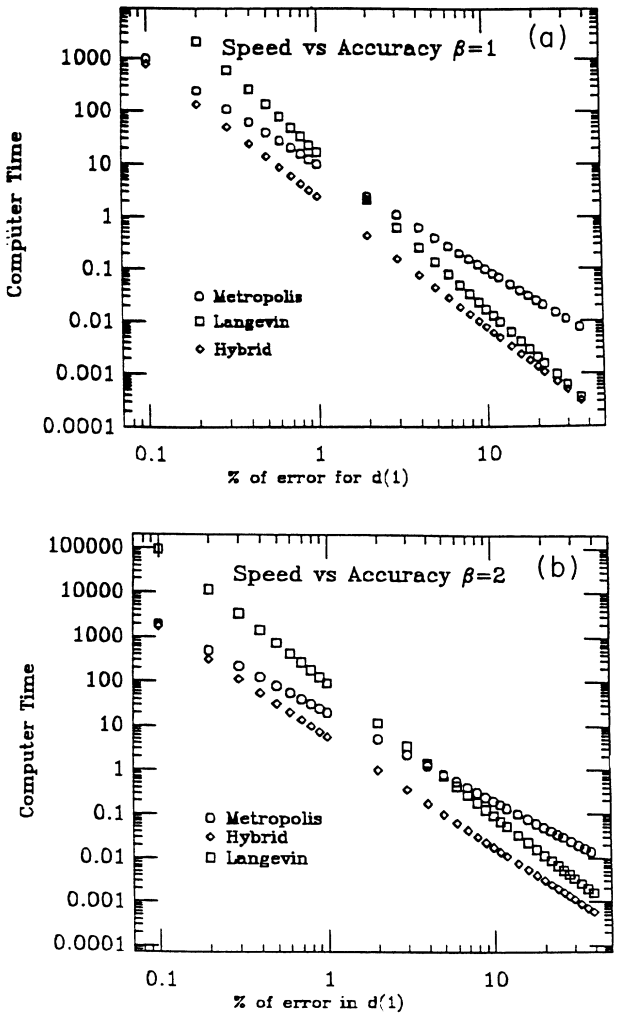

FIG. 2. (a) and (b). Computer time vs the percentage of error in the density-density correlation function at one unit of distance 1, $d(1)$ for $\beta=1$ and 2.

the percentage of error in the density-density correlation time at one unit of distance $d(1)$. We choose $d(1)$ because it is the quantity that consistently has the biggest error. To make these graphs, we arbitrarily assign a value of $t_M = 10$ (20) for the computer time that takes the Metropolis algorithm to generate results with an error of 1% for $\beta = 1$ (2).

Notice that x_0 is very small for $\beta = 1,2$, so, in practice, the hybrid is always faster than the Metropolis, unless we want to have errors of approximately 0.06% or less. Also, we can see that the first-order Langevin algorithm is always slower than the hybrid, but faster than the Metropolis if we can accept errors above a few percent (see Table V).

If we kept decreasing the temperature (i.e., $\beta = 3,4$), we found that the Langevin and the hybrid algorithms start to perform quite badly, we must substantially decrease the size of the time step and perform proportionally more sweeps, increasing the computer time considerably. The minimum error x_0 we must accept before the Langevin and the hybrid algorithms start to become faster than the Metropolis, must depend on the size of the system. The computer time per sweep increases faster with the size for the Metropolis-BSS algorithm ($\sim$size,[3] to update a single site) than for the Langevin or the hybrid ($\sim$size, to perform a complete sweep), but at low temperatures we must perform many more sweeps for the dynamical algorithms (due to the smaller size of the time step), so it is not obvious which method will give better results at low temperatures in bigger lattices.

VIII. CONCLUSIONS

In this work we present a comparative study of the efficiency of different techniques (Metropolis, Langevin, hybrid) in the simulation of a 1D spinless fermion model. Our study shows that all the techniques presented are able to simulate the correct behavior of the system. We also show how the BSS technique of writing the change in the effective action in terms of the Green's function can be applied successfully to the Langevin and the hybrid techniques.

We conclude that at $\beta = 1,2$, and for the system with eight spatial sites, the hybrid method definitely represents the best choice. The Langevin algorithm is faster than the Metropolis for errors above a few percent but, in practice, is always slower than the hybrid. We expect that for larger systems, at these temperatures, the advantage of the Langevin and the hybrid algorithms with respect to the Metropolis will be even more accentuated.

When we kept decreasing the temperature ($\beta = 3,4$), we found the discouraging fact that, in order to keep the stability of the Langevin and the hybrid updated, we needed to decrease the step size in such amount that the system evolves so slowly that these techniques become even more computationally expensive than the exact updating. However, since the exact algorithm becomes very costly for large volumes, it is not obvious that it will continue outperforming the Langevin and the hybrid if the lattice size increases. There is the hope that the slowing down in the two dynamical algorithms due to the decreasing values of the step size is still small compared with the cost of performing the exact updating when the size increases. Lamentably, it is not clear that this would happen.

The fermion matrix becomes a rapidly varying function of the HS variables at low temperatures, so does the Green's function. We believe that the step size in the Langevin and the hybrid methods is inversely proportional to the highest eigenvalue of the Green's function and this eigenvalue increases abruptly when the a phase transition is approached, i.e., the temperature is lowered. Something similar happens for a free-field theory[19] where the time step must be adjusted depending on the highest-frequency mode $k_{\max}$ such that $\Delta < 1/(k_{\max}^2 + m^2)$. This fact and the big errors that we get for these small values of the step size, due in part to the fact that the long-wavelength modes are not efficiently equilibrated, make it hard to decide if these techniques will be able to outperform the exact updating at low temperatures.

We conclude that the Langevin and the hybrid algorithms, in particular, the last one, are fast alternatives to the simulation of fermionic systems not very close to a transition point. Actually, they can be applied quite successfully to search for phase transitions. Near phase transitions, the increasing steps sizes required by these techniques, and the consequent slowing down in the algorithms, make it unclear whether they can be considered a real alternative to the exact updating. It will be interesting to repeat this study with the recently introduced fast Fourier acceleration techniques[9] and to verify if they effectively improve the performance of the Langevin and the hybrid simulations at low temperature.

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