Comparative study of the discrete and the continuous Hubbard-Stratonovich transformation for a one-dimensional spinless fermion model

G. M. Buendia
Department of Physics, University of California, San Diego, La Jolla, California 92093
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A comparative study of the discrete and the continuous Hubbard-Stratonovich transformation is presented. With the use of the Metropolis algorithm, the Monte Carlo time correlation functions for a one-dimensional spinless fermion model are calculated for both methods. The results show the discrete method to be more efficient.

I. INTRODUCTION

In the last few years there has been considerable effort to develop techniques to make possible the numerical study of systems with fermionic degrees of freedom. As a result of this interest considerable progress has been made in this field, and at the moment several different techniques are available.

Recently Hirsch[1] introduced a procedure to eliminate the fermion-fermion interaction by the introduction of an auxiliary discrete variable. The aim of this work is to present a comparative study in terms of the autocorrelation function of this method and a more conventional Hubbard-Stratonovich[2] (HS) transformation where a continuous field is introduced.

We use the one-dimensional spinless fermion model with nearest-neighbor interactions and half-filled band. The Hamiltonian of the system is

$$H=-t\sum_i (c_i^\dagger c_{i+1}+c_{i+1}^\dagger c_i)+u\sum_i (n_i-\tfrac{1}{2})(n_{i+1}-\tfrac{1}{2}) , \tag{1.1}$$

where t is the single fermion transfer integral between sites and u is the strength of the nearest-neighbor repulsion.

In order to perform a Monte Carlo simulation we use the algorithm introduced by Blankenbecler, Scalapino, and Sugar[3] (BSS), that gives an exact calculation of the change in the fermion determinant in terms of the Green function.

We calculate the density-density correlation function, the order parameter, and the autocorrelation function of the sequence of measurements using both methods.

In Secs. II and III we present a brief review of the discrete and continuous HS transformations, the Monte Carlo method used, and the BSS algorithm. For a more detailed explanation see, for example, the appendix of Gubernatis, Scalapino, Sugar, and Toussaint.[4]

II. HUBBARD-STRATONOVICH TRANSFORMATIONS

The HS transformation is based on the identity[2]

$$\exp(\tfrac{1}{2}A^2)=(2\pi)^{1/2}\int_{-\infty}^{\infty} dx\,\exp(-\tfrac{1}{2}x^2-xA) . \tag{2.1}$$

This allows the mapping of an interacting fermion system to a system of noninteracting fermions coupled to a fluctuating external field.

The Hamiltonian of our system can be written as the sum of two parts

$$H=H_0+H_1 , \tag{2.2}$$

where H_1 contains the interacting term and H_0 the bilinear. We use a path integral formulation in order to apply the HS transformation to eliminate the interacting term. We divide the imaginary-time interval into L equal subintervals of width $\Delta\tau$, such that $L\Delta\tau=\beta$. After doing that, the partition function of the system can be written as

$$Z=\mathrm{Tr}\,e^{-\beta(H_0+H_1)}=\mathrm{Tr}\prod_{l=1}^{L} e^{-\Delta\tau(H_0+H_1)}$$
$$\approx\mathrm{Tr}\left[T\exp\left[-\int_0^\beta d\tau(H_0+H_1)\right]\right]+O((\Delta\tau)^2[H_0,H_1]) . \tag{2.3}$$

Now are going to describe how the two methods work in our particular case.

A. Gaussian (continuous)

Using the well-known relation for the occupation number

$$n_i n_{i+1}=-\tfrac{1}{2}(n_i-n_{i+1})^2+\tfrac{1}{2}(n_i+n_{i+1}) , \tag{2.4}$$

we can write the interacting term of the Hamiltonian as

$$H_1=u\sum_i (n_i-\tfrac{1}{2})(n_{i+1}-\tfrac{1}{2})=-\frac{u}{2}\sum_i (n_i+n_{i+1})^2+\frac{u}{4} . \tag{2.5}$$

Using the HS transformation we get for each time subinterval

$$\exp\left[\int_0^\beta d\tau\frac{u}{2}\sum_i (n_i+n_{i+1})^2\right]=(2\pi)^{-N/2}\int\prod_{i=1}^{N} dx_{i,i+1}\exp\int_0^\beta d\tau[-\tfrac{1}{2}x_{i,i+1}^2-x_{i,i+1}\sqrt{u}\,(n_1-n_{i+1})] , \tag{2.6}$$

where $x_{i,i+1}$ is a bosonic field associated with the link $i \rightarrow i+1$.

Since now the Hamiltonian is quadratic in the fermion operators, the trace over the fermionic degrees of freedom can be performed analytically, and the partition function takes the form

$$Z=(2\pi)^{-N/2}\int \prod_{i=1}^{N} dx_{i,i+1} e^{-S_\beta} \times \det\left[1+T\exp\left[\int_0^\beta d\tau h(\tau)\right]\right], \tag{2.7}$$

where

$$S_\beta = \int_0^\beta d\tau \sum_i \tfrac{1}{2} x_{i,i+1}^2 , \tag{2.8}$$

is the bosonic part of the action.

For our one-dimensional model $h(\tau)$ is an $N\times N$ matrix, where N is the size of the system. Its elements are

$$h_{i,j}(\tau_l) = -t(\delta_{i,j-1}+\delta_{i,j+1}) + \sqrt{u}\,[x_{i,i+1}(\tau_l)+x_{i,i-1}(\tau_l)]\delta_{i,j} . \tag{2.9}$$

If we define an $N\times N$ matrix for each time subinterval

$$B_l = \exp(-\Delta\tau\, h(\tau_l)) \tag{2.10}$$

then we can write

$$Z=(2\pi)^{-NL/2}\int \prod_{i=1}^{N} dx_i\, e^{-S_\beta} \det(1+B_L B_{L-1}\cdots B_1) . \tag{2.11}$$

B. Discrete

The idea behind this method is that since the fermi occupation number can take only the values 0 or 1, a field that takes only two values must be enough to eliminate the fermion interaction.[1]

The following identity is used:

$$\exp\{[-\Delta\tau u(n_i-\tfrac{1}{2})(n_{i+1}-\tfrac{1}{2})]\} = \frac{e^{-\Delta U/4}}{2}\sum_{S_i=\pm 1} e^{\Delta\tau J(n_i-n_{i+1})s_{i,i+1}}, \tag{2.12}$$

$$J=(\Delta\tau)^{-1}\cosh^{-1}\left[\exp\frac{\Delta\tau u}{2}\right], \tag{2.13}$$

now $s_{i,i+1}$ is the spin variable associated with the lattice link $i\rightarrow i+1$.

Performing the trace over the fermion degrees of freedom

$$Z=\sum_{S_i=\pm 1}\det\left[1+T\exp\left[-\Delta\tau\sum_l h(l)\right]\right], \tag{2.14}$$

where $h(\tau_l)$ has a similar expression as before, with the discrete variable s instead of the continuous x.

$$h_{i,j}(\tau_l) = -t(\delta_{i,j-1}+\delta_{i,j+1})+J[s_{i,i+1}(\tau_l)+s_{i,i-1}(\tau_l)]\delta_{i,j} . \tag{2.15}$$

Using the same expression for B_l than in the continuous case, the partition function has the form

$$Z=\sum_{S_i=\pm 1}\det(1+B_L B_{L-1}\cdots B_1) . \tag{2.16}$$

It is important to notice the absence of the bosonic part of the action in the partition function for the discrete method.

III. MONTE CARLO CALCULATIONS

The Metropolis *et al.*[5] algorithm requires the calculation of the change in the action corresponding to each field change. Field configurations are generating by sweeping through the lattice and making a random change in the field variable at each link or, in the discrete method, flipping the spin variable. 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 it the action of the system. For a system with interacting fermions the effective action $\exp(-S)=\exp(-S_b)\det M$, is, in general, nonlocal and repeated calculations of its variations can be very time consuming.

In this work we follow the procedure proposed by BSS, in which the updating of the effective action requires N^2 steps, instead of the N^3 required in the direct calculation of the fermion determinant.

IV. RESULTS

We work with a lattice of 8 spatial sites, at $\beta=1$.

Figure 1 shows the results for the density-density correlation function

$$D(j)=\langle n(i)n(i+j)\rangle , \tag{4.1}$$

where the fermion occupation number is obtained from the Green function using the relation

$$n(i)=1-g_1(i,i) . \tag{4.2}$$

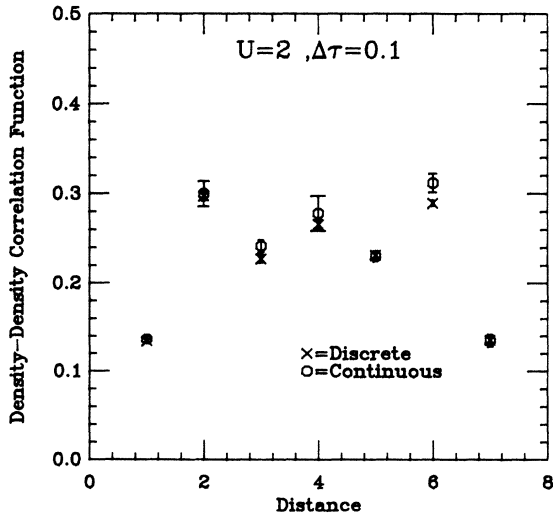

FIG. 1. Density-density correlation function in terms of the distance.

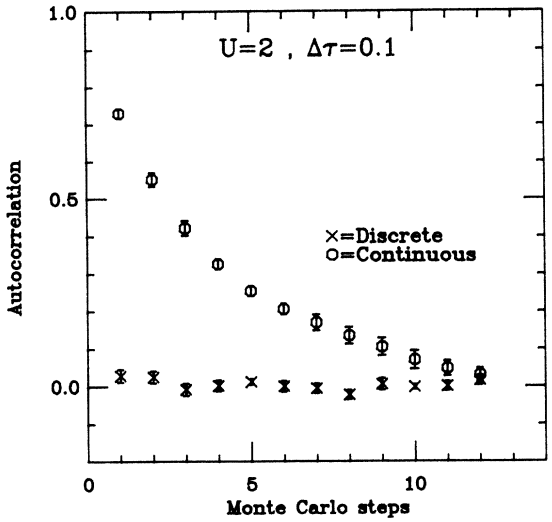

FIG. 2. Autocorrelation function in terms of the number of Monte Carlo steps.

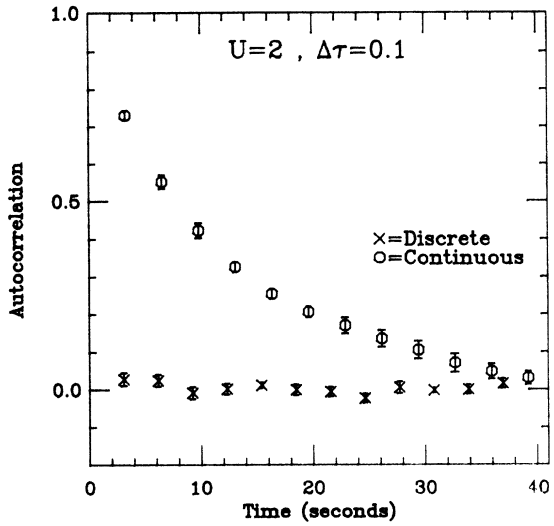

FIG. 3. Autocorrelation function in terms of the computer time.

As we can see both methods produce basically the same results, but the error bars are larger for the continuous method. The graphs show the symmetry with respect to the middle point expected from the periodic boundary conditions imposed.

We repeated the calculations for different sizes of the time subinterval, because we were interested in seeing how big we can make the time slices (which implies an important reduction in computer time) and still obtain the same physical results. We found that $\Delta\tau=0.1$ and $\Delta\tau=0.05$ gives the same values for the density-density correlation function, but the values were different when calculated for $\Delta\tau=0.5$, so we choose $\Delta\tau=0.1$ as the size that gives the best compromise between accuracy and efficiency.

Due to the particle-hole symmetry, positive and negative values of the order parameter are equivalent, so it is not necessarily interesting to consider changes in sign. We use the absolute value of the order parameter

$$O'=|O|=\left|\frac{1}{N}\sum_{i=1}^{N}(-1)^i(n_i-\tfrac{1}{2})\right| , \tag{4.3}$$

to calculate the autocorrelation function in terms of the number of Monte Carlo steps,

$$C(mcs)=\frac{\langle O'(mcs)O'(0)\rangle-\langle O'(0)\rangle^2}{\langle O'^2(0)\rangle-\langle O'(0)\rangle^2} , \tag{4.4}$$

where

$$\langle O'(mcs)O'(0)\rangle=\frac{1}{N-mcs}\sum_{i=1}^{N-mcs}O'(i)O'(i+mcs) , \tag{4.5}$$

and N is the size. The results are shown in Fig. 2.

Since we are interested in comparing the efficiency of the two methods, it is important to take into account the computer time employed for each one. In Fig. 3 we show the time correlation function in terms of the computer time. The relation between the time per step, for the continuous to the discrete is around 1.4.

The error bars are calculated by taking all the measurements and grouping them in five blocks. The values obtained in this way are statistically independent, and we use the standard deviation of the mean as an error estimate.

V. CONCLUSIONS

The results favored the discrete method in quite a conclusive way; it takes less computer time per sweep, and the correlation function decays in fewer sweeps, so it is easier to produce statistically independent quantities with this formulation.

Calculations for other values of u, and for time slices of different sizes, again support this conclusion.

By changing the distance between successive values of the parameter we can change the acceptance fraction in the continuous method. We check that this does not affect our results.

We speculate that the origin of the differences between both methods must be due to the size of the phase space which is much smaller for the discrete formulation than for the continuous, so can it be covered faster.

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[1]J. E. Hirsch, Phys. Rev. B **28**, 4049 (1983).
[2]J. Hubbard, Phys. Rev. Lett. **3**, 77 (1959).
[3]R. Blankenbecler, D. J. Scalapino, and R. L. Sugar, Phys. Rev. D **24**, 2278 (1981); D. J. Scalapino and R. L. Sugar, Phys. Rev. B **24**, 4295 (1981).
[4]J. E. Gubernatis, D. J. Scalapino, R. L. Sugar, and W. D. Toussaint, Phys. Rev. B **32**, 103 (1985).
[5]N. Metropolis, A. Rosenbluth, M. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. **21**, 1087 (1953).