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Stable Monte Carlo algorithm for fermion lattice systems at low temperatures

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We discuss Monte Carlo algorithms for fermion lattice systems based on exact updating of the fermion Green's function. A space and a space-time algorithm are shown to be limiting cases of a formulation that smoothly interpolates between them. This new formulation can to a large extent preserve the desirable features of both limits and suppress the undesirable ones.

The study of strongly interacting quantum many-body systems by numerical techniques is of great current interest. We discuss here fermion lattice systems, and, in particular, the Hubbard model,

$$H=\sum_{\substack{i,j\\ \sigma}} t_{ij}(c_{i\sigma}^{\dagger}c_{j\sigma}+\text{H.c.})+U\sum_i n_{i\uparrow}n_{i\downarrow}-\mu\sum_{i\sigma}n_{i\sigma}\,, \tag{1}$$

as a typical example. Here, $c_{i\sigma}^{\dagger}$ is a creation operator for a fermion of spin σ at lattice site i, and $n_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$. Simplified models such as (1) and generalizations are thought to capture the essential physics of various many-body phenomena in solids, perhaps including high-temperature superconductivity.

Often, it is the properties of the ground state, or of the system at very low temperatures, that one is most interested in. Unfortunately, no Monte Carlo approach to deal directly with fermion lattice systems such as Eq. (1) at zero temperature exists (except in one spatial dimension). Thus, Monte Carlo studies of these models are performed at finite temperatures using a path-integral formulation, and it is then desirable to reach as low a temperature as possible.

In this paper we discuss Monte Carlo approaches based on exact updating of the fermion Green's function. The basic approach was introduced by Blankenbecler, Scalapino, and Sugar[1] (BSS) and has been used for a variety of studies of lattice systems[2,3] and magnetic-impurity systems.[4] However, that approach becomes unstable at low temperatures. A modified approach was introduced recently by Hirsch and Fye[5] (HF) for magnetic impurity systems, which was found to be stable at low temperatures. That approach can also be used for lattice systems[6] (where it remains stable), but is considerably more time consuming than the BSS approach. Here we discuss an approach that interpolates between BSS and HF that can be kept stable at low temperatures and is considerably more efficient than the HF approach for lattice systems. Very recent work by White and co-workers[7] discusses somewhat related ideas in the context of molecular-dynamics simulations of the Hubbard model.

The partition function for the model Eq. (1) on an N-site lattice is written as

$$Z=\text{Tr}e^{-\beta H}=\text{Tr}\prod_{l=1}^{L}e^{-\Delta\tau H}\cong\text{Tr}\prod_{l=1}^{L}e^{-\Delta\tau H_0}e^{-\Delta\tau H_1}\,, \tag{2}$$

with $H=H_0+H_1$. The error in thermodynamic averages caused by the Trotter approximation in Eq. (2) is of order $\Delta\tau^2$.[8] We take as H_1 the interaction part of the Hamiltonian, and decouple it by introducing auxiliary Ising variables[9]

$$\exp(-\Delta\tau U n_{i\uparrow}n_{i\downarrow})=\tfrac{1}{2}\,\text{Tr}_{\mu=\pm 1}\exp[\lambda\mu(n_{i\uparrow}-n_{i\downarrow})-\Delta\tau U(n_{i\uparrow}-n_{i\downarrow})/2] \tag{3}$$

with $\cos(h\lambda)=\exp(\Delta\tau U/2)$. The trace over fermion degrees of freedom can now be explicitly taken, and one obtains, in a "space formulation"[1]

$$Z=\text{Tr}_{\mu}\det\tilde{O}_{+}(\mu)\det\tilde{O}_{-}(\mu) \tag{4}$$

with $\tilde{O}_{\sigma}$ and $N\times M$ matrix:

$$\tilde{O}_{\sigma}=1+\prod_{l=1}^{L}B_l^{\sigma}(\mu)\,, \tag{5a}$$

$$B_l^{\sigma}(\mu)=e^{-\Delta\tau K}e^{V_l^{\sigma}(\mu)}\,; \tag{5b}$$

K is the bilinear part of the Hamiltonian:

$$K_{ij}=t_{ij}-\left(\mu-\frac{U}{2}\right)\delta_{ij} \tag{6a}$$

and

$$[V_l^{\sigma}(\mu)]_{ij}=\lambda\sigma\mu_i(l)\delta_{ij}\,. \tag{6b}$$

An equivalent expression to (4) in a space-time formulation is[1,5]

$$Z=\text{Tr}_{\mu}\det O_{+}(\mu)\det O_{-}(\mu) \tag{7}$$

with O_{σ} an $NL\times NL$ matrix which, written out in the time direction is given by

$$O_{\sigma}=\begin{pmatrix} 1 & 0 & \cdots & \cdots & B_L^{\sigma}\\ -B_1^{\sigma} & 1 & & & \\ 0 & -B_2^{\sigma} & 1 & & \\ \vdots & & & & \\ 0 & \cdots & \cdots & -B_{L-1}^{\sigma} & 1 \end{pmatrix}. \tag{8}$$

The space-time Green's function is defined as the inverse of O_{σ}

$$g^{\sigma}=O_{\sigma}^{-1} \tag{9}$$

and its equal time components are given by the $N \times N$ matrix

$$g^{\sigma}(l,l) = (1 + B_l B_{l-1} \ldots B_1 B_L \ldots B_{l+1})^{-1} . \tag{10}$$

Green's functions corresponding to two different potentials V and V' are related by the Dyson equation[5] (we omit spin indices for simplicity)

$$g' = g + (g-1)(e^{V'-V} - 1) g' . \tag{11}$$

from which the ratio of determinants corresponding to two configurations differing by flipping the spin $\mu_i(l)$ is obtained as

$$\frac{\det O_{\sigma}(-\mu_i(l))}{\det O_{\sigma}(\mu_i(l))} = 1 + [1 - g_{ii}(l,l)](\exp\{V_f^{\sigma}[\mu_i(l)] - V_f^{\sigma}[\mu_i(l)]\} - 1) . \tag{12}$$

This ratio determines whether the spin flip is accepted in a Monte Carlo process. Thus one needs to know the equal time Green's function at the space-time point being updated. For a single spin flip, one easily derives from (11) the relation between the old and new Green's function in terms of the single-site t matrix

$$g^{\sigma'} = g^{\sigma} + (g^{\sigma} - 1) t_i^{\sigma}(l) g^{\sigma} , \tag{13a}$$

$$t_i^{\sigma}(l) = \frac{e^{V_f^{\sigma}[-\mu_i(l)] - V_f^{\sigma}[\mu_i(l)]} - 1}{1 + [1 - g_{ii}^{\sigma}(l,l)](\exp\{V_f^{\sigma}[-\mu_i(l)] - V_f^{\sigma}[\mu_i(l)]\} - 1)} |i,l><i,l| , \tag{13b}$$

i.e., $t_i^{\sigma}(l)$ has a single nonvanishing diagonal matrix element at site i, time slice l.

In the BSS algorithm, the equal time Green's function is constructed from Eq. (10) and, after a spin flip, the equal time components of the Green's function are updated using Eq. (13). After updating an entire time slice, the Green's function for the next time slice is obtained from

$$g^{\sigma}(l+1,l+1) = B_f^{\sigma} g^{\sigma}(l,l) (B_f^{\sigma})^{-1} . \tag{14}$$

This approach takes $O(N^2)$ operations per update, $O(N^3)$ per time slice and $O(N^3 L)$ for an entire sweep through the lattice. Equation (14) involves $O(N^2)$ operations if the matrices B are sparse, as is usually the case, and so has negligible incidence on the overall computer time.

In the HF approach proposed for magnetic impurities, Eqs. (10) and (14) are not used. Instead, the Green's function at the sites where interactions occur only (impurities) is constructed from the Dyson equation (11), and all time components of the Green's function elements involving impurity sites only are updated through Eq. (13). This approach then takes $O((nL)^2)$ operations per update and $O((nL)^3)$ operations per sweep, with n the number of impurities. For the Hubbard model $n = N$, and so this approach takes $O((NL)^3)$ operations, considerably more than the BSS algorithm.

Unfortunately, the BSS algorithm is found to become unstable at low temperatures, typically $\beta \sim 4$ for the Hamiltonian Eq. (1) with $t = 1$. This first shows up in the need to either correct or recompute the Green's function from scratch after a few updatings, and soon thereafter in the impossibility of even computing $g^{\sigma}(l,l)$ from Eq. (10) by standard Gaussian elimination. In contrast, one can easily obtain $g^{\sigma}(l,l)$ from Eq. (9) even at low temperatures.[5,6] The different behavior is related to the different eigenvalue structure of the matrices O_{σ} and $\tilde{O}_{\sigma}$. The spatial matrix $\tilde{O}_{\sigma}$ develops exponentially large eigenvalues as β increases; since it also has $O(1)$ eigenvalues it becomes highly singular at low temperatures. In contrast, the ratio of largest to smallest eigenvalue of O_{σ} grows only algebraically (in fact, linearly) with L. Thus, inversion O_{σ} through Gaussian elimination is stable at low temperatures.

In the HF algorithm it is found that the updating step, Eq. (13), does not lead to instabilities at low temperatures.[5] Since in the BSS algorithm the same updating is used, it is not there where errors first are introduced but in the process of going to the next time slice through Eq. (14). These errors are rapidly amplified by subsequent updating and use of Eq. (14) at low temperatures. In the HF algorithm, Eq. (14) is not used at the expense of updating the entire space-time Green's function instead of just the equal time one.

An approach intermediate between the impurity and lattice algorithms can be constructed as follows. We collapse L_0 time slices of the matrix Eq. (8) into a new matrix with $p = L/L_0$ time slices (we omit spin indices for simplicity)

$$O_{L_0}(1) = \begin{pmatrix} 1 & 0 & & & B_{pL_0} \cdots B_{(p-1)L_0+1} \\ -B_{L_0} B_{L_0-1} \cdots B_1 & 1 & & & \\ & -B_{2L_0} \cdots B_{L_0+1} & 1 & & \\ & & & & \\ & & -B_{(p-1)L_0} \cdots B_{(p-2)L_0+1} & & 1 \end{pmatrix} \tag{15}$$

where $O_{LO}(1)$ is an $Np \times Np$ matrix, and its largest eigenvalue is of order $e^{\beta_0 \varepsilon}$ with ε a typical single-particle energy and

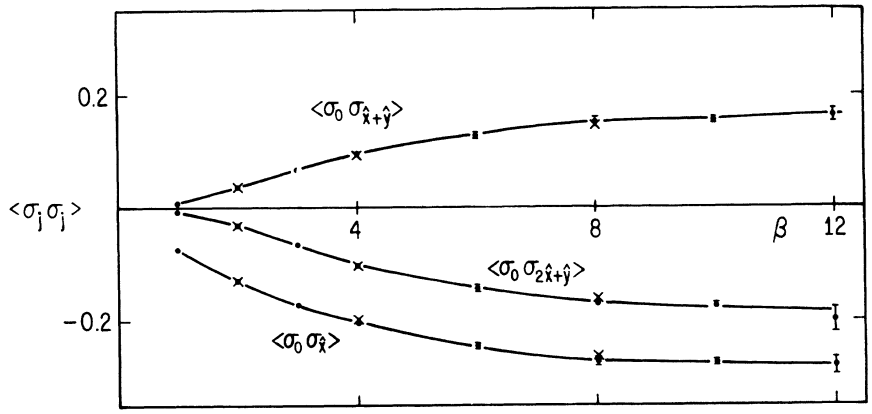

FIG. 1. Spin-spin correlation functions for the $\frac{1}{2}$-filled Hubbard model on a 4×4 lattice. $U=4$, $\Delta\tau=0.167$ (●) and 0.133 (×). Note that correlations reach their low-temperature limit only around $\beta\sim 10$.

$\beta_0=L_0\Delta\tau$. The inverse of O_{L_0} contains a subset of the full Green's function Eq. (9):

$$O_{L_0}^{-1}(1)=g_{L_0}(1)=\begin{pmatrix} g(1,1) & g(1,L_0+1) & \cdots & g[1,(p-1)L_0+1] \\ g(L_0+1,1) & & & \\ \vdots & & & \\ g[(p-1)L_0+1,1] & \cdots & & g[(p-1)L_0+1,(p-1)L_0+1] \end{pmatrix}. \tag{16}$$

Similarly, we define $O_{L_0}(l)$ and $g_{L_0}(l)$, $1\le l\le L_0$. $O_{L_0}(l)$ is given by the form Eq. (15) with all indices of the B matrices increased by $l-1$, and $g_{L_0}(l)$ has the form Eq. (16) with all time indices shifted by $l-1$.

We start by constructing $O_{L_0}(1)$ and $g_{L_0}(1)$ by standard matrix inversion in $O[(Np)^3]$ operations. We then perform Monte Carlo updatings at all sites in the p times slices $1, L_0+1, \ldots, (p-1)L_0+1$, and after each accepted move we update the Green's function Eq. (16) in $(Np)^2$ operations through Eq. (13). This updating takes also $O[(Np)^3]$ operations for all sites in the p time slices. Next, we need the Green's function $g_{L_0}(2)$ to update time slices $2, L_0+2, \ldots, (p-1)L_0+2$. The elements of $g_{L_0}(2)$ are obtained through the relations

$$g_{L_0}(l_1+1,l_2+1)=B_{l_1}g_{L_0}(l_1,l_2)B_{l_2}^{-1}. \tag{17}$$

For an entire sweep, the above procedure is repeated $L_0=L/p$ times. Because Eq. (17) is used L_0 rather than L times, it does not lead to instabilities if L_0 is small enough. The computer time scales as $N^3p^3L_0$, or equivalently N^3L^3/L_0^2. For $p=1$ this reduces to the BSS algorithm. As the temperature is lowered, L_0 is kept fixed at the maximum value that gives a stable algorithm (which corresponds to $\beta_0\sim 3$ or 4) and p is increased. Thus, asymptotically the computer time scales qualitatively similar to the HF algorithm but with a reduction of a factor L_0^2; for typical applications L_0 can be ~ 15–30. Because we always have some of the time components of the Green's function the procedure to calculate imaginary time-dependent quantities and zero-frequency susceptibilities is simpler than in the BSS case and is also stable.

We have implemented this algorithm for the two-dimensional Hubbard model and it performs as expected. As an example, Fig. 1 shows spin-spin correlation functions versus temperature for a 4×4 lattice down to $\beta=12$. At the lowest temperatures, $p=3$ was used. The computer time used to obtain the data in Fig. 1, with 2200 Monte Carlo sweeps, was 78 min. The lowest temperature point took 22 min. Applications of this approach to a variety of questions in Hubbard and other two-dimensional models are under way. The algorithm remains stable down to arbitrarily low temperatures. Lattice sizes of 8×8 and β values of 20 can be studied with reasonable amounts of supercomputer time (several hours on a Cray X-MP supercomputer).

Finally, we comment on the comparison between this approach and other Monte Carlo approaches to Hubbard-like models based on equations of motion methods.[10,7] In a hybrid Monte Carlo approach[7,11] one proposes a global move of all variables, and the computer time for determining the acceptance scales only as N^3, as a single determinant is needed. However, for the molecular-dynamics equations one needs the values of g for all time slices; if an approximate g is used, the acceptance will decrease as N and L increase. It appears to us that asymptotic scaling of the computer time as $(NL)^3$ is inescapable for Hubbard-like models at low temperatures; therefore, it is the prefactor that will determine which of the different algorithms is most efficient. One advantage of our approach is that we can deal with Ising rather than Gaussian auxiliary fields, which have been shown to lead to significantly shorter autocorrelation times in the simulations.[12]

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