Ground State of the Extended One-Dimensional Hubbard Model: A Green's Function Monte Carlo Algorithm

Michael A. Lee and Kazi A. Motakabbir
Department of Physics, Kent State University, Kent, Ohio 44242

and

K. E. Schmidt[a]
Los Alamos National Laboratory, Los Alamos, New Mexico 87545
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A Monte Carlo method for obtaining exact ground-state properties of a class of Hubbard Hamiltonians is described. Results are presented for two special cases, nearest-neighbor Coulomb and on-site interactions, where previous exact results are known. The straightforward applicability of the method to a wider variety of interactions is demonstrated.

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The extended Hubbard model[1] has enjoyed a rich variety of applications in the study of quasi-one-dimensional conductors[2] and, more recently, in the study of solitons in polyacetylene.[3] Although not limited to a one-dimensional system, it is not trivially solvable even there. Many analytic results exist,[4] but perturbation theory or variational calculations[1,5] have been necessary in the general case.

A widely used form of the Hubbard Hamiltonian in one dimension is

$$H = -t\sum_{l,\sigma}[c^{\dagger}_{l,\sigma}c_{l+1,\sigma} + c^{\dagger}_{l,\sigma}c_{l-1,\sigma}] + V\sum_{l,\sigma',\sigma}\rho_{l,\sigma}\rho_{l+1,\sigma'} + \tfrac{1}{2}U\sum_{l,\sigma}\rho_{l,\sigma}\rho_{l,-\sigma}. \quad (1)$$

This form contains the "hopping" term where the fermion operators $c^{\dagger}_{l,\sigma}$ and $c_{l,\sigma}$ create and destroy particles of spin σ, a "Coulomb" term (here only a nearest-neighbor interaction) of strength V, and a contact potential when particles of opposite spin occupy the same site. In our notation, L is the number of sites on a circle, N_{σ} is the number of particles of spin σ, and $\rho_{l,\sigma} = c^{\dagger}_{l,\sigma}c_{l,\sigma}$ is the number operator for particles of spin σ on site l. t, U, and V are coupling constants. We will set $t = 1$.

There have recently been a number of investigations[6] of the properties of one-dimensional Hubbard models at finite temperatures using Monte Carlo techniques. Hirsch and co-workers[6] have developed a simulation method which exploits Suzuki's[7] ideas of mapping a one-dimensional finite-temperature problem onto a two-dimensional (space, inverse temperature) coordinate system. Their method, like the earlier finite-temperature Monte Carlo work by Barker[8] requires that the inverse temperature coordinate be discretized. They find, as did Barker, that the number of discrete inverse temperature segments (and computer time) necessary to maintain the accuracy of the discretization approximation grows as the temperature approaches zero. This behavior is apparently not unique to these methods since Whitlock and Kalos[9] encountered low-temperature slowing down in their work on quantum hard spheres, even though no discretization approximations were evoked.

The Monte Carlo solution which we wish to describe is designed to yield the zero-temperature (ground-state) solution to the Hubbard Hamiltonian. The solution method is essentially the lattice equivalent of a Green's function Monte Carlo (GFMC) algorithm. These techniques were developed by Kalos and co-workers[10] for application to the ground state of boson quantum fluids, particularly ^{4}He. With one exception,[11] these have not been successfully applied to obtain exact results for the many-fermion ground state; however, accurate approximate methods exist.[12] The very first use of quantum Monte Carlo techniques on a lattice can be traced to Metropolis[13] who demonstrated the feasibility for single-particle problems. More recently, the GFMC has been applied to lattice field theory problems by Heys and Stump.[14]

The GFMC method derives its name from the use of a stochastic procedure to iterate the integral equivalent of the time-independent Schrödinger equation,

$$\psi(R) = E\int G(R,R')\psi(R')\,dR', \quad (2)$$

to obtain the ground state of the Hamiltonian. The Green's function is defined as the inverse of the Hamiltonian:

$$HG = I. \quad (3)$$

The conditions necessary to perform the integration in Eq. (2) by Monte Carlo methods require that the energy E, the wave function ψ, and the Green's function G all be positive definite. Then $EG(R,R')$ can be interpreted as the density of configurations arriving at R from a starting position R'. A random-walk procedure which moves a set (or population) of configurations from their initial positions $\{R'\}$ to the final positions $\{R\}$ achieves one iteration of Eq. (2). When an equilibrium distribution of positions $\{R\}$ has been achieved after many iterations, that distribution satisfies Eq. (2) and is said to be sampled from ψ. A demonstration that the above procedure converges to the ground state of H is described in Ref. 11. The exact ground-state energy may be obtained directly, but general structural information and correlation functions require the use of importance sampling and extrapolation procedures.[10] These results, although normally accurate, cannot be said to be exact.

Since the Schrödinger equation does not contain information about the Fermi or Bose statistics, the standard GFMC method converges to the lowest-energy positive-definite eigenstate, which cannot, therefore, be antisymmetric. It has been stated[12] that if the location of the nodes (zeros) of the fermion ground state is known, then the GFMC technique could be modified to obtain the exact ground state. It is a property peculiar to one-dimensional fermion problems that the ground-state nodes are known when the number of fermions N_σ is odd. The only nodes in the ground-state wave function are those which occur when two particles of like spin occupy the same position. It is easily seen, by solving the problem for $N=2$ and $N=3$ noninteracting fermions, that the even-particle wave function has extra nodes.

The appropriate modification of the GFMC method when the nodes of the wave function are known can be understood as follows. If the wave function of N (for the moment spinless) fermions is known in one region of the N-dimensional coordinate space of particle positions where it is positive and bounded by nodes, then it can be known in the negative regions by the interchange of pairs of particles. There are normally $N!$ such equivalent regions. If one redefines the eigenvalue problem to be restricted to this one positive region of space, with the boundary condition that the wave function go to zero at the node, then the original fermion ground state satisfies this new problem, but no other lower-energy wave function can. It is then sufficient to restrict Eq. (1) to one such region of space by adding the additional boundary condition that the Green's function be zero at the nodes.

To implement a GFMC procedure, it is necessary to develop a random walk which samples the Green's function. It will become clear that the only nontrivial obstacles to this are contained in the hopping term. For simplicity, we first consider spinless fermions. We will denote the basis states consisting of N particles on sites $j_1,j_2,\ldots,j_N$ by

$$|J\rangle \equiv |j_1,j_2,\ldots,j_N\rangle \equiv \prod_{i=1}^{N} c_{j_i}^{\dagger}|0\rangle . \tag{4}$$

The linearly independent subset which spans the space of all N-particle states on L lattice sites may be chosen to be the ordered set with $j_1 < j_2 < \ldots < j_N$.

The technical requirement that the eigenvalue spectrum be positive is easily satisfied without modifying the eigenstates by adding to H a constant diagonal term V_0+2N. Let

$$H \rightarrow H + V_0 + 2\textstyle\sum_l c_l^{\dagger} c_l . \tag{5}$$

The matrix elements of H in the ordered basis are

$$\langle I|H|M\rangle = V_I\delta_{I,M} - \sum_i \{\delta_{I,M(i+1)} - 2\delta_{I,M} + \delta_{I,M(i-1)}\} . \tag{6}$$

Here V_I includes the effect of the entire potential (which is diagonal). The notation $M(i\pm1)$ means the state M with the i th particle moved one site to the right $(+1)$ or left (-1).

By substitution of this expression for H into the defining relation for G, Eq. (2), a matrix equation for G results:

$$\delta_{I,J} = \sum_{i=1}^{N} [2G_{I,J} - G_{I,J(i+1)} - G_{I,J(i-1)}] + V_I G_{I,J} . \tag{7}$$

This simple formula for G does not require explicit antisymmetrization only when the number of fermions is odd. The periodic boundary conditions which allow subscripts like $J(i\pm1)$ to take on values outside of the ordered basis can then be mapped back to the ordered basis with an even number of particle interchanges. There are no sign problems when the number of fermions is odd.

We may rearrange the terms in Eq. (7) to get an infinite-series representation of the Green's function. A procedure for sampling a configuration I from $EG_{I,J}$ is akin to doing such an iteration by use of a random walk. In order to interpret the various coefficients in the random-walk equation as probabilities for absorption or as probabilities of making a

move, it is convenient to add a quantity $WG_{I,J}$ to both sides of Eq. (7) before rearrangement. The resulting equation for G which can be sampled by a random walk is

$$G_{I,J}=\frac{\delta_{I,J}}{2N+W}+\left(\frac{W-V_J}{2N+W}\right)G_{I,J}+\frac{2N}{2N+W}\sum_{i=1}^{N}\left[\frac{G_{I,J(i+1)}+G_{I,J(i-1)}}{2N}\right]. \quad (8)$$

Multiplying this equation by a trial energy E leads to three types of random-walk processes. Given an initial configuration J, the first term says that the configuration stays at J (i.e., $I=J$) with likelihood $E/(2N+W)$. The second term says that with probability $(W-V)/(2N+W)$, we sample a value of I from $EG_{I,J}$. Since we may choose $W=V_j$, this term may be avoided. The movement of particles occurs in the last term. With probability $2N/(2N+W)$, we sample one of the $2N$ terms at random, i.e., change J to $J(i\pm1)$ for random i and sample I from $EG_{I,J(i\pm1)}$. If $J(i\pm1)$ is a configuration with two overlapping particles, this term is zero; if not, the sampling of G returns us to the repetition of this process with a new configuration $J(i\pm1)$.

In practice several hundred configurations form the ensemble representing the wave function. The calculation proceeds by iteration of this ensemble according to Eq. (2) until it converges to the ground state. Each iteration requires that every configuration in the ensemble move from its initial location J to zero, one, or more final locations I as required to sample $EG_{I,J}$. The unknown eigenvalue E is determined by the condition that the number of configurations in the population remain stable.

The extension of the above procedure to fermions with spin is straightforward. We would like to report the results of this procedure for a few trial cases, some of which have known analytical or numerical results for the energy. Figure 1 shows that if the on-site potential is zero, then the energy per site for spinless fermions can be obtained to high accuracy. The statistical uncertainty of these results is less than the size of the symbol plotted. In this and other results we have set $t=1$. For the extreme values of $V=\pm2$, the correlation lengths exceed the size of the lattice employed, so that although the energy may be near the infinite-system limit, structural information particularly at large distances will be affected. There is no particular reason to limit this calculation to small systems; the algorithm is extremely fast and the computer requirements grow only linearly with N, not like N^2 or N^3 as is the case for some fermion calculations.

As a final example, the solution for the ground-state energy with only the on-site interaction and equal numbers of spin-up and spin-down fermions is shown in Fig. 2. Exact results in this special case have been calculated previously.[4] These agree within statistical uncertainty with our Monte Carlo results for all densities and interaction strengths as expected.

In summary, we have described a Monte Carlo procedure for obtaining exact ground-state properties of a certain class of Hubbard-like Hamiltonians.

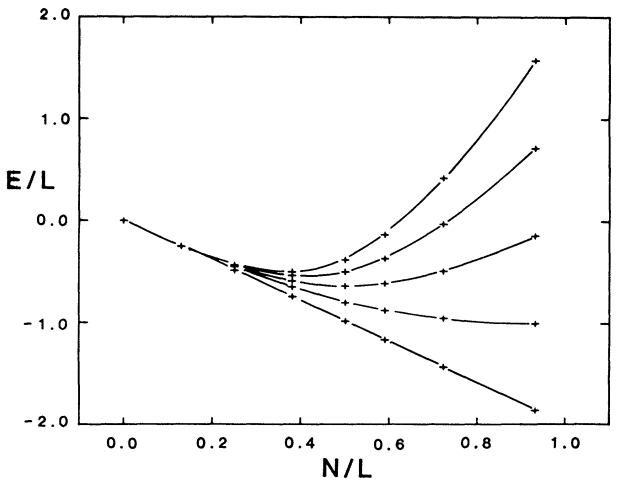

FIG. 1. Energy per site vs density with nearest-neighbor interaction $V=-2, -1, 0, +1, +2$. V increases from the bottom; $N=13$.

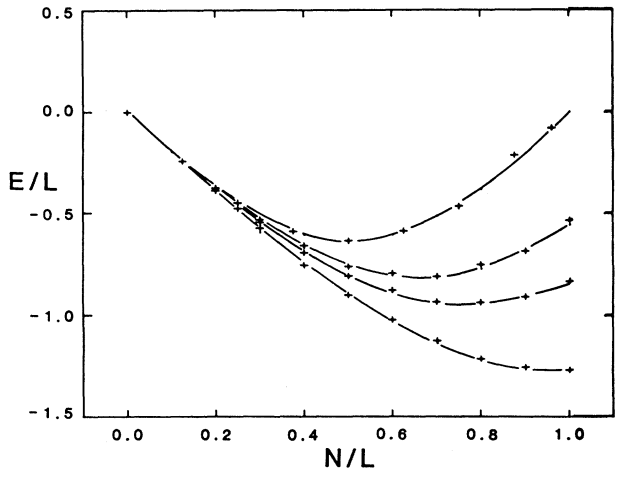

FIG. 2. Energy per site vs density with on-site repulsion $U=0, 2, 4, \infty$. Solid lines are exact results (Ref. 4) for an infinite lattice; the symbols are GFMC calculations for $N=26$.

The method is quite general in that any potential which is diagonal in both particle configuration and spin can be treated with equal ease. The computer time required to obtain the energy to an accuracy of better than 1% was typically 15 min on a VAX class machine.

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[a]Present address: The Courant Institute of Mathematical Sciences, New York, New York 10012.

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