Monte Carlo Study of the Two-Dimensional Hubbard Model

J. E. Hirsch
Department of Physics, University of California, San Diego, La Jolla, California 92093
(Received 6 September 1983)

A two-dimensional model of interacting electrons on a lattice, the Hubbard model, has been studied by means of a numerical simulation technique. Results for the half-filled-band sector are presented for lattices of up to 6×6 spatial sites, as a function of temperature and electron-electron repulsion U. In the ground state, the system is found to exhibit antiferromagnetic long-range order for all values of U, although greatly reduced from the mean-field-theory predictions.

PACS numbers: 75.10.Lp, 71.10.+x

Recently, various techniques have been developed to study interacting quantum systems on a lattice with use of Monte Carlo (MC) methods.[1-3] These techniques open up the possibility of studying in a nonperturbative way previously intractable many-electron problems where both features of band structure and interactions play an essential role. This approach should be useful in bridging the gap between localized and itinerant-electron descriptions of magnetism in narrow-band systems.[4] Here, I begin a study of these questions by considering the two-dimensional half-filled Hubbard model on a square lattice.

The Hubbard Hamiltonian[5] is a simple model for interacting electrons on a lattice: It describes a single band formed by overlapping s orbitals, with a repulsive interaction between electrons of opposite spin at the same site. It is thought to be able to describe many of the features of narrow-band magnetism.[6-8] In one dimension, it has been solved exactly with use of Bethe *Ansatz* techniques.[9] Furthermore, finite-lattice exact[10] and MC[11] calculations have provided information on thermodynamic properties and correlation functions. In more than one dimension, essentially no exact calculations exist although a variety of approximate studies have been performed.[5-8]

The model is defined by the Hamiltonian

$$H=\sum_{i,j,\alpha} c_{i\alpha}^{\dagger}K_{ij}c_{j\alpha}+U\sum_{i} n_{i\uparrow}n_{i\downarrow}-\mu\sum_{i\alpha}(n_{i\alpha}-0.5), \tag{1}$$

with $n_{i\alpha}=c_{i\alpha}^{\dagger}c_{i\alpha}$ the fermion occupation number for spin $\alpha=\uparrow,\downarrow$ at site i, and $K_{ij}=-t$ if i,j are nearest neighbors on a square lattice, and zero otherwise. $\mu=U/2$ for the half-filled-band case. The single-particle eigenstates for the case $U=0$ have energy

$$\epsilon(k_x,k_y)=-2t(\cos k_x+\cos k_y).$$

The bandwidth is $W=8t$, and I will use units so that $t=1$.

I write a functional integral formulation for the partition function, using a transformation recently proposed to eliminate the fermion-fermion interaction, introducing auxiliary Ising variables $\sigma_i(\tau)=\pm 1$. The procedure is similar to the usual Hubbard-Stratonovich transformation and is discussed in detail elsewhere.[12] The result is

$$Z=\mathrm{Tr}\,e^{-\beta H}\cong\mathrm{Tr}_{\{\sigma_i(\tau_l)\}}\mathrm{Tr}\prod_{l=1}^{L}\exp(-\Delta\tau\sum_{i,j,\alpha}c_{i\alpha}^{\dagger}K_{ij}c_{j\alpha})\exp[\sum_{i}\lambda\sigma_i(\tau_l)(n_{i\uparrow}-n_{i\downarrow})], \tag{2}$$

$$\lambda=2\,\mathrm{arctanh}\{[\tanh(\Delta\tau U/4)]^{1/2}\}. \tag{3}$$

The error in obtaining Eq. (2) is $O(\Delta\tau^2 tU)$. I have used $\Delta\tau U=0.5$, which should give systematic errors of a few percent at most.[12]

Taking the trace over fermion degrees of freedom in Eq. (2) yields[2]

$$Z=\mathrm{Tr}_{\{\sigma_i(\tau_l)\}}\prod_{\alpha}\det[1+B_L(\alpha)B_{L-1}(\alpha)\cdots B_1(\alpha)]\equiv\mathrm{Tr}_{\sigma}\det(O_{\uparrow})\det(O_{\downarrow}), \tag{4a}$$

$$B_l(\alpha)=\exp(-\Delta\tau K)\exp[V_l(\alpha)], \tag{4b}$$

$$[\exp V_l(\alpha)]_{ij}=\delta_{ij}\exp[\lambda\alpha\sigma_i(\tau_l)], \tag{4c}$$

$(K)_{ij}=K_{ij}$, and $\alpha=\pm 1$. The equal-time Green's function is given by

$$G_{ij}{}^{\alpha}=\langle\langle c_{i\alpha}c_{j\alpha}{}^{\dagger}\rangle\rangle=\mathrm{Tr}_{\sigma}\langle c_{i\alpha}c_{j\alpha}{}^{\dagger}\rangle\det(O_{\uparrow})\det(O_{\downarrow})/Z\,, \tag{5a}$$

$$\langle c_{i\alpha}c_{j\alpha}{}^{\dagger}\rangle=\left(\frac{1}{1+B_L(\alpha)B_{L-1}(\alpha)\cdots B_1(\alpha)}\right)_{ij}\,, \tag{5b}$$

and averages over more products of fermion operators are obtained by performing Wick's contractions, i.e.,

$$\langle c_{i1\alpha}{}^{\dagger}c_{i2\alpha}c_{i3\alpha'}{}^{\dagger}c_{i4\alpha'}\rangle=\langle c_{i1\alpha}{}^{\dagger}c_{i2\alpha}\rangle\langle c_{i3\alpha'}{}^{\dagger}c_{i4\alpha'}\rangle+\delta_{\alpha\alpha'}\langle c_{i1\alpha}{}^{\dagger}c_{i4\alpha}\rangle\langle c_{i2\alpha}c_{i3\alpha}{}^{\dagger}\rangle\,. \tag{6}$$

Similar relations hold for time-dependent correlation functions. In addition, there exists a simple proportionality relation between correlation functions of the Ising spins and fermion spin-spin correlation functions.[12]

I use the heat-bath algorithm to perform a Monte Carlo calculation of the trace over Ising spins, using the product of fermion determinants as the Boltzmann weight. For the half-filled-band case on bipartite lattices, the following relation holds as a result of particle-hole symmetry:

$$\det(O_{\uparrow})=\det(O_{\downarrow})\exp[-\lambda\sum_{i,l}\sigma_i(\tau_l)]\,, \tag{7}$$

so that the product of determinants is positive definite. For the non-half-filled-band case, I have numerical evidence that the product of determinants can become negative at low temperatures, complicating the situation somewhat.

To compute the change in the fermion determinant for a change in an Ising spin, I use the algorithm introduced by Blankenbecler, Scalapino, and Sugar,[2] which updates the fermion Green's function at each step exactly. It involves N^2 operations per update, with N the number of spatial sites. In addition, after sweeping through ten to fifteen time slices the Green's function has to be recomputed because of degradation due to rounding errors. For large lattices ($>4\times4$), it is convenient to do a checkerboard breakup[3] of the kinetic-energy operator in Eq. (4b), so that the resulting matrices are sparse.[13] Because of the relation (7), I only need to work with the Green's function for one spin. A sweep through a $6\times6\times32$ lattice (the largest size studied) took approximately 70 sec on a VAX 11/750 computer. A typical simulation involved 200 warmup sweeps and 1000 measurement sweeps. I have compared results of my simulations with exact results by Shiba[10] for a six-site chain and found good agreement.

At finite temperatures, the two-dimensional Hubbard model is not expected to have magnetic order because of the Mermin-Wagner theorem. At $T=0$, however, the existence of long-range magnetic order is an open question. Hartree-Fock theory predicts antiferromagnetic long-range order for any value of U and all spatial dimensionalities (d). In $d=1$, however, it is known that quantum fluctuations destroy the long-range order for all values of U. I have investigated this question in $d=2$ by studying the spin-spin correlation function:

$$S(\vec{k})=\sum_R e^{i\vec{k}\cdot\vec{R}}\langle(n_{0\uparrow}-n_{0\downarrow})(n_{R\uparrow}-n_{R\downarrow})\rangle\,. \tag{8}$$

For $\vec{k}=(\pi,\pi)$, this quantity is found to grow as the temperature is lowered and the lattice size increased. To extrapolate the size dependence, it is essential to consider finite lattices that can accommodate the Néel state using periodic bound-

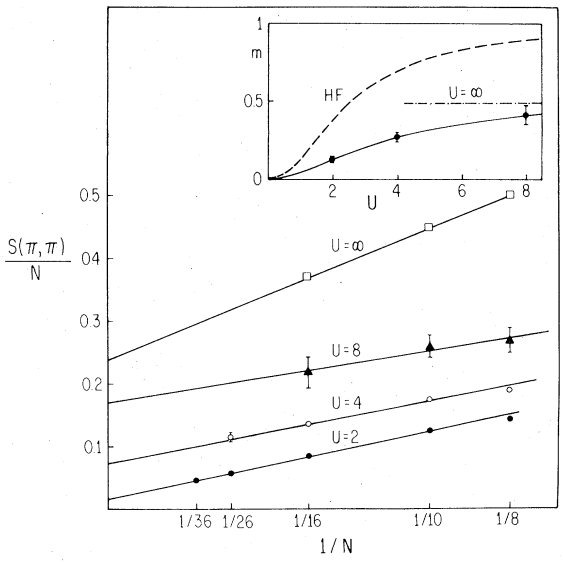

FIG. 1. Extrapolation of the ground-state antiferromagnetic long-range order. The $U=\infty$ results are taken from Ref. 14. The $N=8$ results were not used in the extrapolation for $U=2$ and $U=4$. For $N=10$, antiperiodic boundary conditions were used. The inset shows the staggered magnetization m vs U (here and in the following, the full line through the MC points is to guide the eye) and the Hartree-Fock predictions (dashed line).

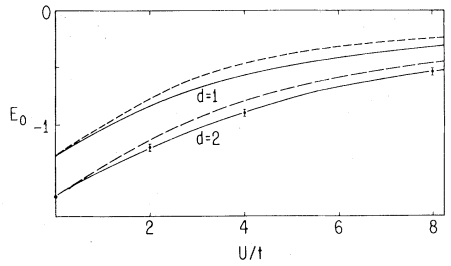

FIG. 2. Ground-state energy vs U for $d=2$ (MC results) and $d=1$ (exact, from Ref. 8). The dashed lines are Hartree-Fock results.

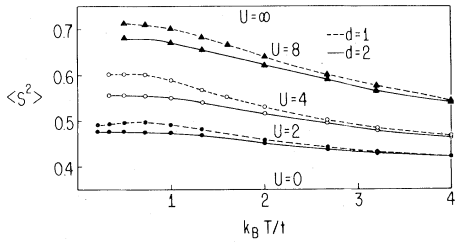

FIG. 3. Local magnetic moment vs temperature on a 6×6 two-dimensional lattice and a six-site one-dimensional lattice.

ary conditions, as pointed out by Oitmaa and Betts.[14] Such lattices with square cells in $d=2$ can be constructed for any number of sites N satisfying $N=r^2+s^2$, with r and s integers and $r+s$ even. Figure 1 shows $S(\pi,\pi)/N$ at temperatures $\beta=0.75\sqrt{N}$ plotted versus $1/N$ for $N=8$, 10, 16, 26, and 36. The Oitmaa and Betts ground-state results[14] for the antiferromagnetic Heisenberg model, which is the $U\to\infty$ limit of the Hubbard model in the half-filled sector, are also shown. My results fit a linear dependence well except for $N=8$, and suggest that the model has long-range antiferromagnetic order in the ground state for all values of U. The inset shows the ground-state staggered magnetization versus U, which is greatly reduced from the predictions of Hartree-Fock theory as a result of quantum fluctuations.

Figure 2 shows the extrapolated ground-state energy versus U. Hartree-Fock theory yields a reasonable upper bound. Exact and Hartree-Fock results for $d=1$ are also shown for comparison.

Figure 3 shows the temperature dependence of the local magnetic moment, defined by

$$\langle S^2\rangle=\langle\tfrac{3}{4}(n_{i\uparrow}-n_{i\downarrow})^2\rangle, \tag{9}$$

on a 6×6 lattice. This quantity was found to be very insensitive to the lattice size. It takes the value $\frac{3}{8}$ in the noninteracting limit, and $\frac{3}{4}$ in the $U=\infty$ limit where the electrons are completely localized. For any finite U the local moment takes the noninteracting value at high temperatures, and increases gradually as T is lowered. Note that the behavior is smooth and very similar to the one-dimensional case. The two-dimensional system has a smaller magnetic moment for a given value of the Coulomb interaction, because of the fact that the electrons have more paths to delocalize.

Figure 4 shows the magnetic susceptibility versus temperature on a 6×6 lattice. From comparison with results for smaller lattices, I expect finite-size effects to start becoming noticeable around $T\sim0.75$. In the noninteracting case, χ diverges logarithmically as $T\to0$ because of a logarithmic singularity in the density of states at the Fermi surface. It is not clear whether this behavior persists as the interaction is turned on. The interaction enhances the magnetic susceptibility, although less than in the $d=1$ case (not shown). Again the behavior is smooth as a function of temperature.

Because of the nested Fermi surface, the system considered here is expected to be insulating for all values of U. Results for the imaginary time dependence of various correlation functions appear to confirm this prediction. The extraction of the value of the gap is subtle because the results do not fit a simple mean-field behavior, and will be discussed elsewhere.

In summary, I have reported results of Monte Carlo simulations of the two-dimensional half-

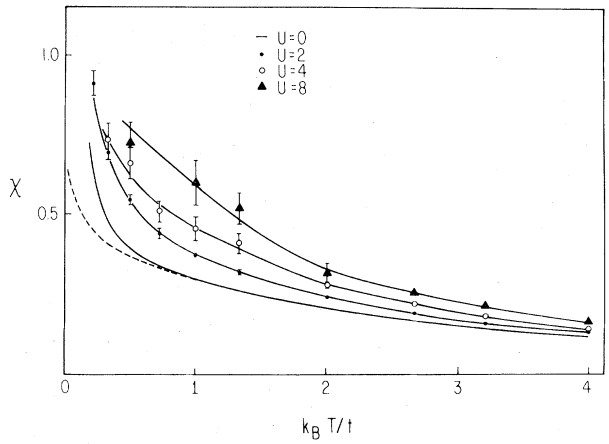

FIG. 4. Magnetic susceptibility vs temperature on a 6×6 lattice. The dashed line is the $U=0$ susceptibility for an infinite lattice.

filled Hubbard model. This is the first Monte Carlo study of an electronic lattice model of interest to condensed matter physics in more than one dimension. I conclude that the system is an antiferromagnetic insulator in the ground state as predicted by mean-field theory, although the staggered magnetization is greatly reduced from the mean-field prediction. At finite temperatures, the behavior is qualitatively similar to the one-dimensional case: The system is a paramagnetic insulator, and the magnetic susceptibility and local moment increase smoothly as the temperature is decreased. It will be of interest to consider the model with further than nearest-neighbor hopping, so that the Fermi surface is nonnested, as well as the non-half-filled-band sectors where ferromagnetism could possibly occur. In addition, calculations for small lattices in three dimensions ($4\times4\times4$) appear to be quite feasible.

This work was supported by the National Science Foundation under Grant No. DMR-82-17881.

[1]"Monte Carlo Methods in Quantum Problems," edited by M. Kalos (Reidel, Dordrecht, to be published), and references therein.

[2]R. Blankenbecler, I. 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).

[3]J. E. Hirsch, D. J. Scalapino, R. L. Sugar, and R. Blankenbecler, Phys. Rev. Lett. 47, 1628 (1981), and Phys. Rev. B 26, 5033 (1982).

[4]T. Moriya, in *Electron Correlation and Magnetism in Narrow-Band Systems*, edited by T. Moriya (Springer-Verlag, New York, 1981), p. 2.

[5]J. Hubbard, Proc. Roy. Soc. London, Ser. A 276, 238 (1963), and 281, 401 (1964).

[6]D. Penn, Phys. Rev. 142, 350 (1966).

[7]B. Brandow, Adv. Phys. 26, 561 (1977), and references therein.

[8]S. Doniach, Adv. Phys. 18, 819 (1969), and references therein.

[9]E. Lieb and F. Wu, Phys. Rev. Lett. 20, 1445 (1968).

[10]H. Shiba and P. Pincus, Phys. Rev. B 5, 1966 (1972); H. Shiba, Prog. Theor. Phys. 48, 2171 (1972).

[11]J. Hirsch and D. Scalapino, Phys. Rev. B 27, 7169 (1983), and to be published.

[12]J. Hirsch, Phys. Rev. B (to be published).

[13]This was first used in this context by R. Sugar (private communication). I am grateful to him for a helpful discussion on this point.

[14]J. Oitmaa and D. Betts, Can J. Phys. 56, 897 (1978).