Renormalization-group study of the Hubbard model

Jorge E. Hirsch*
The James Franck Institute and Department of Physics, University of Chicago, Chicago, Illinois 60637
(Received 7 September 1979)

The ground state of the half-filled Hubbard model is studied using a real-space renormalization-group technique. We first study in detail the one-dimensional case. We find the ground state to be insulating for all finite coupling, in agreement with the exact solution. We compute the ground-state energy, localization length, energy gap, magnitude of the local moment, and spin-density autocorrelation function. For those quantities that are exactly known we find good agreement with the exact results. Using a simple extension of our one-dimensional calculation, we are able to study approximately two- and three-dimensional lattices. We find a Mott transition at finite interaction for these cases. The critical exponents for these transitions are found to satisfy an approximate interdimensional scaling law.

I. INTRODUCTION

The Hubbard model[1] is the simplest model one can study to examine the effects of correlations between electrons in narrow energy bands. The Hamiltonian consists of a nearest-neighbor hopping term and an electron-electron repulsion U which acts when two electrons are sitting at the same site. In this paper we study the half-filled Hubbard model using a zero-temperature renormalization-group (RG) technique. The method consists in constructing iteratively a variational ground state by dividing the system into cells and keeping at each step only the lowest-lying energy states in each cell. This method has been extensively used for studying spin systems at zero temperature.[2–7] One of the purposes of this work is to show that it is useful also to study systems with fermions defined on a lattice with short-ranged interactions. We concentrate mainly on the one-dimensional (1D) chain. For this case, a closed expression has been found for the ground state.[8] For the half-filled band, the results show that there is a Mott transition at $U=0$; the system is insulating for any nonzero U. Our approximate analysis reproduces correctly this feature of the exact solution. We compute the ground-state energy and the magnitude of the local moment, and find good agreement with the exact results.[8,9] We also study the behavior of the localization length and the energy gap near the Mott transition. The method correctly predicts an essential singularity at zero coupling, although it fails to reproduce the detailed behavior near the singularity. We can also compute arbitrary ground-state correlation functions, which cannot be simply obtained from the exact solution. As an illustration, we show the static q-dependent spin-spin correlation function.

It should be mentioned that there exists a related calculation for the 1D Hubbard model,[10] where the authors keep many energy states at each iteration, and are thus able to study approximately temperature-dependent properties. In this paper, however, we concentrate on ground-state properties and we emphasize the fact that we want the renormalized Hamiltonian to be of the same form as the original one, which makes the physics of the problem more transparent.

By a simple extension of our one-dimensional calculation, we are able to treat approximately two- and three-dimensional (2D and 3D) hypercubic lattices. It is generally thought that because of the special form of the free-electron Fermi surface for these lattices when only nearest-neighbor hopping is considered in the Hamiltonian, the ground state is insulating for any nonzero U, as in one dimension.[11,12] However, any small distortion of the Fermi surface, introducing further-than-nearest-neighbor hopping, will change this result. Our approximate method is not sensitive to that special feature of the nearest-neighbor-only case, and it predicts a Mott transition for finite U, whether we include longer-range hopping or not. In any case, any realistic model of a metal should include longer-range hopping,[13] so that our results are relevant for those cases. We obtain the critical exponents for the transition and verify that an approximate interdimensional scaling law, recently proposed for disordered electronic systems[14] and critical phenomena[15] is well satisfied.

II. ONE DIMENSION

In one dimension, the Hubbard Hamiltonian is given by

$$H=-t\sum_{i,\sigma}[c_{i\sigma}^{\dagger}c_{i+1,\sigma}+c_{i+1,\sigma}^{\dagger}c_{i,\sigma}]+U\sum_{i}n_{i\uparrow}n_{i\downarrow}-\mu\sum_{i,\sigma}n_{i\sigma}+\tfrac{1}{2}UN\ , \tag{1}$$

where $c_{i\sigma}^{\dagger}$ and $c_{i\sigma}$ are the creation and annihilation operators for an electron of spin σ at site i, and $n_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$. t gives the kinetic energy in the band and U is the Coulomb repulsion between electrons on the same site. The chemical potential μ is $\frac{1}{2}U$ for the half-filled band case.[16]

We divide the chain into (nonoverlapping) cells of three sites (we want an odd number of sites per cell if we want the renormalized Hamiltonian to describe fermions) and the Hamiltonian into an intracell part, H_0, and an intercell coupling V. V is the hopping part of the Hamiltonian that transfers an electron from one cell to the next. The intracell Hamiltonian, H_0, can be written as a sum over cells (labeled by p) of cell Hamiltonians

$$H=\sum_{p}H_0^p\ . \tag{2}$$

Next, we diagonalize exactly the intracell Hamiltonian H_0^p. Our Hilbert space has four states per site: $|0\rangle$; $c_{i\uparrow}^{\dagger}|0\rangle\equiv|+\rangle$; $c_{i\downarrow}^{\dagger}|0\rangle\equiv|-\rangle$; and $c_{i\uparrow}^{\dagger}c_{i\downarrow}^{\dagger}|0\rangle\equiv|+-\rangle$ so that we have 64 states per cell. There are, however, several conserved quantities: number of particles, z component of spin (S_z), total spin (S), and parity. We are interested in the half-filled band case, so that we consider the states with $n=2$, 3, and 4 particles; we find one nondegenerate ground state in each of the subspaces $n=2$ and 4, with $S=0$ and $S_z=0$, and two degenerate ground states in the subspace $n=3$, with $S=\frac{1}{2}$, and $S_z=\pm\frac{1}{2}$. These states are

$$\begin{aligned}
|0'\rangle &= a_1|1,0\rangle+a_2|2,0\rangle+a_3|3,0\rangle, & E_{0'}&=-2\mu+\lambda_a\ ,\\
|+'\rangle &= b_1|1,+\rangle+b_2|2,+\rangle+b_3|3,+\rangle, & E_{+'}&=-3\mu+\lambda_b\ ,\\
|-'\rangle &= b_1|1,-\rangle+b_2|2,-\rangle+b_3|3,-\rangle, & E_{-'}&=-3\mu+\lambda_b\ ,\\
|+-'\rangle &= a_1|1,+-\rangle+a_2|2,+-\rangle+a_3|3,+-\rangle, & E_{+-'}&=-4\mu+\lambda_a+U\ .
\end{aligned} \tag{3}$$

TABLE I. States that form the lowest-lying eigenstates for three-site cells in the 1D Hubbard model.

n	S_z	S	States
2	0	0	$\|1,0\rangle=\frac{1}{\sqrt{2}}(\|+\rangle\|0\rangle\|-\rangle-\|-\rangle\|0\rangle\|+\rangle)$ $\|2,0\rangle=\frac{1}{2}(\|+\rangle\|-\rangle\|0\rangle-\|-\rangle\|+\rangle\|0\rangle+\|0\rangle\|+\rangle\|-\rangle-\|0\rangle\|-\rangle\|+\rangle)$ $\|3,0\rangle=\frac{1}{\sqrt{6}}(\|+-\rangle\|0\rangle\|0\rangle+2\|0\rangle\|+-\rangle\|0\rangle+\|0\rangle\|0\rangle\|+-\rangle)$
3	$\frac{1}{2}$	$\frac{1}{2}$	$\|1,+\rangle=\frac{1}{\sqrt{2}}(-\|+-\rangle\|+\rangle\|0\rangle+\|0\rangle\|+\rangle\|+-\rangle)$ $\|2,+\rangle=\frac{1}{2}(-\|+-\rangle\|0\rangle\|+\rangle-\|0\rangle\|+-\rangle\|+\rangle+\|+\rangle\|0\rangle\|+-\rangle+\|+\rangle\|+-\rangle\|0\rangle)$ $\|3,+\rangle=\frac{1}{\sqrt{6}}(\|+\rangle\|+\rangle\|-\rangle-2\|+\rangle\|-\rangle\|+\rangle+\|-\rangle\|+\rangle\|+\rangle)$
3	$-\frac{1}{2}$	$\frac{1}{2}$	$\|1,-\rangle=\frac{1}{\sqrt{2}}(-\|+-\rangle\|+\rangle\|0\rangle+\|0\rangle\|-\rangle\|+-\rangle)$ $\|2,-\rangle=\frac{1}{2}(-\|+-\rangle\|0\rangle\|-\rangle-\|0\rangle\|+-\rangle\|-\rangle+\|-\rangle\|0\rangle\|+-\rangle+\|-\rangle\|+-\rangle\|0\rangle)$ $\|3,-\rangle=\frac{1}{\sqrt{6}}(-\|-\rangle\|-\rangle\|+\rangle+2\|-\rangle\|+\rangle\|-\rangle-\|+\rangle\|-\rangle\|-\rangle)$
4	0	0	$\|1,+-\rangle=\frac{1}{\sqrt{2}}(\|-\rangle\|+-\rangle\|+\rangle-\|+\rangle\|+-\rangle\|-\rangle)$ $\|2,+-\rangle=\frac{1}{2}(\|+\rangle\|-\rangle\|+-\rangle+\|+-\rangle\|+\rangle\|-\rangle-\|-\rangle\|+\rangle\|+-\rangle-\|+-\rangle\|+\rangle\|-\rangle)$ $\|3,+-\rangle=\frac{1}{\sqrt{6}}(\|0\rangle\|+-\rangle\|+-\rangle+2\|+-\rangle\|0\rangle\|+-\rangle+\|+-\rangle\|+-\rangle\|0\rangle)$

The states $|1,0\rangle$, $|2,0\rangle$, etc., are listed in Table I. The quantities λ_a and (a_1,a_2,a_3) are the lowest eigenvalue and corresponding eigenvector of

$$A=\begin{bmatrix} 0 & -\sqrt{2}t & 0 \\ -\sqrt{2}t & 0 & -\sqrt{6}t \\ 0 & -\sqrt{6}t & U \end{bmatrix} , \tag{4}$$

while λ_b and (b_1,b_2,b_3) are the lowest eigenvalue and corresponding eigenvector of

$$B=\begin{bmatrix} U & -\sqrt{2}t & 0 \\ -\sqrt{2}t & U & -\sqrt{6}t \\ 0 & -\sqrt{6}t & 0 \end{bmatrix} . \tag{5}$$

We will keep only these states per cell in defining our renormalized Hamiltonian. Note that these 4 states very much resemble the original site states $|0\rangle$, $|+\rangle$, $|-\rangle$, $|+-\rangle$ in that the spin quantum numbers are the same and their occupation number also if we subtract two from n in all the new states. We define new cell-fermion operators by the relations

$$\begin{aligned} &c_\uparrow^{\dagger\prime}|0'\rangle=|+'\rangle , \\ &c_\downarrow^{\dagger\prime}|0'\rangle=|-'\rangle , \\ &c_\uparrow^{\dagger\prime}c_\downarrow^{\dagger\prime}|0'\rangle=-c_\downarrow^{\dagger\prime}c_\uparrow^{\dagger\prime}|0'\rangle=|+-'\rangle . \end{aligned} \tag{6}$$

The intracell Hamiltonian restricted to the subspace of these four states only can be written in terms of the new cell-fermion operators as

$$\begin{aligned} H_0'=&E_{0'}+(E_{+'}-E_{0'})(n_\uparrow'+n_\downarrow') \\ &+(E_{+-'}+E_{0'}-2E_{+'})n_\uparrow'n_\downarrow' \end{aligned} \tag{7}$$

with $n_\sigma'=c_\sigma^{\dagger\prime}c_\sigma'$, so that it has the same form as the original Hamiltonian for one site. For obtaining the intercell coupling we compute the matrix elements of the old fermion operators on the boundary site of the cell, c_σ^b, with the states we are keeping, and we find

$$\begin{aligned} \langle 0'|c_\uparrow^b|+'\rangle=\langle -'|c_\uparrow^b|+-'\rangle=\langle 0'|c_\downarrow^b|-'\rangle \\ =-\langle +'|c_\downarrow^b|+-'\rangle=\lambda \end{aligned} \tag{8}$$

with

$$\lambda=\frac{1}{2\sqrt{2}}(a_1b_2+a_2b_1+\frac{3}{2\sqrt{6}}(a_2b_3+a_3b_2) \tag{9}$$

so that we can identify

$$c_\sigma^b=\lambda c_\sigma' \tag{10}$$

and our renormalized Hamiltonian has exactly the same form as the original one (except for an additive constant). We can then iterate this procedure, and obtain after the nth iteration a Hamiltonian of the form

$$\begin{aligned} H^{(n)}=&-t_n\sum_{i,\sigma}(c_{i\sigma}^\dagger c_{i+1,\sigma}+c_{i+1,\sigma}^\dagger c_{i,\sigma}) \\ &+U_n\sum_i n_{i\uparrow}n_{i\downarrow}-\mu_n\sum_{i,\sigma}n_{i\sigma}+\sum_i d_n , \end{aligned} \tag{11}$$

with the coefficients determined by the recursion relations

$$\begin{aligned} &U_{n+1}=U_n+2(\lambda_a^{(n)}-\lambda_b^{(n)}) , \quad t_{n+1}=\lambda_n^2 t_n , \\ &\mu_{n+1}=\mu_n+\lambda_a^{(n)}-\lambda_b^{(n)} , \quad d_{n+1}=3d_n+\lambda_a^{(n)}-2\mu_n , \end{aligned} \tag{12}$$

with λ_n, $\lambda_a^{(n)}$, $\lambda_b^{(n)}$ given by Eq. (8) and the diagonalization of (4) and (5), with t_n, and U_n replacing t and U. The initial conditions are

$$U_0=U , \quad t_0=t , \quad \mu_0=\tfrac{1}{2}U , \quad d_0=\tfrac{1}{2}U . \tag{13}$$

Note that the relation $\mu_n=\frac{1}{2}U_n$ is preserved at all steps of our iteration if we start with $\mu_0=\frac{1}{2}U_0$.

We analyze the recursion relations for $y=U/t$ and find only two fixed points, $y=0$ and ∞. That is, the ground state is analytic as a function of y, except at the origin, as found in the exact solution. Starting with any nonzero y, the recursion relations lead to the $y=\infty$ fixed point; i.e., at each iteration the intercell hopping term becomes weaker with respect to the Coulomb interaction. This shows that the ground state is insulating for any nonzero interaction, so that the Mott transition occurs for $U=0$.

From the constant term in the Hamiltonian we obtain the ground-state energy

$$E_G=\lim_{n\to\infty}\frac{d_n}{3^n}=\sum_{n=1}^{\infty}\frac{\lambda_a^{(n)}-2\mu_n}{3^n}+\tfrac{1}{2}U . \tag{14}$$

This is shown in Fig. 1, compared with the exact results of Lieb and Wu.[8] This method always yields an upper bound to the exact ground-state energy. The reason is that the Hamiltonian after n steps, $H^{(n)}$, equals the original Hamiltonian H truncated to some subspace of the original Hilbert space. Thus, the ground-state energy of $H^{(n)}$ equals the expectation value of the ground state of $H^{(n)}$ with the original Hamiltonian H and is, by the variational principle, an upper bound to the true ground-state energy

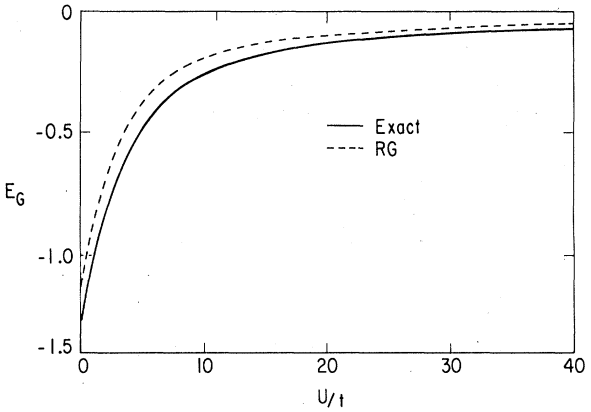

FIG. 1. Ground-state energy of 1D Hubbard model. Comparison betweem RG calculation and exact result.

of H. When n increases, the constant term in $H^{(n)}$ grows as 3^n while the rest of $H^{(n)}$ remains of the same order, so that the ground-state energy will be given by the constant term in $H^{(n)}$ as $n \to \infty$.

We have also computed the magnitude of the local moment, defined by

$$L_0 = \langle S^2 \rangle = \tfrac{3}{4} \langle n_\uparrow + n_\downarrow - 2 n_\uparrow n_\downarrow \rangle \quad . \tag{15}$$

This quantity is $\frac{3}{4}$ in the $U = \infty$ limit, when the electrons are completely localized, and $\frac{3}{8}$ in the free-electron limit $U = 0$ and it gives therefore an idea of the degree of localization of the electrons for all U. To compute the average of an operator, we calculate the part of it contained in the subspace spanned by the states we are keeping by calculating the matrix elements of the operator with those states. This gives the renormalized operator, and its ground-state average will be approximately the same as that of the original operator. For a site operator like the local moment, we take it always at the center of the cell to minimize end effects. The renormalized operator for the local moment has the same form as the original one, except for an additive and a multiplicative constant. We obtain the recursion relation

$$L_0 = \tfrac{3}{4} a_2^2 + (b_1^2 + b_3^2 - a_2^2) L_0' \quad , \tag{16}$$

where L_0' is the local moment for the system described by the renormalized Hamiltonian. Iterating this relation we obtain L_0. Our results are plotted in Fig. 2 and compared with the exact results, which can be obtained from the exact ground-state energy by[9]

$$L_0 = \tfrac{3}{4} - \tfrac{3}{2} \frac{dE_G}{dU} \quad . \tag{17}$$

We obtain the limits $U = 0$ and ∞ correctly, and the agreement for all U is very good.

We want to define a length that measures the distance over which the electrons are localized in the ground state. Consider the correlation function

$$F(R) = \frac{1}{N} \sum_i \langle c^\dagger_{i+R,\sigma} c_{i,\sigma} \rangle \quad . \tag{18}$$

This function will presumably decay exponentially in the large U region, as can be seen from the following perturbation-theory argument: start from the ground state for $U = \infty$, with all sites singly occupied (the antiferromagnetic Heisenberg chain ground state in the 1D case) and construct the ground state for large but finite U in perturbation theory in t/U. For obtaining a nonvanishing result for $F(R = na)$ (a the lattice spacing) we have to go to nth order in perturbation theory, so that

$$F(r) \sim \left(\frac{t}{U} \right)^n \sim e^{-R |\ln t/U|} \quad . \tag{19}$$

On the other hand, in the free-electron limit

$$F(R) = \frac{1}{N} \sum_k e^{ikR} \langle n_k \rangle = \frac{1}{N} \sum_{k < kF} e^{ikR} \quad . \tag{20}$$

It is easy to convince oneself that $F(R)$ will decay algebraically (with oscillations) for any reasonable Fermi surface. In particular, one obtains $F(R) \sim 1/R^d$ for a d-dimensional hypercubic lattice with nearest-neighbor hopping only and R in the direction of an axis, and $F(R) \sim 1/R^{(d+1)/2}$ for a spherical Fermi surface in d dimensions. This suggests that quite generally $F(R)$ will have an algebraic decay

$$F(R) \sim 1/R^\eta \tag{21}$$

on the metallic side of the Mott transition (with η possibly depending on the coupling strength) and an exponential decay

$$F(R) \sim e^{-R/\xi} \tag{22}$$

on the insulating side. ξ gives then a measure of the localization of the electrons in the insulator and it diverges at the Mott transition.

Let us compute this correlation function for the one-dimensional case with our RG approach: by the method previously discussed we obtain

$$F(R) = \tfrac{2}{3} \lambda^2 F'(R/3) \tag{23}$$

so that for $R = 3^n$ we obtain after n iterations

$$F(3^n) = (\tfrac{2}{3})^n \left(\prod_{j=1}^{n} \lambda_j \right) \langle c^\dagger_{i\sigma} c_{2\sigma} \rangle H^{(n)} \quad . \tag{24}$$

In the free-electron limit $\lambda = 1/\sqrt{2}$, so that we obtain for the exponent

$$\eta = \frac{-\ln \frac{2}{3} \lambda^2}{\ln 3} = 1 \tag{25}$$

in agreement with the exact result. In the case of

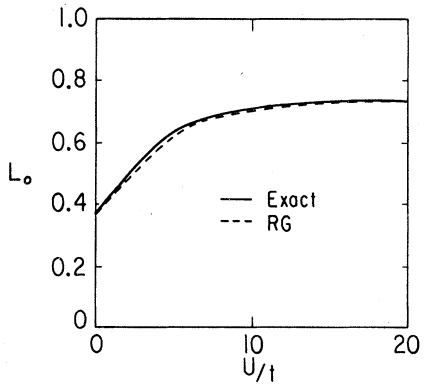

FIG. 2. Magnitude of the local moment in 1D Hubbard model. Comparison between RG calculation and exact result.

nonzero U, we scale to the large-U regime; taking into account that the nearest-neighbor average goes to zero as

$$\langle c^{\dagger}_{1\sigma} c_{2\sigma} \rangle_{H(n)} \sim t_n / U_n \tag{26}$$

and that the large-U recursion relations are

$$\frac{U_{n+1}}{t_{n+1}} = \frac{1}{\lambda_n^2} \frac{U_n}{t_n} \tag{27}$$

with $\lambda_n = \sqrt{3/4}$, we obtain

$$F(3^n) \sim (\tfrac{2}{3}\lambda^4)^n \ . \tag{28}$$

We see that we again obtain algebraic decay of the correlation function, this time with an exponent

$$\eta = \frac{-\ln \frac{2}{3}\lambda^4}{\ln 3} = 3.42 \ . \tag{29}$$

This failure of the RG method to display exponential decay of the correlation functions is well known to occur in other models also and has been discussed in detail by Fradkin and Raby.[17] Nevertheless, we obtain a much faster decay of the correlation function in the large-U region.

Even within this limitation of our method we can obtain an estimate of the localization length near the Mott transition as the distance over which a crossover occurs from the free-electron rate of decay of $F(R)$ to a faster rate of decay: start with a system with small y_0 and assume after n_0 iterations we have scaled to the large coupling region $y \sim 1$; i.e., $U \sim t$. The localization length will be given approximately by

$$\xi \sim 3^{n_0} \ . \tag{30}$$

For obtaining n_0, we consider the recursion relation for small y, which is

$$y_{n+1} = y_n + a y_n^3 \tag{31}$$

with $a = 0.047$. We can then write

$$dy = a y^3 d_n \tag{32}$$

and integrating we find

$$n_0 \approx \frac{1}{2a y_0^2} \tag{33}$$

so that the localization length goes as

$$\xi \sim e^{bt^2/U^2} \tag{34}$$

with $b = 11.7$. We see that the localization length diverges extremely rapidly for small U/t (faster than any power) due to the very slow growth of y under iterations for small y.

A similar behavior is obtained for the energy gap of the system. The electrical conductivity at zero temperature is determined by the energy gap between the ground state and the lowest excited state that is connected to the ground state by a nonzero matrix element of the current operator. Within our RG treatment, this energy gap is given by the limiting value of U after infinite iterations: $E_g = U_\infty$. (The recursion relations for t and U separately give $t_n \to 0$, $U_n \to U_\infty > 0$ as $n \to \infty$.) For small initial U/t we obtain the behavior

$$E_g \sim e^{-ct^2/U^2} \tag{35}$$

with $c = 7.4$. The behavior of the localization length and the energy gap show that the system has an essential singularity at $U = 0$ in one dimension.

The energy gap for the 1D Hubbard model can be calculated exactly from the Lieb and Wu solution, and one finds for small U[18]

$$E_g \sim e^{-2\pi t/U} \ .$$

That is, although the RG method succeeds in predicting an essential singularity at $U = 0$, it predicts the wrong power in the exponent (note, however, that the coefficient c in the exponent is close to the exact result). The behavior (35) is related to the fact that the quadratic term in y_n is missing in the recursion relation (31). This cannot be corrected by taking larger cells in the RG calculation, since it has been shown by Pfeuty (private communication) that the same behavior would be obtained by taking odd-site cells of any size, if only the four states around the half-filled band occupation are kept. Clearly, further work is needed in this direction.

Finally, we have computed the q-dependent spin-spin correlation function, defined by

$$G(q) = \frac{1}{N} \sum_{i,j} e^{iq(R_i - R_j)} \langle \sigma_z^i \sigma_z^j \rangle \ . \tag{36}$$

By the method previously discussed we obtain a recursion relation that involves only the same correlation function for wave vector three times as large and the local moment, both in the renormalized system

$$G(q) = 1 + \tfrac{4}{3} e_3 \cos(qa) + \tfrac{2}{3} e_5 \cos(2qa) + \tfrac{4}{9}[4e_4 \cos(qa) + 2e_6 \cos(2qa)] L_0' + \tfrac{1}{3}[2e_1^2 + e_2^2 + 4e_1 e_2 \cos(qa) + 2e_1^2 \cos(2qa)][G'(3q) - 1] \ , \tag{37}$$

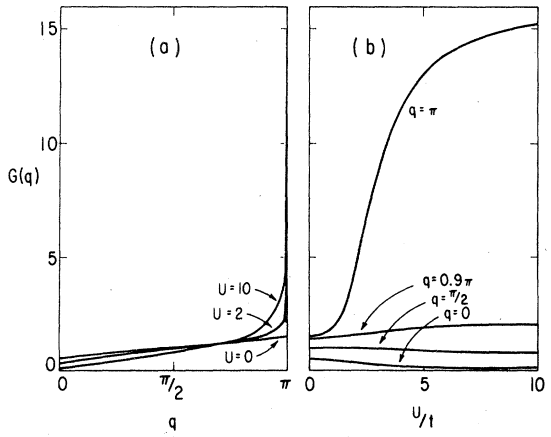

FIG. 3. Spin-spin correlation function $G(q)$ in 1D Hubbard model from the RG calculation. (a) For fixed U as a function of q. (b) For fixed q as a function of U.

with

$$
\begin{aligned}
e_1 &= \tfrac{1}{2}b_2^2 + \tfrac{2}{3}b_3^2 \ , \\
e_2 &= b_1^2 - \tfrac{1}{3}b_3^2 \ , \\
e_3 &= -\tfrac{1}{2}a_2^2 \ , \\
e_4 &= -\tfrac{2}{3}b_3^2 + \tfrac{1}{2}a_2^2 \ , \\
e_5 &= -a_1^2 \ , \\
e_6 &= \tfrac{1}{3}b_3^2 + a_1^2 \ ,
\end{aligned}
\tag{38}
$$

so that iterating Eq. (37) together with Eq. (16) we obtain the correlation function. In Fig. 3 we plot $G(q)$: (a) as a function of q for several values of U; and (b) as a function of U for several values of q. Note the sharp increase in the correlation function for large U and $q \sim \pi$. In the large U limit, the system is equivalent to an antiferromagnetic Heisenberg model with coupling t^2/U and the increase in $G(q)$ at $q \sim \pi$ signals the tendency to antiferromagnetic ordering. In the antiferromagnetic Heisenberg chain, the ground-state spin-spin correlation function is believed to decay with distance as $\langle \sigma_z^0 \sigma_z^{R=na} \rangle \sim (-1)^n/R$ (Ref. 19), and hence the $q=\pi$ Fourier transform is divergent. We obtain in the large U limit $\langle \sigma_z^0 \sigma_z^R \rangle \sim (-1)^n/R^{1.07}$, which is close to the above result. Unfortunately, this small error in the exponent causes our calculated $G(q)$ to go to a large finite value instead of diverging for $q \to \pi$, and $U \to \infty$.

III. TWO AND THREE DIMENSIONS

We next apply our method to a two-dimensional square lattice. The smallest sensible choice for a cell in this case is a 3×3 square (we want an odd number of sites per cell). This is, however, not simple, since we have to deal with $4^9 = 262\,144$ states (although there are simplifications due to symmetries). For that reason, we implement the simplifying scheme shown in Fig. 4. We perform our transformation in two steps; in the first step we take three-site linear cells in the x direction and treat all the couplings in the y direction approximately, and in the second step we do the same procedure with a 90° rotation. Remarkably, we recover after these two steps an isotropic system.

As mentioned earlier, this system with only nearest-neighbor hopping is believed to exhibit the same behavior as the 1D model, a Mott transition at $U=0$. Any small distortion of the free-electron Fermi surface, however, by introducing longer range hopping, will change this very special feature. We have performed calculations with nearest-neighbor hopping only and including small second- and third-nearest-neighbor hopping terms and find a Mott transition for finite U in all cases. That is, our method is insensitive to that subtle property of the model with nearest-neighbor hopping only. Nevertheless, a Mott transition for a finite U is what one would expect in any higher-dimensional real material. Since our results do not change significantly by introducing second- and third-nearest-neighbor hopping terms, we will discuss for simplicity the nearest-neighbor hopping model only. Our recursion relations are now

$$
\begin{aligned}
U_{n+1} &= \bar{U}_{n+1} + 2(\bar{\lambda}_a^{(n+1)} - \bar{\lambda}_b^{(n+1)}) \ , \\
t_{n+1} &= 2\bar{\lambda}_{n+1}^2 \bar{t}_{n+1} \ ,
\end{aligned}
\tag{39}
$$

where $\bar{U}_{n+1}$ and $\bar{t}_{n+1}$ are obtained from U_n and t_n by the 1D recursion relations (II) and $\bar{\lambda}_a^{(n+1)}$, $\bar{\lambda}_b^{(n+1)}$, and $\bar{\lambda}_{n+1}$ are given by the same functions of $\bar{U}_{n+1}$ and $\bar{t}_{n+1}$ as in the 1D case. Analyzing these recursion relations, we now find a nontrivial fixed point at

$$
\left(\frac{U}{t} \right)_c = 3.72 \tag{40}
$$

which describes a Mott transition; below this point, we scale to the free-electron fixed point $U/t=0$, above this to the strong interaction limit $U/t=\infty$. The value one obtains from the Hubbard III calcula-

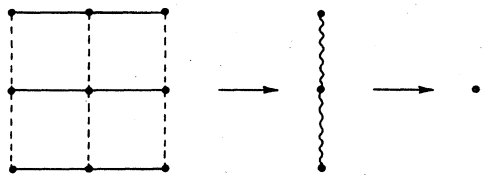

FIG. 4. Approximate RG transformation in 2D. First we take three-site cells in the x direction, then in the y direction. After the first step the couplings in the x and y direction are different, but they are again equal after the second step.

tion[1] for a two-dimensional lattice with a parabolic density of states is $(U/t)_c = 6.93$. This discrepancy is not surprising, if we take into account that the densities of states for both calculations are quite different. Also, our method probably underestimates y_c since we are neglecting transitions to higher states that could enhance delocalization.

We study the behavior of the localization length near the fixed point. In this case, the localization length has a power-law behavior

$$\xi \sim |y - y_c|^{-\nu} \ . \tag{41}$$

We can obtain the exponent ν by the same arguments discussed in the 1D case or by the standard method of linearizing the recursion relations around the fixed point; we find

$$\nu = 1.40 \ . \tag{42}$$

For the energy gap above the transition, we also obtain an algebraic behavior

$$E_g = U_\infty \sim |U - U_c|^s \ . \tag{43}$$

Plotting $\log E_g$ vs $\log |U - U_c|$ we obtain

$$s = 1.34 \ . \tag{44}$$

This can also be obtained via the scaling relation $s = \nu z$, where z is the "dynamic exponent" which is related to the factor by which the energy scales at the fixed point under the RG transformation, $c(l) : c(l) = 1/l^z$ (l being the length scale change). In this case, $z = 0.963$.

It is interesting to compare our result for the gap exponent with the exponent obtained from Hubbard's calculation. For that case, one obtains $s = 1.5$, which is close to our result. In another calculation, however,[20] it is predicted that the gap exponent at the Mott transition should be $s = 0.5$. This result is obtained by taking into account the localization of the pseudoparticle states near the band edges of the Hubbard band. Our result, however, lends support to the original value of s, at least in two dimensions.

Finally, we can also extend this calculation to three dimensions by the same method, although one might expect it to be much less accurate. Again we find a Mott transition, now at

$$\left[\frac{U}{t}\right]_c = 4.76 \tag{45}$$

and the critical exponents are $\nu = 0.826$ and $s = 1.08$.

It is interesting to note that our exponents satisfy an approximate interdimensional scaling law recently proposed for electronic problems in disordered media[14] and for critical phenomena[15]

$$\nu_d = \nu_{d-1} \frac{5-d}{4-d-2\nu_{d-1}} \ . \tag{46}$$

In one dimension, we have $\nu_1 = \infty$; substituting in Eq. (44), we find $\nu_2 = 1.5$, which is satisfied by our result [Eq. (40)] within 7%. Putting $\nu_2 = 1.40$, we find $\nu_3 = 0.74$, which differs from our result by about 10%. Note that even for the Ising model this scaling relation is only approximately satisfied. These arguments lend further support to our higher-dimensional calculation.

We have also computed the exponent η in the metallic region for the two- and three-dimensional cases. We find $\eta = 2$ and 3, respectively, independently of the coupling, which are the exact results for $U = 0$. This happens because we scale always to the $U = 0$ fixed point on the metallic side of the transition. However, one cannot rule out the possibility that there may be a line of fixed points in the metallic region with continuously varying critical exponents which is missed in this simple RG analysis.

IV. SUMMARY

In summary, we have studied the half-filled Hubbard model at zero temperature using a real-space RG technique. Although the method is approximate, we believe it gives a good qualitative description of the behavior of these models, as it has for other cases. In one dimension, we obtained correctly the fact that the ground state is insulating for any nonzero U. We calculated the ground-state energy and the magnitude of the local moment and found good agreement with the exact results. We defined and calculated the localization length for the electrons in the ground state, and found that it diverges exponentially fast as $U \to 0$. A similar behavior is found for the energy gap, which goes to zero exponentially fast, in agreement with the exact solution. However, the power of the exponent is not given correctly by the RG method. We also calculated the spin-spin static correlation function and found a strong tendency towards antiferromagnetic ordering at large U, although we failed to obtain the divergency for $U = \infty$ that occurs in the antiferromagnetic Heisenberg chain. We extended the calculation to two and three dimensions and found a Mott transition at a finite U for these cases. The critical exponents for the transition were found to satisfy an approximate interdimensional scaling law recently proposed. We believe that the method will be useful for studying other fermionic Hamiltonians in one and higher dimensions.

ACKNOWLEDGMENTS

I acknowledge helpful discussions with Professor G. Mazenko and his constant encouragement, as well as his careful reading of the manuscript. A useful

discussion with Professor J. Hertz is also acknowledged. This work was supported by the Materials Research Laboratory program of the National Science Foundation at the University of Chicago. In addition, the author was supported by a Victor J. Andrew Memorial Feliowship.

---

*Present address: Institute for Theoretical Physics, University of California, Santa Barbara, Calif. 93106.

[1]J. Hubbard, Proc. R. Soc. London Ser. A 276, 238 (1963); 281, 401 (1964).
[2]S. D. Drell, M. Weinstein, and S. Yankielowicz, Phys. Rev. D 14, 1769 (1977).
[3]R. Jullien, P. Pfeuty, J. N. Fields, and S. Doniach, Phys. Rev. B 18, 3568 (1978); R. Jullien, J. N. Fields, and S. Doniach, *ibid.* 16, 4889 (1977).
[4]J. E. Hirsch and G. F. Mazenko, Phys. Rev. B 19, 2656 (1979); J. E. Hirsch, Phys. Rev. B 20, 3907 (1979).
[5]J. N. Fields, Phys. Rev. B 19, 2637 (1979); J. N. Fields, H. W. J. Blöte, and J. C. Bonner, J. Appl. Phys. 50, 1807 (1979).
[6]R. Jullien and P. Pfeuty, Phys. Rev. B 19, 4646 (1979); W. A. Penson, R. Jullien, and P. Pfeuty, *ibid.* 19, 4653(1979).
[7]D. C. Mattis and J. Gallardo (unpublished).
[8]E. Lieb and F. Wu, Phys. Rev. Lett. 20, 1445 (1968).
[9]H. Shiba and P. A. Pincus, Phys. Rev. B 5, 1966 (1972).
[10]S. T. Chui and J. W. Bray, Phys. Rev. B 18, 2426 (1978).
[11]P. Richmond, Solid State Commun. 7, 997 (1969).
[12]P. M. Chaikin, P. Pincus, and G. Beni, J. Phys. C 8, L65 (1975).
[13]B. H. Brandow, J. Phys. C 8, L357 (1975).
[14]K. F. Freed, J. Phys. C 12, L17 (1979).
[15]Y. Imry, G. Deutscher, and D. J. Bergmann, Phys. Rev. A 7, 744 (1973).
[16]S. Methfessel and D. Mattis, in *Handbuch der Physik,* edited by S. Flügge (Springer Verlag, Berlin, 1968), Vol. 18, Pt. 1.
[17]E. Fradkin and S. Raby, Phys. Rev. D 20, 2566 (1979).
[18]A. A. Ovchinnikov, Sov. Phys. JETP 30, 1160 (1970).
[19]A. Luther and I. Peschel, Phys. Rev. B 12, 3908 (1975).
[20]F. Yonezawa and M. Watabe, Phys. Rev. B 8, 4540 (1973).