Renormalization-group study of the Anderson-Hubbard model

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We study the half-filled Hubbard model with random on-site energies with the use of a real-space renormalization group. For $d=1$, we find a transition from an Anderson insulator to a Hubbard insulator as the Hubbard U is increased. We find no metallic phase. For $d=3$, we find a metallic phase which, surprisingly, is stabilized against Anderson localization by a small Hubbard U.

I. INTRODUCTION

In disordered systems a metal-insulator transition can occur due to electronic states at the Fermi surface becoming localized.[1,2] A model commonly used to describe this is the Anderson Hamiltonian[1]—a tight binding model with randomness introduced by having the on-site energies vary independently from site to site. For fixed electron density the transition from metal to insulator occurs when the ratio of the random energy spread W to the hopping term t exceeds a critical value.

A metal-insulator transition can also be the result of electron-electron interactions. In the Hubbard model[3,4] the only interaction present is that between two electrons on the same atom. When this term U is large compared to the hopping term t, the band splits into two subbands with a gap between them. If there is one electron per site, the lower subbands for both spins will be full and the upper ones empty, and the system will be an insulator.

Thus both the Anderson transition and Hubbard transition are favored by a small hopping term. Although it is not well understood what the combined effects of the disorder and the repulsion term are, the following are expected to be true: (1) Introducing weak disorder in the Hubbard model causes the subbands to broaden and overlap if the gap is small; hence, a larger U is needed for the Hubbard transition. (2) The Coulomb term provides additional localizing influence and so less disorder is needed for localization.

In this paper we present a renormalization-group (RG) calculation for the half-filled Hubbard-Anderson Hamiltonian at $T=0$. The method we use is that developed for quantum-mechanical spin systems.[5–8] Recently, Hirsch has used this method to study the pure Hubbard model[9] and we essentially follow his procedure. An RG calculation to second order for the pure model has also been carried out by Dasgupta and Pfeuty.[10] A more elaborate calculation for the pure system in one dimension (1D) has also been performed by Chui and Bray.[11]

In Sec. II we describe the RG calculation. The description is self-contained although the procedure is just a modification of Hirsch's. In Secs. III and IV we present the results for $d=1$ and $d=3$, respectively. We find that a small U actually hinders localization, contradicting the second expectation mentioned above. Our method is too crude to determine whether this effect can stabilize the metallic phase against localization in 2D. (An elaborate calculation of this type for the noninteracting system in 2D by Lee indicates that finite disorder is needed for localization. The validity of this result is still unclear.[12])

II. PROCEDURE

The Hubbard-Anderson Hamiltonian is given by

$$H=\sum_{i\sigma} W_i n_{i\sigma} - \sum_{\substack{\langle ij\rangle \\ \sigma}} t_{ij} C_{i\sigma}^{\dagger} C_{j\sigma} + \sum_i U n_{i\uparrow} n_{i\downarrow} , \tag{2.1}$$

where $C_{i\sigma}^{\dagger}, C_{i\sigma}$ creates and destroys an electron of spin σ at site i, respectively, and $n_{i\sigma}=C_{i\sigma}^{\dagger}C_{i\sigma}$. U is the effective on-site Coulomb repulsion, taken to be positive ("negative U" is possible in a strongly polarizable medium and leads to interesting behaviors[13]). The hopping constants t_{ij}, taken to be i,j independent initially, connect only nearest neighbors. The site energies W_i are chosen independently from a Gaussian distribution (for numerical convenience) with a width W. We consider the half-

filled band case, and so there is on the average one particle per site.

The calculation for 1D is as follows. We generate 300 random energies W_i using a Gaussian random number generator and place them on a chain. We then divide the chain into cells of three sites (odd number of sites to preserve fermionic character) and rewrite the Hamiltonian as

$$H=\sum_{\alpha} H_{\alpha}-\sum_{\alpha\sigma} t_{3\alpha,3\alpha+1}(C^{\dagger}_{3\alpha,\sigma}C_{3\alpha+1,\sigma}+\text{H.c.}) , \tag{2.2}$$

where α is a cell index (the cell α contains the sites $3\alpha-2,3\alpha-1,3\alpha$). H_{α}, the cell Hamiltonian, is given by the terms in the original Hamiltonian involving only the sites in cell α. The hopping terms between boundary sites couple neighboring cells.

Next, we diagonalize each H_{α} exactly. Since there are four states per site ($|0\rangle$, $C^{\dagger}_{i\uparrow}|0\rangle \equiv |\uparrow\rangle$, $C^{\dagger}_{i\downarrow}|0\rangle \equiv |\downarrow\rangle$, $C^{\dagger}_{i\uparrow}C^{\dagger}_{i\downarrow}|0\rangle \equiv |\uparrow\downarrow\rangle$), we are dealing with a possible 64 states for three sites. However, H_{α} conserves the number of particles n, total spin S, and total z component of spin S_z; this allows us to decouple different subspaces. We ignore charge fluctuations for length scales larger than the size of the cell and consider only $n=2,3,4$ (we will return to this later). We keep only the lowest energy states for each particle number—singlets with $S=0$ for $n=2,4$ ($|2\rangle, |4\rangle$), and a doublet with $S=\frac{1}{2}$, $S_z=\pm\frac{1}{2}$ for $n=3$ ($|3\uparrow\rangle, |3\downarrow\rangle$); the corresponding energies are $E^{(2)},E^{(4)},E^{(3)}$. There are six states with $S=0$ for $n=2,4$, and eight states with $S=\frac{1}{2}$, $S_z=\pm\frac{1}{2}$ for $n=3$; and so we must diagonalize (numerically) 6×6 and 8×8 matrices. The various states are listed in the Appendix.

We define new states

$$\begin{aligned}&|0'\rangle\equiv|2\rangle, |\uparrow'\rangle\equiv|3\uparrow\rangle, |\downarrow'\rangle\\ &\quad\equiv|3\downarrow\rangle, |\uparrow\downarrow'\rangle\equiv|4\rangle .\end{aligned} \tag{2.3}$$

Associated with these states are new fermion operators,

$$\begin{aligned}&C'^{\dagger}_{\uparrow(\downarrow)}|0'\rangle=|\uparrow(\downarrow)'\rangle ,\\ &C'^{\dagger}_{\uparrow}C'^{\dagger}_{\downarrow}|0'\rangle=-C'^{\dagger}_{\downarrow}C'^{\dagger}_{\uparrow}|0'\rangle=|\uparrow\downarrow'\rangle ,\\ &n'_{\sigma}=C'^{\dagger}_{\sigma}C'_{\sigma} .\end{aligned} \tag{2.4}$$

Restricting ourselves to these states, we can write the Hamiltonian as

$$H=\sum_{i\sigma} W'_i n'_{i\sigma}-\sum_{\substack{\langle ij\rangle\\ \sigma}} t'_{ij}C'^{\dagger}_{i\sigma}C'_{j\sigma}+\sum U'_i n'_{i\uparrow}n'_{i\downarrow} +\text{const} , \tag{2.5}$$

where i,j refer to cell indices. The renormalized parameters are given by

$$\begin{aligned}&W'_i=E^{(3)}_i-E^{(2)}_i ,\\ &U'_i=E^{(4)}_i-2E^{(3)}_i+E^{(2)}_i ,\end{aligned} \tag{2.6}$$

and t'_{ij} are obtained by insisting that the matrix elements between new states on neighboring cells are the same whether we use the old or the new Hamiltonian:

$$t'_{i,i+1}=t_{3i,3i+1}\langle\uparrow'_i 0'_{i+1}|C^{\dagger}_{3i+1,\uparrow}C_{3i,\uparrow}|0'_i\uparrow'_{i+1}\rangle , \tag{2.7a}$$

$$t'_{i,i+1}=t_{3i,3i+1}\langle\uparrow'_i\downarrow'_{i+1}|C^{\dagger}_{3i+1,\uparrow}C_{3i,\uparrow}|0'_i\uparrow\downarrow'_{i+1}\rangle , \tag{2.7b}$$

$$t'_{i,i+1}=t_{3i,3i+1}\langle\uparrow\downarrow'_i 0'_{i+1}|C^{\dagger}_{3i+1,\uparrow}C_{3i,\uparrow}|\downarrow'_i\uparrow'_{i+1}\rangle , \tag{2.7c}$$

$$t'_{i,i+1}=t_{3i,3i+1}\langle\uparrow\downarrow'_i\downarrow'_{i+1}|C^{\dagger}_{3i+1,\uparrow}C_{3i,\uparrow}|\downarrow'_i\uparrow\downarrow'_{i+1}\rangle . \tag{2.7d}$$

If there is particle-hole symmetry on a microscopic scale, the matrix elements in Eqs. (2.7a)—(2.7d) will all be the same and $t'_{i,i+1}$ calculated from one equation will satisfy the other three. However, for the random system, there is no such symmetry and the matrix elements are all different. We define the magnitude of $t'_{i,i+1}$ as the root mean square of the four values obtained from the four equations (there is spin inversion symmetry and so it is only necessary to consider these four equations).

The new energies W'_i no longer obey a Gaussian distribution and the t_{ij} and U_i are no longer site independent. In order to iterate the RG, we adopt the following procedure:

(1) We force the distribution of W'_i back into a Gaussian with new width

$$W'^2=\overline{W'^2_i}-(\overline{W'_i})^2 \tag{2.8}$$

(the overbar implies average). The new Gaussian is not centered at zero since there is a constant shift due to the repulsion term but can be taken to be so (we can do this formally by introducing the chemical potential).

(2) We force U'_i back into a constant,

$$U'=\overline{U'_i} . \tag{2.9}$$

(3) We force the distribution of t'_{ij} into a Gaussian with mean

$$t'=\overline{|t'_{ij}|} \tag{2.10a}$$

and width

$$t_2' = \overline{t_{ij}'^2} - (\overline{|t_{ij}'|})^2 . \quad (2.10b)$$

We then use these parameters to generate again a lattice of 300 sites. This process is iterated and the flows of the parameters observed.

The above define our RG procedure. We now discuss the approximations involved.

(1) The usual approximation of truncation of eigenstates is employed. In a pure system this allows one to construct a variational ground state. However, because it is necessary to generate an N-site random system from an $(N/3)$-site one in a nonperiodic way, this is no longer true in the present case. Nevertheless, the truncation process is still within the spirit of RG theory.

(2) Charge fluctuations are ignored at every iteration except for those within each cell. Although this does not mean that a cell of N sites (of the original lattice) must be occupied by N particles, it does mean that the cell can be occupied by no less than $N-1$ particles and no more than $N+1$ particles. The effect of unfavorable occupation is to increase the renormalized potential spread; hence we expect to obtain Anderson localization of states near the Fermi surface with less disorder than is actually required. Also, this means that even for the case $t_{ij}, U \equiv 0$, the energy scale does not change with length scale correctly; and the calculation does not give the correct density of states even in the most trivial case.

(3) The distributions of W_i and t_{ij} are forced into Gaussians at every iteration. For $t_{ij}, U \equiv 0$, after one iteration, the distribution of W_i' can be calculated and is found to be

$$P'(W_i') \sim e^{-W_i'^2/2}[1-\mathrm{erf}^2(W_i'/\sqrt{2})] ,$$

not appreciably different from a Gaussian. So, at least for this trivial case, this approximation is probably acceptable.

(4) A finite-sized lattice is used at every iteration. In fact, we are forced to use a rather small lattice because of all the matrix diagonalizations involved. However, we have checked a few values with a larger lattice ($N=900$) and do not notice any qualitative differences.

We also perform the calculation for 3D using a $12\times12\times12$ cubic lattice. To carry out the RG, we divide the lattice into cells of $3\times3\times3$. Following Hirsch, we perform the RG procedure first in the x direction (for example), then in the y direction and then in the z direction. After the RG process is performed for each direction, a new set of parameters (W_i', t_{ij}', U_i') is obtained; the RG procedure for the next direction is done using these parameters. Only after the RG process is completed for all three directions and the final set of parameters for that iteraction obtained are the distributions of W_i' and t_{ij}' forced into Gaussians and the U_i' set to a constant. Unlike the case of 1D, the sign of t_{ij} is important in 3D ("frustration"), and t_{ij}' instead of $|t_{ij}'|$ is now used in (2.10a) and (2.10b).

III. RESULTS FOR 1D

In Fig. 1 we show the flows of $t/W, U/W$ for 1D as the RG procedure is iterated. t_2/W is found to iterate to zero for all initial $t_2=0$ and is not shown. The phases are also indicated in the figure.

There are two stable fixed points, at $P_H=(t/W=0,\ U/W=\infty)$ and $P_A=(0,0.48)$. Hence, there are two phases, both insulating. The fixed point at $P_M=(\infty,0)$ is unstable and there is no metallic phase. This is to be expected since neither the Hubbard nor the Anderson model has a metallic phase in 1D.[14,15]

The Hamiltonian of the fixed point P_H has $t \sim t_2 \ll W \ll U$. For $t, t_2, W=0$, each site is occupied by one particle and there are 2^N degenerate ground states since the energy is independent of the spins of the electrons. This degeneracy is not broken by W_i for $W \ll U$. However, in second order, this degeneracy is broken by introducing small hopping terms t_{ij}. In fact, the system is equivalent to a spin-$\frac{1}{2}$ Heisenberg antiferromagnetic chain with couplings $J_{ij}=2t_{ij}^2/U$.[16] If t_{ij} obey a Gaussian distribution, the distribution of J_{ij} is given by

$$P(J) \sim \theta(J) \int \exp[-(t'-t)^2/2t_2^2] \times \delta(J-2t'^2/U)dt' \sim \theta(J)/\sqrt{J}\exp[-\tfrac{1}{2}(\sqrt{J}-\sqrt{J_a})^2/J_0] , \quad (3.1)$$

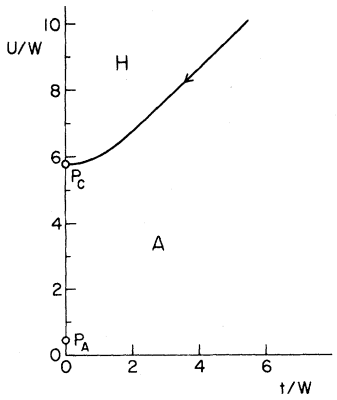

FIG. 1. Phase diagram of the 1D Anderson-Hubbard Hamiltonian as obtained by our RG calculation.

where $J_a = 2t^2/U$, $J_0 = 2t_2^2/U$.

At P_A, $t \sim t_2 \ll U \lesssim W$. For $t, t_2 = 0$, a site i is double occupied if $W_i < -U/2$, singly occupied if $-U/2 < W_i < U/2$, and unoccupied if $W_i > U/2$. Thus, single spins occupy sites with probability p,

$$p = \frac{1}{\sqrt{2\pi W^2}} \int_{-u/2}^{u/2} e^{-x^2/2W^2} dx = \mathrm{erf}\left[\frac{u}{\sqrt{8W}}\right]. \tag{3.2}$$

There is no energy gap. Introducing small t_{ij} again couple the single spins. But, as has been shown by Theodorou and Cohen,[17] now the couplings J_{ij} obey a distribution $P(J) \overset{J \to 0}{\sim} J^{-\alpha}$, where α depends on p [if we set the decay length in their equation equal to the lattice spacing, then $\alpha = 1 - |\ln(1-p)| \approx 0.8$ for the fixed point value of U/W].

Thus, as U increases, there is a transition from a gapless insulator to one with a gap equal to U_∞, where U_∞ is the value of U at the fixed point P_H. The critical fixed point is at $P_c = (0, 5.8)$. Close to the phase boundary on the phase H side, the gap is $U_\infty \sim (U - U_c)$, where U_c is the value of U at the phase boundary (for $t = 0$, $U_\infty = U - U_c$).

IV. RESULTS FOR 3D

The flows of the parameters for 3D are shown in Fig. 2. The fixed point $P_M = (\infty, 0)$ is now stable and so there is now a metallic phase M. The three phases meet at the triple point $P_T = (1.1, 5.8)$. The phase-A fixed point is now at $P_A = (0, 1.26)$ and the critical fixed point for the $A \leftrightarrow H$ transition is at $P_c = (0, 8.3)$. The fact that these are different from their values for 1D is due to the inaccuracy of the calculation, since for $t_{ij} \equiv 0$, the system is essentially zero dimensional. As in 1D, close to the $A \leftrightarrow H$ phase boundary (but far away from P_T), the gap is $U_\infty \sim U - U_c$.

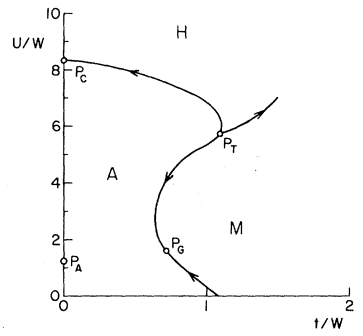

FIG. 2. Phase diagram of the 3D Hamiltonian.

The Anderson fixed point on the $U = 0$ axis is totally unstable and the critical point for the Anderson transition (M-A) is at P_G (actually, the fixed point has nonzero t_2, and this is a projection). For a small but finite U, the critical value of t/W actually decreases from its value at $U = 0$, implying that more disorder is needed for localization. This is contrary to what is expected if we consider U as an additional localizing influence from what we know about the pure Hubbard model. On the other hand, because of the Coulomb repulsion, the presence of a spin-up electron causes the potential on a site with a favorable W_i to be less so for the spin-down electron and vice versa; hence, the electrons are less likely to be trapped by the random potential. Our calculation seems to indicate that the latter is the dominating effect for small U. As U increases, the critical value of t/W begins to increase again, indicating that the localizing influence of U is now the important effect.

For $t/W > 1.1$, the system goes directly from phase M to phase H as U increases. The critical fixed point for this transition is just the Hubbard Hamiltonian critical point (∞, ∞). The ratio of U/t is 4.76, the same as that obtained by Hirsch.[9] Close to the phase boundary (but not close to P_T), the gap is $U_\infty \sim (U - U_c)^{1.08}$.

V. SUMMARY

We studied the half-filled Anderson-Hubbard model using an RG method which is a modification of the one used by Hirsch to study the pure Hubbard model. Our calculation treated the randomness rather crudely and expected errors were discussed.

In 1D we found that, as expected, there is no metallic phase. As U increases an energy gap develops and the system undergoes a transition from an "essentially" Anderson insulator to an "essentially" Hubbard insulator. For t_{ij} small, we discussed the magnetic properties far away from the phase boundary.

In 3D we found that the metallic phase is also present. We also found that more disorder is needed for the metal—Anderson-insulator transition for increasing U if U is small, indicating that the metallic phase is actually stabilized by a small Coulomb repulsion. For larger U the localizing effect of the correlation dominates.

For $d = 2$ all states are expected to be localized in

the Anderson model no matter how small the disorder is as long as it is finite.[18,19] It would be interesting to investigate whether the stabilizing effect of the metallic phase by a small U can cause a phase transition to occur at finite disorder. Unfortunately, our method is too crude to handle this case.

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APPENDIX

The states needed for the RG calculation, are as follows: For $n=2, S=0, S_z=0$,

$$\frac{1}{\sqrt{2}}(|\uparrow\rangle|0\rangle|\downarrow\rangle-|\downarrow\rangle|0\rangle|\uparrow\rangle),$$

$$\frac{1}{\sqrt{2}}(|\uparrow\rangle|\downarrow\rangle|0\rangle-|\downarrow\rangle|\uparrow\rangle|0\rangle),$$

$$\frac{1}{\sqrt{2}}(|0\rangle|\uparrow\rangle|\downarrow\rangle-|0\rangle|\downarrow\rangle|\uparrow\rangle),$$

$$|\uparrow\downarrow\rangle|0\rangle|0\rangle,$$

$$|0\rangle|\uparrow\downarrow\rangle|0\rangle,$$

$$|0\rangle|0\rangle|\uparrow\downarrow\rangle.$$

For $n=3, S=\frac{1}{2}, S_z=\frac{1}{2}$,

$$\frac{1}{\sqrt{6}}(|\uparrow\rangle|\uparrow\rangle|\downarrow\rangle-2|\uparrow\rangle|\downarrow\rangle|\uparrow\rangle+|\downarrow\rangle|\uparrow\rangle|\uparrow\rangle),$$

$$\frac{1}{\sqrt{2}}(|\uparrow\rangle|\uparrow\rangle|\downarrow\rangle-|\downarrow\rangle|\uparrow\rangle|\uparrow\rangle),$$

$$|\uparrow\rangle|\uparrow\downarrow\rangle|0\rangle,$$

$$|\uparrow\rangle|0\rangle|\uparrow\downarrow\rangle,$$

$$|\uparrow\downarrow\rangle|\uparrow\rangle|0\rangle,$$

$$|\uparrow\downarrow\rangle|0\rangle|\uparrow\rangle,$$

$$|0\rangle|\uparrow\downarrow\rangle|\uparrow\rangle,$$

$$|0\rangle|\uparrow\rangle|\uparrow\downarrow\rangle.$$

For $n=3, S=\frac{1}{2}, S_z=-\frac{1}{2}$,

$$\frac{1}{\sqrt{6}}(-|\downarrow\rangle|\downarrow\rangle|\uparrow\rangle+2|\downarrow\rangle|\uparrow\rangle|\downarrow\rangle-|\uparrow\rangle|\downarrow\rangle|\downarrow\rangle),$$

$$\frac{1}{\sqrt{2}}(-|\downarrow\rangle|\downarrow\rangle|\uparrow\rangle+|\uparrow\rangle|\downarrow\rangle|\downarrow\rangle),$$

$$|\downarrow\rangle|\uparrow\downarrow\rangle|0\rangle,$$

$$|\downarrow\rangle|0\rangle|\uparrow\downarrow\rangle,$$

$$|\uparrow\downarrow\rangle|\downarrow\rangle|0\rangle,$$

$$|\uparrow\downarrow\rangle|0\rangle|\downarrow\rangle,$$

$$|0\rangle|\uparrow\downarrow\rangle|\downarrow\rangle,$$

$$|0\rangle|\downarrow\rangle|\uparrow\downarrow\rangle.$$

For $n=4, S=0, S_z=0$,

$$\frac{1}{\sqrt{2}}(-|\uparrow\rangle|\uparrow\downarrow\rangle|\downarrow\rangle-|\downarrow\rangle|\uparrow\downarrow\rangle|\uparrow\rangle),$$

$$\frac{1}{\sqrt{2}}(|\uparrow\rangle|\downarrow\rangle|\uparrow\downarrow\rangle-|\downarrow\rangle|\uparrow\rangle|\uparrow\downarrow\rangle),$$

$$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle|\uparrow\rangle|\downarrow\rangle-|\uparrow\downarrow\rangle|\downarrow\rangle|\uparrow\rangle),$$

$$|0\rangle|\uparrow\downarrow\rangle|\uparrow\downarrow\rangle,$$

$$|\uparrow\downarrow\rangle|0\rangle|\uparrow\downarrow\rangle,$$

$$|\uparrow\downarrow\rangle|\uparrow\downarrow\rangle|0\rangle.$$

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