PHYSICAL REVIEW B VOLUME 37, NUMBER 13 1 MAY 1988

Mean-field hopping solution in the Anderson-Hubbard model

R. Allub*
International Centre for Theoretical Physics, 34100 Trieste, Italy

(Received 25 September 1987)

The tight-binding diagonally disordered Anderson model with on-site Coulomb interaction is solved in the mean-field hopping approach. Phase diagrams of the metal-insulator transition are obtained from the free energy for the half-filled band and the binary-alloy distribution. For attractive interaction ($U<0$), the Coulomb term gives additional localizing effect and for some values of the microscopic parameters the temperature induced two transitions (insulator to metal to insulator). For $U>0$ two different types of behavior are distinguished. For small disorder ($W \leq U/2$), the metallic phase can be induced by disorder, while for large W, the disorder always destroys the phase of extended states.

I. INTRODUCTION

There has been a considerable amount of theoretical effort in recent years devoted to the understanding of disordered media.[1,2] Many aspects of the problem are still far from being understood; in particular, the interplay of the Coulomb interaction and disorder. This important question has been studied theoretically within the framework of certain simplified models, most commonly the so-called Anderson-Hubbard Hamiltonian.[3] This model consists of Anderson's Hamiltonian[4] for disordered media plus an on-site electron-electron interaction (U) term.

Anderson's model is a tight-binding Hamiltonian in which a band is formed from atomic orbitals associated with lattice points. Randomness is introduced in the model by assuming that the site energies (i.e., the diagonal matrix elements of the Hamiltonian) are statistical variables having given probability distribution of width W, which is taken as a measure of the degree of randomness. It has been demonstrated[4–11] within Anderson's model that a critical value of W, W_c may exist such that all eigenstates are localized for $W>W_c$. This disappearance of extended eigenstates has been termed the Anderson transition.

This limit ($U=0$) of the Anderson-Hubbard model (AHM) is still a difficult problem and only the solution in one dimension is known.[12–14]

Without disorder ($W=0$), the AHM reduces to Hubbard's model.[15] As simple as this Hamiltonian is, it still represents a truly interacting system. Without interacting ($U=0$) one obtains a pure band behavior due to the small but finite overlap of the atomic wave functions. For zero hopping term ($t=0$), the atomic limit occurs and the particles are localized. Thus, the Hubbard Hamiltonian describes a system which allows for both these limits; naturally, the intermediate regime $t \simeq U$ is of particular interest, as in this range of parameters the competition between band effects and localization due to correlations is most subtle. So far, only the one-dimensional case has been solved exactly.[16]

One may consequently anticipate that the competition between Anderson localization and Hubbard localization should lead to a very interesting phase diagram. Unfortunately, only numerical approximations exist for the Anderson-Hubbard Hamiltonian.

Renormalization-group calculations[3] show that a small interaction U (as compared to the degree of disorder) actually hinders localization. Results for various correlation functions,[17] using Monte Carlo simulation, show an increase of the on-site correlation when the disorder is increased. Similar results are obtained in more recent numerical work[18] for the localization length.

At present, it seems then that the common result from many different numerical approaches is that the Coulomb term does not provide additional localizing effect for small U.

The aim of this work is to present a very simple approach to the AHM, but one that still retains the essential features of competition between disorder and Coulomb interaction. In this sense, the disorder and the interaction terms are treated exactly, but the kinetic energy of the electrons is considered in a mean-field approach. Its solution allows, due to its simplicity, a better physical understanding of the results.

In Sec. II we set up the model Hamiltonian and obtain the free energy for the binary-alloy distribution. Finally, in Sec. III we present the results and discuss their physical implications.

II. THE MODEL

The Anderson-Hubbard Hamiltonian is given by

$$H=\sum_{i,\sigma}(\varepsilon_i-\mu)n_{i\sigma}-t'\sum_{\langle i,j\rangle,\sigma}c_{i\sigma}^{\dagger}c_{j\sigma}+U\sum_i n_{i\uparrow}n_{i\downarrow}+\tfrac{1}{2}UN\ , \quad (1)$$

where $c_{i\sigma}^{\dagger}$, $c_{i\sigma}$ creates and destroys an electron of spin σ at site i, respectively, and $n_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$; ε_i is the energy level at site i, t' the hopping parameter between nearest neighbors, U the on-site Coulomb interaction, and μ the chemical potential. The site energies are statistical variables having a given probability distribution $P_{(\varepsilon_i)}$.

In order to obtain an exactly solvable model we make the following approximation in the hopping term:

$$(c_{i\sigma}^{\dagger}c_{j\sigma}+\text{H.c.})=(c_{i\sigma}^{\dagger}+c_{j\sigma}^{\dagger})(c_{i\sigma}+c_{j\sigma})-n_{i\sigma}-n_{j\sigma}$$
$$\approx\Delta(c_{i\sigma}+c_{j\sigma})+(c_{i\sigma}^{\dagger}+c_{j\sigma}^{\dagger})\Delta-\Delta^{2}-n_{i\sigma}-n_{j\sigma}\ , \qquad (2)$$

with

$$\Delta=\langle c_{i\sigma}+c_{j\sigma}\rangle=\langle c_{i\sigma}^{\dagger}+c_{j\sigma}^{\dagger}\rangle\ . \qquad (3)$$

In this approximation, the Hamiltonian [Eq. (1)] can be written in site-diagonal form,

$$H=\sum_{i,\sigma}(\varepsilon_i-\mu+t)n_{i\sigma}+Nt\Delta^{2}-t\Delta\sum_{i,\sigma}(c_{i\sigma}^{\dagger}+c_{i\sigma})+U\sum_{i}n_{i\uparrow}n_{i\downarrow}+\tfrac{1}{2}UN\ . \qquad (4)$$

The new hopping parameter is $t=zt'$, where z is the number of nearest neighbors.

In this Hamiltonian [Eq. (4)], the sites are coupled only by the mean-field parameter Δ (to be determined from the minimum of the total free energy) and therefore each site can be solved independently in a subspace of four states.

If we define

$$H_i=(\varepsilon_i-\mu+t)\sum_{\sigma}n_{i\sigma}+t\Delta^{2}-t\Delta\sum_{\sigma}(c_{i\sigma}^{\dagger}+c_{i\sigma})+Un_{i\uparrow}n_{i\downarrow}+\tfrac{1}{2}U\ , \qquad (5)$$

the eigenstates of this Hamiltonian are the following:

(a) two states involving zero and one particle (a linear combination of $|0\rangle$ and $(1/\sqrt{2})(c_{i\uparrow}^{\dagger}+c_{i\downarrow}^{\dagger})|0\rangle$) with energies

$$U/2+t\Delta^{2}+(\varepsilon_i-\mu+t)/2\pm[(\varepsilon_i-\mu+t)^{2}/4+2t^{2}\Delta^{2}]^{1/2}\ ; \qquad (6)$$

(b) two states mixing one and two particles (a linear combination of $c_{i\uparrow}^{\dagger}c_{i\downarrow}^{\dagger}|0\rangle$ and $(1/\sqrt{2})(c_{i\uparrow}^{\dagger}-c_{i\downarrow}^{\dagger})|0\rangle$) with energies

$$U+t\Delta^{2}+3(\varepsilon_i-\mu+t)/2\pm[(\varepsilon_i-\mu+t+U)^{2}/4+2t^{2}\Delta^{2}]^{1/2}\ . \qquad (7)$$

The free energy for any particular site is

$$F_i=-T\ln(2)+t\Delta^{2}+U/2+(\varepsilon_i-\mu+t)/2-T\ln(Z)\ , \qquad (8)$$

where

$$Z=\cosh\{\beta[(\varepsilon_i-\mu+t+U)^{2}/4+2t^{2}\Delta^{2}]^{1/2}\}\times\{\exp[-\beta(\varepsilon_i-\mu+t+U/2)]\}+\cosh\{\beta[(\varepsilon_i-\mu+t)^{2}/4+2t^{2}\Delta^{2}]^{1/2}\}$$

and β is the inverse of the temperature T.

For the total free energy we perform a configurational average. Using the "quenched-type" average[19] we get

$$F_T=\sum_{i}\langle F_i\rangle=N\langle F_i\rangle=N\int P_{(\varepsilon_i)}F_{i(\varepsilon_i)}d\varepsilon_i\ . \qquad (9)$$

In order to have a simple solution, we take the following probability distribution (bindary-alloy approximation) of the site energies:

$$P_{(\varepsilon_i)}=\tfrac{1}{2}\delta_{(\varepsilon_i-W)}+\tfrac{1}{2}\delta_{(\varepsilon_i+W)}\ . \qquad (10)$$

In this approximation, the mean free energy per site is trivially obtained as

$$F=F_T/N=-T\ln(2)+t\Delta^{2}+U/2+(t-\mu)/2-\frac{T}{2}\ln(Z_{+})-\frac{T}{2}\ln(Z_{-})\ , \qquad (11)$$

where

$$Z_{+}=\cosh\{\beta[(W-\mu+t+U)^{2}/4+2t^{2}\Delta^{2}]^{1/2}\}\{\exp[-\beta(W-\mu+t+U/2)]\}+\cosh\{\beta[(W-\mu+t)^{2}/4+2t^{2}\Delta^{2}]^{1/2}\}$$

and

$$Z_{-}=\cosh\{\beta[(-W-\mu+t+U)^{2}/4+2t^{2}\Delta^{2}]^{1/2}\}\{\exp[-\beta(-W-\mu+t+U/2)]\}+\cosh\{\beta[(-W-\mu+t)^{2}/4+2t^{2}\Delta^{2}]^{1/2}\}\ .$$

For the half-filled band case, the chemical potential μ is $t+U/2$ and the free energy reduces to

$$F=-T\ln(2)+t\Delta^{2}+U/4-W/2-T\ln(Z_1)\ , \qquad (12)$$

with

$$Z_1=\cosh\{\beta[(W+U/2)^{2}/4+2t^{2}\Delta^{2}]^{1/2}\}[\exp(-\beta W)]+\cosh\{\beta[(W-U/2)^{2}/4+2t^{2}\Delta^{2}]^{1/2}\}\ ,$$

where the order parameter Δ takes on a value corresponding to the minimum of this F for a given W, U, and T. If the minimum corresponds to $\Delta=0$, the sites are decoupled [see Eq. (4)] and the system is an insulator. For $\Delta=\Delta_{\min}\neq0$, the metallic phase is obtained. At the transition,

$$F_{M(\Delta=\Delta_{\min})}=F_{I(\Delta=0)}\ , \qquad (13)$$

where the subscripts M and I refer to metallic and insulating phases, should hold. We find first- and second-order transitions.

III. RESULTS AND DISCUSSION

It is a very simple exercise in statistical mechanics to calculate the energy and the mean-field parameter $\Delta_{\min}$ for the model Hamiltonian at zero temperature. We find that for small $U(\,|U|<4t)$ a critical value of W, $W_{\mathrm{CA}}=U/2+2t$, exists such that all eigenstates are localized for $W \geq W_{\mathrm{CA}}$ and the system is an Anderson insulator (AI). The ground state has $N/2$ sites with $(\varepsilon_i>0)$ 0 particle and $N/2$ sites with $(\varepsilon_i<0)$ 2 particles, for a mean energy per site of $E_A=-W+U/2$. For $W<W_{\mathrm{CA}}$, the metallic phase $(\Delta_{\min}\neq 0)$ occurs and the mean energy per site is given by

$$E_M=-(t/2)[1+(W-U/2)/(2t)]^2 \ . \tag{14}$$

For large U $(U\geq 4t)$ a new critical value of W appears: $W_{\mathrm{CH}}=U/2-2t$. For $W\leq W_{\mathrm{CH}}$ the system is a Hubbard insulator (HI). The fundamental state is degenerate because each site has one particle with two possible values of the spin $(\uparrow,\downarrow)$ and the mean energy per site is $E_H=0$. Thus, for large U, two possible metal-insulator transitions can occur (HI to metal to AI) and the metallic phase only exists when $W_{\mathrm{CH}}<W<W_{\mathrm{CA}}$.

These results can be interpreted in terms of the energy levels scheme at each site. For small U the conducting states arise from the mixture of zero and one particles at $N/2$ sites and the mixture of one and two particles at the other $N/2$ sites. As U is switched on, for $U<0$, the levels of zero and two particles move away from the one-particle levels and hinder the conducting mixture; as a consequence W_{CA} goes to zero. For $U>0$, the levels of zero and two particles approach the one-particle levels and the mixing is improved; thus, W_{CA} increases with U. This result has been observed in various numerical approaches.[3,17,18]

For $W=0$, it is interesting to note that the energy in the metallic phase [Eq. (14)] reduces to the well-known Gutzwiller result,[20,21]

$$E_{M(W=0)}=-E_0(1-U/U_c)^2 \ , \tag{15}$$

where $E_0=t/2$ and $U_c=8E_0$. In order to solve the Hubbard model at $T=0$, Gutzwiller applied a variational method.[20] At finite temperature, the phase diagrams can be obtained in a straightforward way from the free energy F.

In Fig. 1 we show the variation of the metal-insulator transition temperature T_c as a function of the disorder W for different values of the attractive interaction $(U<0)$. In Fig. 2 the results for small Coulomb repulsion $(0\leq U\leq 4t)$ are presented and the results for $U>4t$ are shown in Fig. 3.

For $U<0$ the phenomenon of reentrance appears. As the temperature is lowered a second-order transition to the metallic phase is observed; at even lower temperature a new transition occurs back to the AI phase (Fig. 1, C and D). In terms of our levels scheme this can be explained as a consequence of the fact that the competing states have different entropy contributions. We have explored the possibility of metallic reentrance in disorder media and have found that it can appear in a small region of the phase diagram.

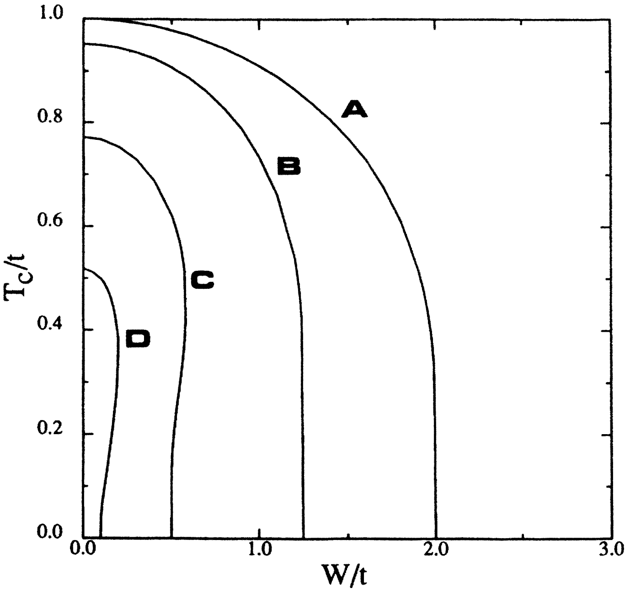

FIG. 1. Variation of the metal-insulator transition temperature T_c as a function of the disorder W for different values of the interaction U: (A) $U=0$, (B) $U=-1.5t$, (C) $U=-3t$, and (D) $U=-3.8t$.

For $U>0$, in the limit of small Coulomb repulsion $(U\leq 2t)$ we observe that increasing the disorder leads to a decrease of the transition temperature down to zero for $W=W_{\mathrm{CA}}$. For $3t\leq U$ a new feature appears: as W is switched on, T_c increases with W. As a consequence, the combined action of both mechanisms gives a function of T_c versus W with a maximum as shown in Fig. 2 and Fig. 3.

For large U $(U>4t)$, the HI phase appears. For $W>W_{\mathrm{CH}}$, at very low temperature a first-order transi-

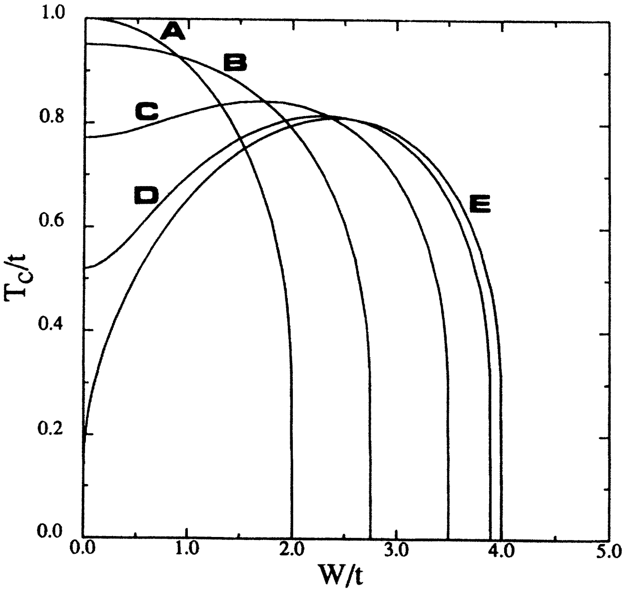

FIG. 2. Variation of T_c as a function of W for U ranging from 0 to $4t$. (A) $U=0$, (B) $U=1.5t$, (C) $U=3t$, (D) $U=3.8t$, and (E) $U=4t$.

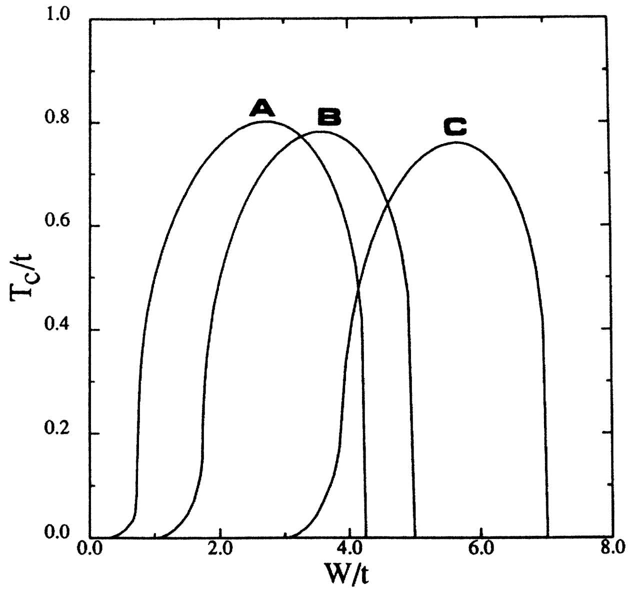

FIG. 3. Variation of T_c as a function of W for U ranging from $4.5t$ to $10t$. (A) $U=4.5t$, (B) $U=6t$, and (C) $U=10t$.

tion occurs between the HI and metallic phase (Fig. 3). Here also we find that the competing states have different entropy contributions.

When the transitions are of second order, it is easy to get an explicit relation for T_c,

$$1-2tA/B=0\ , \tag{16}$$

where

$$A=(1/W_-)\sinh(W_-/2T_c)$$
$$+(1/W_+)[\exp(-W/T_c)]\sinh(W_+/2T_c)\ ,$$
$$B=\cosh(W_-/2T_c)+[\exp(-W/T_c)]\cosh(W_+/2T_c)\ ,$$
$$W_-=W-U/2\ ,$$
$$W_+=W+U/2\ .$$

Finally, it is interesting to analyze the two limiting cases: $W=0$ and $U=0$. In either case, the same law (Fig. 1, A) for T_c is obtained. As the transitions are of second order, Eq. (16) gives

$$T_c/T_{c0}=(W/W_c)[\text{arctanh}(W/W_c)]^{-1} \text{ for } U=0 \tag{17}$$

and

$$T_c/T_{c0}=(U/U_c)[\text{arctanh}(U/U_c)]^{-1} \text{ for } W=0\ , \tag{18}$$

where $T_{c0}=t$, $W_c=2t$, and $U_c=4t$. Therefore, we conclude that the interaction U or the disorder W always destroys the phase of extended states.

IV. SUMMARY

We have studied the competition between disorder and Coulomb interaction in the Anderson-Hubbard model. We solve the problem in the mean-field hopping solution, and recover in this approach Gutzwiller's solution in the Hubbard limit (zero disorder). Despite this simple approximation very interesting phase diagrams are obtained. These results can be interpreted in a very simple energy levels scheme. We believe that this approximation conserves the essential features of the competition between disorder and Coulomb interaction and gives good qualitative results.

For attractive U, we find that the interaction gives additional localizing effect and the possibility of metallic reentrance. For Coulomb repulsion two different types of behavior are distinguished. For small disorder the metallic phase can be induced by disorder, while for large W the phase of extended states is always destroyed.

ACKNOWLEDGMENTS

The author would like to thank Professor Abdus Salam, the International Atomic Energy Agency, United Nations Education, Social and Cultural Organization (UNESCO) and Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET, Argentina.) for financial support and hospitality at the International Centre for Theoretical Physics, Trieste, Italy.

---

*Permanent address: Centro Atómico Bariloche, (8400) S.C. de Bariloche, Río Negro, Argentina.

[1] P. A. Lee and T. V. Ramakrishnan, Rev. Mod. Phys. **57**, 287 (1985).
[2] A. L. Efros and Pollack, *Electron-Electron Interaction in Disorder Systems* (North-Holland, Amsterdam, 1984).
[3] M. Ma, Phys. Rev. B **26**, 5097 (1982).
[4] P. W. Anderson, Phys. Rev. **109**, 1492 (1958).
[5] J. M. Ziman, J. Phys. C **2**, 1230 (1969).
[6] D. M. Thouless, J. Phys. C **3**, 1559 (1970).
[7] M. Kikuchi, J. Phys. Soc. Jpn. **29**, 296 (1970).
[8] E. N. Economou and Morrel H. Cohen, Phys. Rev. Lett. **25**, 1445 (1970); Phys. Rev. B **5**, 2931 (1972).
[9] D. M. Thouless, J. Non-Cryst. Solids **8-10**, 461 (1972).
[10] D. C. Herbert and R. Jones, J. Phys. C **4**, 1145 (1971).
[11] T. Lukes, J. Non-Cryst. Solids **8-10**, 470 (1972).
[12] H. Schmidt, Phys. Rev. **105**, 425 (1957).
[13] P. Erdös and R. C. Herndon, Adv. Phys. **31**, 65 (1982).
[14] E. N. Economou, *Green's Functions in Quantum Physics* (Springer, Berlin, 1983).
[15] J. Hubbard, Proc. R. Soc. London, Ser. A **276**, 238 (1963); **281**, 401 (1964).
[16] E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. **20**, 1445 (1968).
[17] A. Muramatsu and W. Hanke, Phys. Scr. **T13**, 319 (1986).
[18] J. A. Verges, E. Louis, F. Flores, and E. V. Anda, Phys. Rev. B **35**, 7146 (1987).
[19] S. Ma, *Modern Theory of Critical Phenomena* (Benjamin, New York, 1976).
[20] M. C. Gutzwiller, Phys. Rev. Lett. **10**, 159 (1963); Phys. Rev. **134**, A923 (1964).
[21] W. F. Brinkman and T. M. Rice, Phys. Rev. B **2**, 4302 (1970).