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ON THEORY OF ELECTRON LOCALIZATION IN AMORPHOUS SYSTEMS

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1. INTRODUCTION

In recent years enormous efforts have been made to study the properties of disordered or amorphous systems (see [1-3]). Using various kinds of CPA [4-12] and cluster methods [13-15] a substantial progress in understanding the density of states (DS) in such systems could be reached. Especially it was demonstrated that the DS in disordered systems will be determined essentially by the short range order (cf. [14-16]) while the long range effect becomes damped out.

Much more difficulties have arisen when considering the conductivity (or resistivity) in disordered systems. Long ago Mott (see [1,17]) has proposed the concept of mobility edges which truncate the extended states from the localized one. The latter states may occur due to potential fluctuations (cf. [2,18,19]). Then one distinguishes between hopping and band conductivity according to circumstances whether or not the Fermi level lies in the pseudogap, built by localized states. The nature and the conditions for appearance of localized states have been investigated by several authors within different approaches (cf. [3,18-23]). Although a qualitative understanding of electron localization in disor-

dered systems seems to be found (cf. [3]), this subject is yet under current discussion concerning special applied methods and quantitative results for the critical conditions (cf. [2,3,24]).

The basis of localization theories is mostly the Anderson model [18] with disorder only in the diagonal matrix elements of the potential. This kind of disorder causes localized states beginning at the extreme edges of the DS. Under critical disorder conditions an Anderson transition appears where all states become localized (cf. [1-3]). For the application of localization theories to amorphous, especially, to one-component systems it is, however, important to include off-diagonal randomness (ODR), because the fluctuations of the atomic distances cause varying hopping and overlap integrals. In general, the existing localization theories are formulated in such a way that ODR can be included in the consideration without principal difficulties. Economou [25] has formulated a localization theory which formally involves also random hopping integrals. The first numerical estimations on the basis of this theory were made by Herscovici [26] using the simplest approximations. The obtained results have indicated that statistical independent ODR yields an effect of delocalization. Herbert and Jones [22] have tried to treat random hopping potentials in the Anderson model analyzing the residues of the off-diagonal propagator. This treatment was much more difficult than the consideration of diagonal disorder, however, calculations indicate that in three dimensions there is probably a mobility edge in the tail of the DS.

In the present paper the localization theory of Economou and Cohen (E/C) [19] was applied to a generalized tight binding model of amorphous one-component systems involving fluctuations of the hopping integrals which are coupled to the fluctuations of the energy levels and the overlap integrals (Sects. 2 and 3). The obtained expression for the localization functionn L(E) (Sect. 3) is estimated in Sect. 4 with the help of several improved approximations (cf. [3]). Thereby it is found that the coupled diagonal and off-diagonal disorder and the presence of fluctuating overlap integrals lead to an asymmetric change of the mobility edges. Furthermore it is confirmed that the ODR causes an effect of delocalization.

Consequently, an Anderson transition in amorphous systems can only be expected if the diagonal disorder is strong enough, i.e., chemical or other kinds of diagonal disorder are additionally present. As an example, in Sect. 5 we briefly study the influence of diagonal spin disorder due to electron correlation described by the Hubbard model and treated within the alloy analogy (cf. [22,27-29]).

2. MODEL

Let us consider a system containing N identical atoms at the points $\vec{R}_n$ forming an amorphous structure. The Hamiltonian $\mathcal{H}$ for such a system is supposed to be of the form

$$\mathcal{H} = \sum_n h(\vec{w} - \vec{R}_n) + T(\vec{w}), \qquad (1)$$

where $T(\vec{w})$ is the kinetic part and $h(\vec{w} - \vec{R})$ denotes an effective potential due to an

atom at the site $\vec{R}_n$. Now let N linearly independent functions $|\phi_n\rangle$ span the space of N eigenfunctions $|\psi_j\rangle$ of $\mathcal{H}$ with energies E_j from E_a to E_b. These functions $|\phi_n\rangle$ may be approximated by localized atomic orbitals associated with atoms at the point $\vec{R}_n$ (cf. /30/).). Solving the matrix equation

$$(E_j S - h)\nu^j = 0, \tag{2}$$

where the matrix elements of S and h are given by

$$\begin{aligned} S_{nm} &= \langle\phi_n|\phi_m\rangle = \delta_{nm} + \Delta S_{nm}, \\ h_{nm} &= \langle\phi_n|\mathcal{H}|\phi_m\rangle = \epsilon_n \delta_{nm} + V_{nm}, \end{aligned} \tag{3}$$

($V_{nn} = \Delta S_{nn} = 0$), the corresponding eigenfunctions $|\psi_j\rangle$ then are

$$|\psi_j\rangle = \sum_n^N \nu_n^j |\phi_n\rangle. \tag{4}$$

As is shown by Halpern /30/, the density of states between energies E_a and E_b can be calculated by the reduced Green's function which is essentially the projection of the full Green's function (GF) onto the space of the function $|\phi_n\rangle$. In Sect. 3 it is shown that on the basis of the reduced GF the question may be discussed whether or not an eigenstate of $\mathcal{H}$ with energy $E(E_a \leq E \leq E_b)$ is localized.

For the sake of simplicity we will work within the nearest-neighbour approximation (NNA) where

$$V_{nm}, \Delta S_{nm} \begin{cases} \neq 0 & \text{if n,m nearest neighbours (NN)} \\ = 0 & \text{elsewhere.} \end{cases}$$

This approximation is a good one if we assume that the functions are well enough localized and the amorphous structure may be characterized by a well established short range order, e.g., the number of NN Z is nearly constant for various atoms. In the framework of NNA and neglecting three-centre integrals, ϵ_n and V_{nm} are given by

$$\begin{aligned} \epsilon_n &= \langle\phi_n|h(\vec{w} - \vec{R}_n) + T(\vec{w})|\phi_n\rangle + \sum_{m \neq n} \langle\phi_n|h(\vec{w} - \vec{R}_m)|\phi_m\rangle. \\ V_{nm} &= \langle\phi_n|h(\vec{w} - \vec{R}_n) + h(\vec{w} - \vec{R}_m) + T(\vec{w})|\phi_m\rangle. \end{aligned} \tag{5}$$

The variation of the atomic distances $\Delta R_{nm} = |\vec{R}_n - \vec{R}_m|$ in the amorphous structure lead to randomly distributed values of ϵ_n, V_{nm} and ΔS_{nm}. If $|\phi_n\rangle$ is an s-like state these quantities are functions of the distance ΔR_{nm}. Therefore the fluctuations of ϵ_n, V_{nm} V_{nm} and ΔS_{nm} are strong coupled so that really only one random variable exists. As we have assumed no large fluctuations in the NN shell, in a first approximation, expanding ϵ_n, V_{nm} and ΔS_{nm} linearly in the variation of ΔR_{nm}, the following simple relations can be obtained

$$\begin{aligned} \epsilon_n &= a \sum_{m \neq n} (V_{nm} - V_{nm}^{\circ}) + b, \\ \Delta S_{nm} &= s(V_{nm} - V_{nm}^{\circ}) + c, \end{aligned} \tag{6}$$

where V_{nm}° belongs to the averaged atomic positions which determine the type of short range order. For the sake of convenience further we shall choose for $b = 0$ and $c = 0$.

For more complicate atomic orbitals $|\phi_n\rangle$ ϵ_n, V_{nm}, and ΔS_{nm} are only partially correlated. However, for the first estimation of the coupling of diagonal and off-diagonal randomness we can use relation (6) also in this case . As we will see in the next Sections and because of the results obtained in /31/these coupling is of importance in the considered model of amorphous systems.

In recent papers /8, 9, 32/ concerning amorphous or liquid systems the assumption $\epsilon_n = \text{const}$ has been used. Indeed, estimations of the deviation of ϵ_n from the atomic level due to the second part in Eq. (5) yield small corrections for crystalline systems (cf. /32/). However, it does not mean that the fluctuations of ϵ_n can be neglected, although it is expected that ϵ_n fluctuate not so strong as V_{nm}, i.e., $|a| < 1$.

3. EXTENDED E/C-THEORY OF LOCALIZATION

For the derivation of several localization criterions it is, in general, not necessary to restrict the consideration to regular lattices(cf. /33/) and diagonal disorder (cf./22, 25, 26/). In the Anderson sense /18/ an electron is localized if there is a finite probability of rediscovering the electron in the region in which the electron was initially localized. Let the initial state $|\psi(t=0)\rangle$ be $|\phi_n\rangle$,then the probability W_n that the electron will be in the initial state after infinite time evolution $(t \to \infty)$ is given by $W_n = \lim_{t\to\infty} |\langle\phi_n|\psi(t)\rangle|^2$. Analogously to the derivation in /19/, W_n may be expressed in the following way

$$W_n = \lim_{s\to 0+} \frac{s}{\pi} \int_{-\infty}^{\infty} dE\, G_n(E+is) G_n(E-is), \qquad (7)$$

where

$$G_n(E) = \langle\phi_n|(E-\mathcal{H})^{-1}|\phi_n\rangle \qquad (8)$$

represents a projection of GF onto the subspace of such eigenfunctions of $\mathcal{H}$ defined by (4). Therefore G_n is the diagonal element of the reduced GF introduced by Halpern /30/. This quantity may be expressed in terms of the self-energy $\Delta_n(E)$ defined by

$$G_n(E) = (E - \epsilon_n - \Delta_n(E))^{-1}. \qquad (9)$$

Following the arguments used by E/C /19/it can be shown that an eigenstate overlapping with $|\phi_n\rangle$ and with eigenenergy $E\,(E_a \le E \le E_b)$ is localized if and only if the self-energy $\Delta_n(E)$ is analytic at E. In the E/C theory the analytic properties of $\Delta_n(E)$ are considered by the convergence of the perturbation series (PS) for $\Delta_n(E)$. In order to get this PS, we start with the equation of motion for the reduced GF which may be represented in the following matrix form (cf. Eqs.(2,3)and /30/)

$$G = S(ES - h)^{-1}S \equiv S\mathcal{G}S \qquad (10)$$

For the quantity $\mathcal{G}$ the equation

$$\mathcal{G}_{nm} = g_n + g_n \sum_{m'} \bar{V}_{nm'} \mathcal{G}_{m'm} \qquad (11)$$

holds, where $g_n = (E-\epsilon_n)^{-1}$ and $\bar{V}_{nm} = V_{nm} - E\Delta S_{nm}$. If we partially renormalize the PS solution for $\mathcal{G}_{nm}$ we get

$$\mathcal{G}_{nm} = \mathcal{G}_n \delta_{nm} + \mathcal{G}_n \tau_{nm}(E) \mathcal{G}^n_m, \qquad (12)$$

where

$$\mathcal{G}_n = (E - \epsilon_n - d_n(E))^{-1}$$

$$d_n(E) = \sum_{m \neq n} \bar{V}_{nm} g_m \bar{V}_{mn} + \sum_{m,k \neq n} \bar{V}_{nm} g_m \bar{V}_{mk} g_k \bar{V}_{kn} + \cdots,$$

and for $n \neq m$ $(\tau_{nn} = 0)$

$$\tau_{nm}(E) = \bar{V}_{nm} + \sum_{m' \neq n,m} \bar{V}_{nm'} g_{m'} \bar{V}_{m'm} + \cdots . \qquad (13)$$

$\mathcal{G}^n_m$ is defined in the same way as $\mathcal{G}_n$, the superscript n denotes that $\mathcal{G}^n_m$ has been calculated for $\epsilon_n = \infty$. Finally, according to (9)-(13) the self-energy $\Delta_n(E)$ has the solution of the form

$$\Delta_n(E) = (d_n(E) + (E - \epsilon_n) X_n(E))/(1 + X_n(E)), \qquad (14)$$

where

$$X_n(E) = \sum_{m \neq n} S_{nm} \mathcal{G}^n_m \tau_{mn} \mathcal{G}_n + \sum_{m \neq n} S^2_{nm} \mathcal{G}_m + \sum_{m,k \neq n} S_{nm} \mathcal{G}_m \tau_{mk} \mathcal{G}^m_k S_{kn}. \qquad (15)$$

If we assume that for a certain energy E the renormalized perturbation expression (RPE) for the quantities $d_n(E)$, $d_m(E)$, $d^n_m(E)$, $d^m_k(E)$, $\tau_{mn}(E)$ and $\tau_{mk}(E)$ converges, then from /19/ it follows that the only singularity of these quantities are simple poles, consequantly, because of (14) also the self-energy $\Delta_n(E)$ has only simple pole singularities and is analytic elsewhere. The corresponding eigenstate at the energy E is then localized. In the opposite case nonanalytic behaviour of $d_n(E)$ or $X_n(E)$ yields nonanalytic self-energy $\Delta_n(E)$ which is due to a localiz state. Under the assumption that the convergence of the above-mentioned RPE is equivalent to the convergence of the series alone (cf. /3, 19/) the problem is reduced to find the probability distribution of the M-th term of these series in the limit $M \to \infty$. The considered diagrams for the various series are similar but have only different starting and end points which are, however, in a finite region if we use NNA. Therefore these boundary conditions cannot influence the probability distribution of infinite extended diagrams. Thus, the consideration of the analyticity of $\Delta_n(E)$ can be reduced to the study of the convergence of the $d_n(E)$-series alone where the overlap integrals only appear in renormalized hopping integrals $\bar{V}_{nm} = V_{nm} - E\Lambda S_{nm}$.

Supposing, that the amorphous system has a finite structural correlation, we can apply all arguments of E/C /19/ to derive a general localization function L(E) which determines localized states at energy E by the condition $L(E) < 1$. L(E) can be redefined in the following way

$$L(E) = \lim_{M \to \infty} \Big(\sum_{\substack{n_1 \neq 0 \\ n_2 \neq 0, n_1 \\ \vdots \\ n_M \neq 0, n_1 \cdots n_{M-1}}} \tilde{V}_{0n_1} \tilde{\mathcal{G}}^{\circ}_{n_1} \cdots \tilde{V}_{n_{i-1}n_i} \tilde{\mathcal{G}}^{0 \cdots n_{i-1}}_{n_i} \cdots \tilde{\mathcal{G}}^{0 \cdots n_{M-1}}_{n_M} \Big)^{1/M}, \qquad (16)$$

where the products $\tilde{V}\tilde{\mathcal{G}}$ are given by

$$\ln(\tilde{V}_{n_{i-1}n_i} \tilde{\mathcal{G}}^{0 \cdots n_{i-1}}_{n_i}) = \langle \ln(|\bar{V}_{n_{i-1}n_i}/(E - \epsilon_{n_i} - d^{0 \cdots n_{i-1}}_{n_i})|) \rangle. \qquad (17)$$

The symbol $\langle \ldots \rangle$ denotes here a structure averaging according to a distribution function of sites. For doing this calculation further apprpximations are required.

4. APPROXIMATE L(E) AND RESULTS

4.1. Zero-Order Approximation

Neglecting the statistical character of the self-energies $d_{n_i}^{0\ldots n_{i-1}}$ in (17) (cf. /3, 19, 26/), it is possible to omit these quantities. By a constant factor the approximated expression for L(E) is then fitted in such a way that in the ordered case mobility and band edges coincide. Thus, one obtaines

$$L(E) \approx L_0(E) = (K/K_0) Z \exp(\langle \ln(|\bar{V}_{nm}/(E-\epsilon_m)|)\rangle), \qquad (18)$$

where K is the connectivity of the amorphous structure and may be defined as the $1/M$ -th power of the sum of all possible diagrams in (16) in the limit $M \to \infty$. K_0 is the corresponding value of the ordered structure with the same short range order.

The averaging in (18) corresponds to a summation over all possible clusters containing a central atom and the surrounding nearest-neighbour atoms. Here we assume that the NN positions with respect to the central arom fluctuate independently around the mean.

For a qualitative estimation of (18) the fluctuations of the distances in the cluster can be replaced by statistically independent fluctuations of V_{nm} according to a given probability distribution. As an example, we examine the case of Lorentzian distribution which is characterited by the mean value V_0 and the half width Γ. Then one gets

$$L_0(E) = Z((V_0^2 + \Gamma^2(1-Es)^2)/(E^2 + (Za\Gamma)^2))^{1/2}. \qquad (19)$$

The characteristic properties of electron localization are the mobility edges E_c which separate extended from localized states and are determined by $L(E_c)=1$. Here these edges are symmetric to $E_0 = -s(Z\Gamma)^2/(1-(Zs\Gamma)^2)$ and decrease (or increase) with increasing disorder (the measure for it is Γ) if $(1-(Zs\Gamma)^2)a^2 > (<)(1-(ZsV_0)^2)$. It is known that diagonal disorder /1, 3, 18/ leads to an Anderson transition. Including ODR all states become localized only for $(1-(Zs\Gamma)^2)a^2 \geq (1+(V_0/\Gamma)^2-(Zs\Gamma)^2)$. It is seen that random hopping integrals act against localization and if $|a| \leq 1$ no Anderson transition is possible and the E_c increase monotonously with Γ (Fig. 1). The presence of fluctuating overlap integrals yields the interesting result that for $a^2 > (1-(ZsV_0)^2)$ the difference between E_c first decreases but then increases with growing Γ (Fig. 1). This feature of E_c contains the possibility that for a certain value of a and Γ first an Anderson transition takes place but then with increasing Γ a second transition occurs where the states once again become extended. This is caused by an additional delocalization effect due to fluctuations of overlap integrals. This effect is the greater the stronger the fluctuations.

4.2. Second Order Perturbation Theory

In the second order perturbation theory for $d_{n_i}^{0\ldots n_{i-1}}$ the localization function is

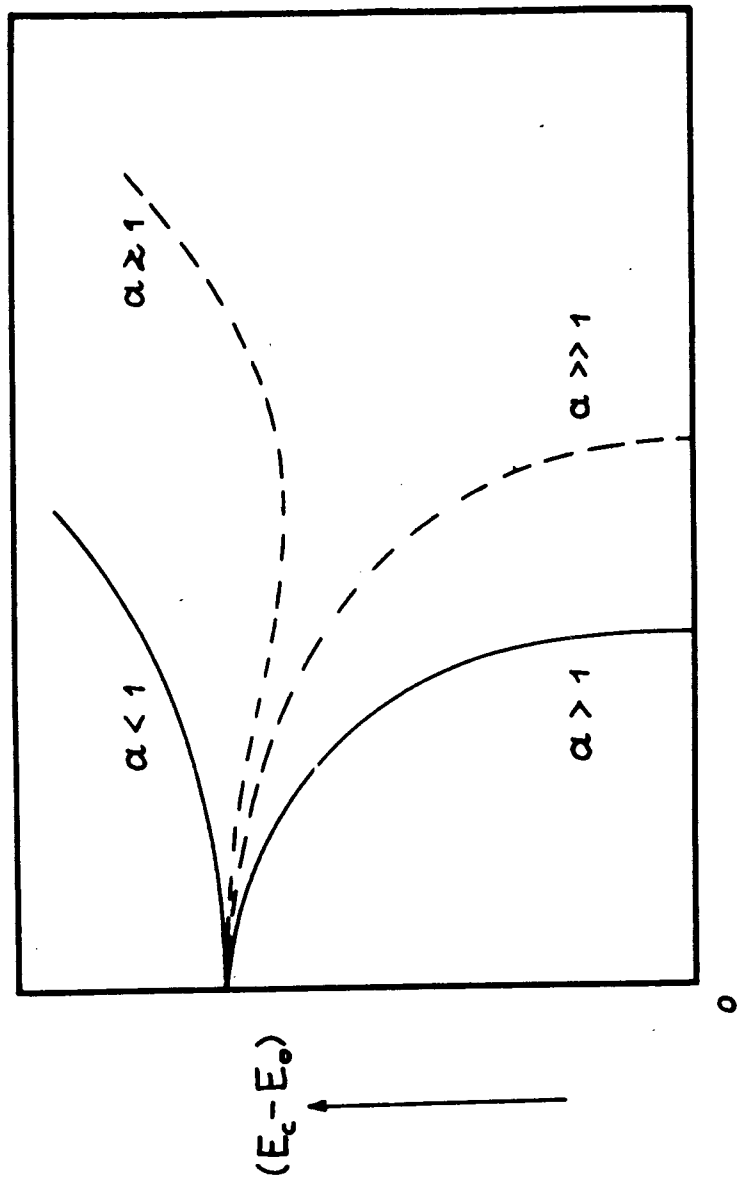


Fig. 1. Mobility edges E_c according to L_0-criterion in dependence upon strength of disorder, $\Gamma_\epsilon = |a|Z\Gamma$. Results are independent of Z.

approximately given by

$$L(E) \approx L_1(E) = K \exp(\langle \ln(|\bar{V}_{n_{i-1}n_i}/(E-\epsilon_{n_i} - \alpha \Sigma_n |\bar{V}_{n_i n}|^2/(E-\epsilon_n))|)\rangle),$$

where $\alpha = Z - K_0$, if we once again require the right behaviour of $L_1(E)$ in the ordered case. It is possible to test this criterion numerically in the same way as $L_0(E)$. Thereby we would get the same formulas as Herscovici in the paper /26/ if we there replace $\Gamma_v \to \Gamma(1-Es)$, $\Gamma_\epsilon \to Z|a|\Gamma$ and choose for simplicity $K = K_0$. Herscovici /26/ has shown for $s=0$ that according to this criterion the mobility edges for $\Gamma_v/\Gamma_c \ll 1$ are displaced to smaller energies (in modulus) compared with the inferior approximation. This result holds also for $s \neq 0$. On the other hand $L_1(E)$ leads to a stronger delocalization comparing with $L_0(E)$ if $\Gamma_\epsilon \to 0$ and $\Gamma_v \neq 0$. Thus $L_1(E)$ is more sensitive to increasing disorder. In spite of this we must criticize this criterion because it completely fails to describe the character of states in the middle of the band. The reason for the wrong behaviour of $L_1(E)$ at $E \simeq 0$ comes from the breakdown of the second order perturbation theory.

4.3. Approximated Renormalization Expansion

An improved expression for L(E), valid at all energies, can be got using the renormalized perturbation expansion (RPE) for $d_{n_i}^{0 \ldots n_{i-1}}$ (cf. /3, 18, 19/) and terminating these series after the first term. To eliminate the difficulties with the restricted occupation of sites in $d_{n_i}^{0 \ldots n_{i-1}}$ we replace approximately (see /20, 26/).

$$d_{n_i}^{0\ldots n_{i-1}} \approx d_{n_i} = a \sum_n |\bar{V}_{n_i n}|^2/(E - \epsilon_n - d_n), \qquad (21)$$

where the sum is taken over all nearest-neighbours of n_i. The obtained simplified RPE can be regarded as a RPE for a fictive Bethe lattice with ϵ_n and $\bar{V}_{nm}$ given by the real amorphous system. Thus, all $\tilde{\mathcal{G}}_{n_i}^{0\ldots n_{i-1}}$ in (16) can be calculated by $\tilde{\mathcal{G}}_{n_i}^{B} = \langle \ln(|\mathcal{G}_{n_i}^{B}|)\rangle$, where $\mathcal{G}_{n_i}^{B}$ is the diagonal element of the lattice GF (cf. Eq. (12)) for the fictive Bethe lattice. A method to obtain the quantity $\tilde{\mathcal{G}}_{n_i}^{B}$ is the self-consistent effective medium approach or CPA [4-12]. The simplest version of CPA, which includes diagonal and off-diagonal randomness, is the single bond CPA [34, 35]. An improved CPA version is the Bethe-Peierls approximation [7] which is also applicable for fluctuating $\bar{V}_{nm}$ coupled with ϵ_n.

Here we do not want to go in details of such calculations. For studying L(E) on principle we consider only the case of Lorentzian distributed hopping integrals and neglect the correlation between different $\bar{V}_{nm}$. Then the CPA is not required because $\tilde{\mathcal{G}}_{n_i}^{B}$ can be exactly solved by contour integration (cf. [19, 36, 37]). Since the $\bar{V}_{nm}$ occur only with the absolute value, no restrictions for the parameter a are necessary to perform the contour integration. Using the abbreviation $\Gamma_v = \Gamma(1 - Es)$ and $\Gamma_\epsilon = Z|a|\Gamma$, L(E) can be written down in the form

$$L(E) \approx L_2(E) = K(V_0^2 + \Gamma_v^2)^{1/2} |\mathcal{G}_0^B(E, \epsilon_0 \to \epsilon_0 - i\Gamma_\epsilon, V_0 \to (a(V_0^2 + \Gamma_v^2))^{1/2})|,$$

where

$$\mathcal{G}_0^B = (E - \epsilon_0 - d)^{-1}$$

and

$$d = Z(E - \epsilon_0 \mp ((E - \epsilon_0)^2 - 4(Z - 1)V_0^2)^{1/2})/2(Z - 1). \qquad (23)$$

The sign - (or +) is used if $(E - \epsilon_0) \geq 0$ (or $(E - \epsilon_0) < 0$). The so far unknown parameter a is fitted by the condition that for the corresponding ordered case ($K \to K_0$, $V_{nm} \to V_0$, $\epsilon_n \to \epsilon_0$, and $S_{nm} \to \delta_{nm}$) the mobility and band edges coincide, i.e., $L_2(\pm ZV_0) = 1$. It follows $a = (Z - K_0)(ZK_0 + Z - K_0)/Z^2$. For the sake of simplicity further we shall choose $K = K_0$. Since K is only a factor in the formula of $L_2(E)$, it follows that the smaller K the easier the electrons become localized. The results for the mobility edges E_c ($L_2(E_c) = 1$) are shown in Fig. 2.

From formula (22) one directly sees the effect of random hopping integrals. It yields an effective increasing of the band width. Analogously to the second order approximation, the diagonal disorder has here a stronger localization effect compared with the results of the L_0-criterion, e.g., for $a \to \infty$, $\Gamma_v \to 0$, $\Gamma_\epsilon \neq 0$, and $s = 0$ an Anderson transition takes place about $(Z - 2)/Z$ times sooner (Fig. 2a). Furthermore the limit for the parameter a at which an Anderson transition becomes impossible is lowered, instead of $|a_L| = 1$ now $|a_L| = K/Z$. The results for

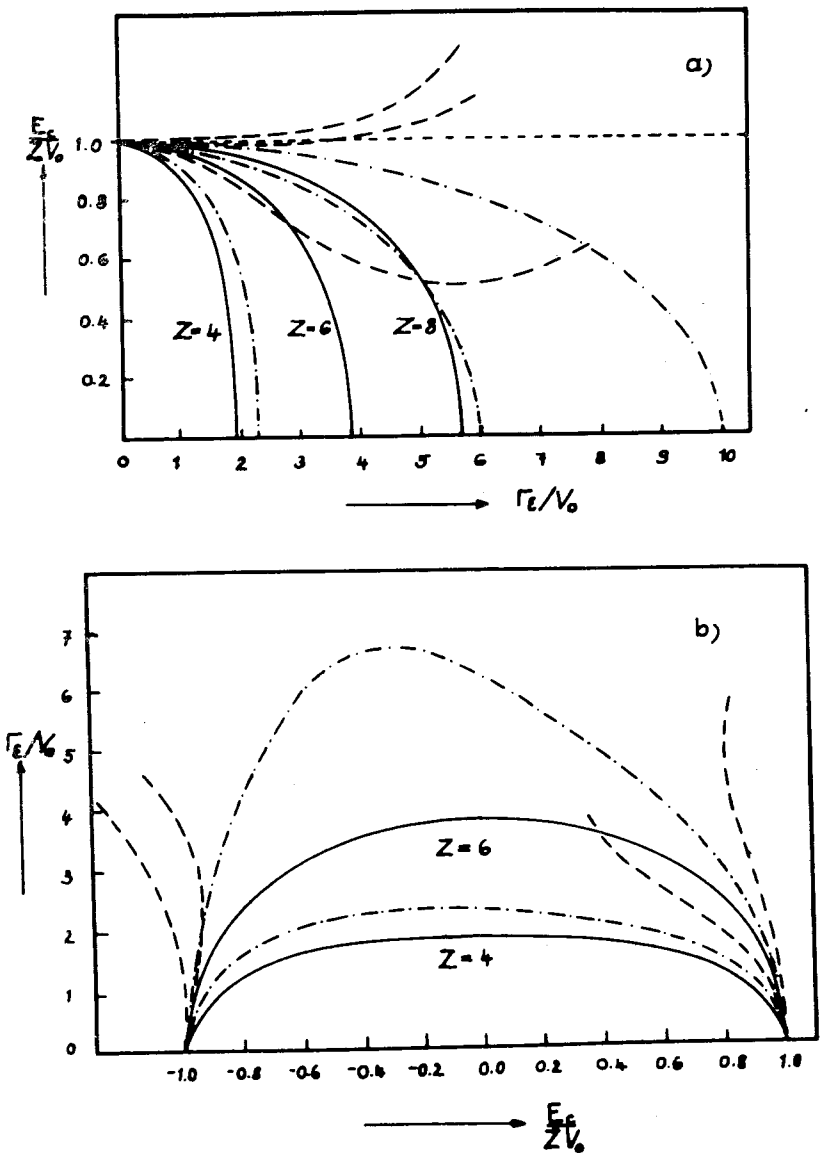


Fig. 2. Dependence of the mobility edges upon Γ_ϵ obtained from L_2-criterion where $V_0>0$, ——— $|a|\to\infty$, $\Gamma\to 0$, -·-·-· $|a|=1$ and - - - $|a|=2/3$. a) $s=0$ and b) $s=0.04$.

$s=0.04$ are shown in Fig. 2b. It is seen that the qualitative picture is the same as for the L_0-criterion.

4.4. The Licardello/Economou Criterion

Licardello and Economou (L/E) /3/ have demonstrated that the function L(E) is not very sensitive to the special restriction when calculating $\tilde{\mathcal{G}}_{n_i}^{0\ldots n_{i-1}}$. Therefore they have proposed to replace all $\tilde{\mathcal{G}}_{n_i}^{0\ldots n_{i-1}}$ by $\tilde{\mathcal{G}}_{n_i}^{m}$ where m is one of the NN of n_i. Using the approximation $\langle\ln(|\mathcal{G}|)\rangle \approx \ln(|\langle\mathcal{G}\rangle|)$, L/E have then calculated this quantity by a single site CPA. Here we apply a cluster version of CPA. We consider a compact cluster formed by a central atom surrounded by its Z nearest-neighbours and embedded in an effective medium which is characterized by an effective Bethe lattice with a coherent hopping integral $\tilde{V}_c$. For such a cluster $\tilde{\mathcal{G}}_{n_i}^{m}$ is calculated (cf. /3, 38/) where the structure averaging over all possible clusters can be performed in the same way as described in Sect. 4.1. The use of the Lorentzian distribution enables us to carry out the integration over the stochastical variable V_{nm} in an exact manner, if the parameter a obeys the condition $|a| \geq |1-Es|$ (cf. /19, 37/). Requiring now the CPA like condition

$$\langle\ln(|\mathcal{G}_{n_i}^{m}|)\rangle_{\text{cluster}} = \ln(|\mathcal{G}_{n_i\,\text{eff}}^{m}|), \qquad (24)$$

the coherent hopping integral $\tilde{V}_c$ can be determined self consistently. It is found

$\bar{V}_c = V_0 - i\Gamma_v \,\mathrm{sign}(a)$. Hence the approximated expression for L(E) has the form

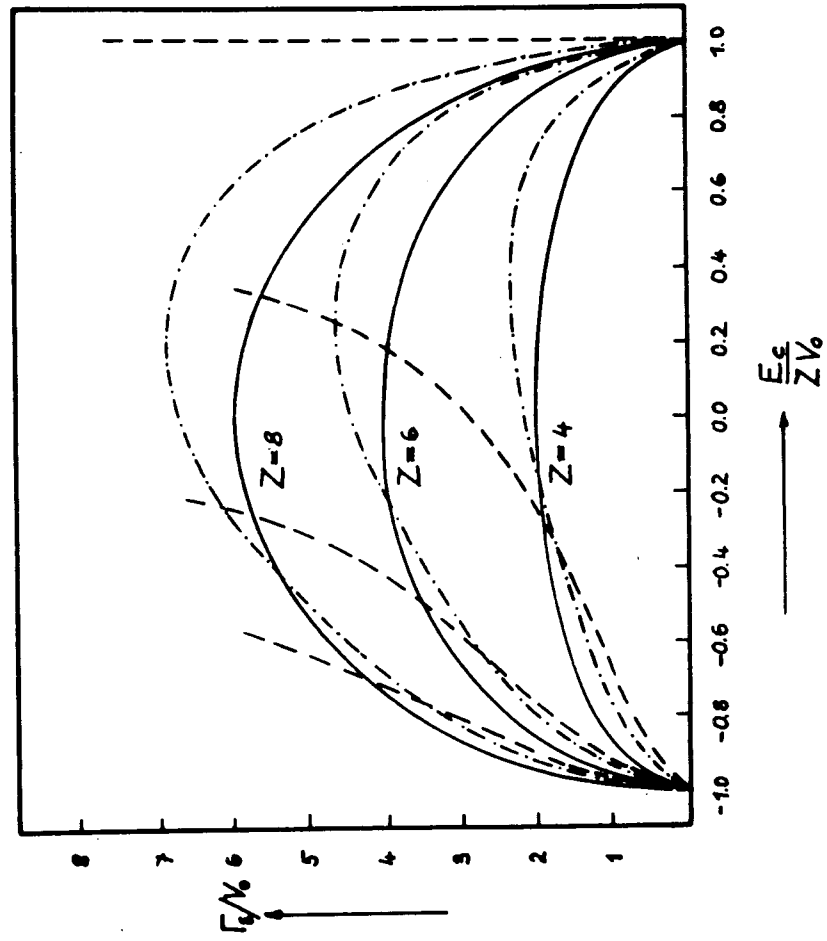
$$L(E) \approx L_3(E) = |EZ \mp (EZ^2 - Z + 1)^{1/2}| \quad (\mathrm{Re}\,EZ \gtrless 0), \qquad (25)$$

where

$$EZ = (E - \epsilon_0 + i\Gamma_\epsilon)/2(V_0 - i\Gamma_v \,\mathrm{sign}(a)).$$

Results based on this criterion are shown in Fig. 3. For diagonal disorder Bishop[38] has analysed the L/E-criterion in the case of Bethe and real lattices. These results show that this criterion is extremely successful qualitatively (cf. [3]). The Z-dependence of the position of E_c is similar to that found for L_2. A further improvement of this criterion is concerned with the asymmetric change of the mobility edges due to the coupling between ϵ_n and V_{nm}. This is expected from the exact results for the density of states in the extended Lloyd model[37]. There an asymmetric damping of the $\vec{k}$-states appears and it should be expected that the electron localization is the stronger the greater the damping of $\vec{k}$-states[33]. This statement is confirmed in the case of small fluctuations where for $aV_0 < 0$ the presence of random hopping integrals enhances (lowers) the damping and the localization effect at the bottom (top) of the band. However, for greater fluctuations the effect of diagonal and off-diagonal disorder on localization does not simply interference in that way as for the $\vec{k}$-state damping. This can be explained by a general delocalization effect of ODR.

Fig. 3. Dependence of the mobility edges upon Γ_ϵ for the L_3-criterion ($s = 0$, $V_0 > 0$, ——— $|a| \to \infty$, $\Gamma \to 0$, --- $a = -2$, - - - $a = -1$).



The quoted results of the L_3-criterion are directly confirmed by the exact investigations of a one-dimensional model involving diagonal and off-diagonal disorder in the used manner /39/.

The influence of fluctuating overlap integral ($s \neq 0$) is qualitatively the same as for the L_2 and L_0-criterions. It gives an additional reason for asymmetric change of the mobility band. After the obtained Anderson transition ($|a| \gg 1$) another transition can appear at higher values of Γ where the states once again become delocalized. It must be pointed out here that the latter result cannot be physically realistic. At first the Lorentzian distribution for V_{nm} represents the real situation, the worse the greater the width of the distribution. On the other hand, there exists a bound for the overlap integral, i.e., $|S_{nm}| \leq 1$. Consequently, the ansatz (6) and the obtained results are quite good only for sufficient small parameters Γ and s.

4.5. Concluding Remarks

We only note that it is still possible to derive an upper bound of $L(E)$ (cf. /19, 26/). In the case of Lorentzian distribution of V_{nm} and under the condition $|a| \geq |1 - Es|$ the resulting $F(E)$-criterion has the same form as L_0.

Overlooking the different approximations in the E/C-theory of electron localization for amorphous one-component systems and regarding all available results of the literature we conclude that ODR acts against localization of electrons, i.e.. has a qualitative opposite influence than diagonal randomness. Therefore, because of the importance of ODR in amorphous systems, this kind of randomness must be included when discussing properties of electronic conductivity in this systems (cf. /29/).

One consequences of that is related to the expected small effect of diagonal disorder ($|a| < 1$) in amorphous one-component systems. This does not allow that a structural stimulated metal-nonmetal transition takes place in such systems. Only other, additional kinds of diagonal disorder, e.g., chemical or spin disorder, can cause such a transition in amorphous samples.

5. Mott-Anderson Transition

In amorphous systems of transition metals the electron correlation has, maybe, an important effect in producing localized states. For instance, it is obtained an effective cellular disorder if we consider the Hubbard model for correlation in narrow energy bands /27/ and use the alloy analogy approximation /22, 27, 28, 29/. On the other hand, there are problems in understanding the dynamical effects which are neglected in the alloy analogy. Here we quote a phenomenological point of view, comparing the dynamical fluctuations in the Hubbard model with the thermodynamical one in the one electron case. It is known that for nonzero temperatures the electrons can be delocalized by thermal activated hopping. In spite of this a relative sharp mobility edge appears for comparable small temperatures.

In this sense we suppose that the dynamical fluctuations of correlated electrons only cause smeared mobility edges which may be detected by the alloy analogy. Such a supposition is justificated if in the energy region of quasi localized states the dynamical corrections only slightly change the results of the static approximation. In the case of fully localized states, i.e., in the atomic limit ($U \to \infty$), the alloy analogy is exact. From that we may expect that also for states, which are only partially extended in space (U finite) - localized in the alloy analogy, the dynamical fluctuations have merely a second order effect.

Let us now derive a localization criterion to determine quasilocalized states for the Hubbard model. For this purpose we reformulate the alloy analogy in the following way. A spin $\uparrow$ electron in the atomic limit can have the energies ϵ_n or $\epsilon_n + U$ depending on the circumstances whether or not an electron with spin $\downarrow$ is present at the same place. In the senses of a static approximation the spin$\downarrow$ electron can be regarded as fixed in position if we switch on hopping for spin$\uparrow$ electrons. Assuming a random distribution of the $\downarrow$ electrons we can apply methods developed for disordered alloys.

In particular, we want to calculate the localization function $L(E)$ for such a system using the L/E approach (Sect. 4.4). The averaging over all spin $\downarrow$ configurations in the expression for $L(E)$ is performed by applying a single site CPA for the quantity $\mathcal{G}_n^m \equiv \ln(|(E - \tilde{\epsilon}_n - d_n^m)^{-1}|)$ where $\tilde{\epsilon}_n$ can have the above-mentioned two values. According to

Shiba's CPA approach[5] the environment of the n-th atom is replaced by an effective medium with coherent potentials $\epsilon_m + \Sigma$ $(m \neq n)$. Then, Σ will be self-consistently determined by the condition that the spin$\downarrow$ configuration and structure average of the local quantity $\mathcal{G}_n^m$ is equal to the corresponding value of the effective medium, i.e.,

$$\langle \mathcal{G}_n^m(E, \epsilon_n + \Sigma) \rangle = n_\uparrow \langle \mathcal{G}_n^m(E, \epsilon_n) \rangle + n_\downarrow \langle \mathcal{G}_n^m(E, \epsilon_n + U) \rangle, \quad (26)$$

where n_σ is the averaged occupation number per atom (see [28]). The structure average in (26) may be performed in the same way as described in Sect. 4.4 for all three quantities and is equivalent to the replacement of all V_{nm} by a coherent hopping integral $V_c = V_0 - i\Gamma \,\mathrm{sign}(a)$ $(|a| \geq 1,\ s = 0)$ in an effective Bethe lattice. When the number of electrons present is one per atom and the system is assumed to be paramagnetic, we have $n_\uparrow = n_\downarrow = 1/2$, and hence the solution of the problem becomes easy. Numerical results are shown in Fig.4 where the mobility edges are plotted against the parameters of disorder U and Γ.

In the case of small Γ and varying the correlation parameter U the mobility bands behave like the density of states bands for $\Gamma = 0$ (cf. [27, 28]). The density of states for the case $\Gamma \neq 0$ has marked tails [37] and therefore is no longer directly related to the metal-nonmetal transition in the Mott-Hubbard sense[27]. The onset of such a transition will now be dependent on the position of the Fermi level E_F in relation to the mobility

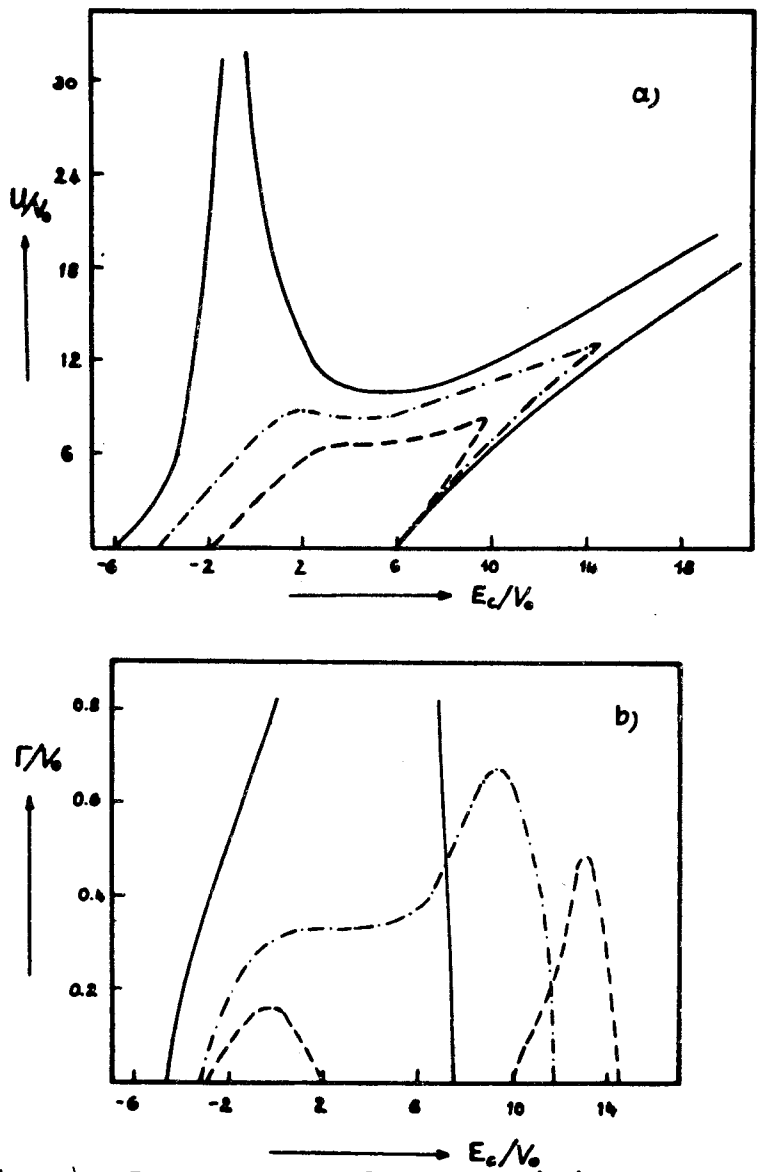


Fig. 4. Dependence of the mobility bands for the Hubbard model treated in alloy analogy upon the disorder parameters a) U(—— $\Gamma = 0$, -·-·- $\Gamma = 0.4$, --- $\Gamma = 0.8$) and b) Γ (—— U=3, -·-· U=9, ---U=12). It is $V_0 > 0$, $\alpha = -1$, $Z = 6$, and $s = 0$.

bands. Because of asymmetric change of the density of states in our model of amorphous systems, E_F changes the position with increasing Γ also in the case n=1 so that the critical value of the parameter U cannot be determined simply by the value at which the mobility gap disappears. With increasing Γ in both subbands an Anderson transition takes place and for a certain value of Γ only one mobility band remains.

Let us assume that U/V_0 and the width of the V_{nm} distribution will be lowered if pressure is applied on amorphous nonmetallic systems. Then we may meet the possibility of realization of nonmetal-metal transition. This transition is a mixed type of Mott and Anderson transition whereas the dominant mechanism is due to electron correlation (cf. /28/). In the connection with our remarks on the dynamical effects in the Hubbard model the found transition cannot be very sharp, although observable in real amorphous systems.

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