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W.John, J.Schreiber

LOCALIZATION THEORY FOR THE RANDOM WAIRE MODEL

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W.John,* J.Schreiber

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*Arbeitsgruppe Theoretische Physik, Sektion Physik, Technische Universitat, GDR.

Ён В., Шрейбер Ю.

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Локализация электронов в модели Уйэра

Для двухзонной модели Уэра аморфных ковалентных полупроводников применяется теория локализации Экономо и Кона. В сравнении с плотностью состояний исследуется поведение краев подвижности для флуктуации в разных потенциальных параметрах, причем их распределение предполагается Лоренцовским.

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John W., Schreiber J.

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Localization Theory for the Random Weaire Model

The localization theory of Economou and Cohen is applied for the random two-band Weaire model of amorphous covalent semiconductors. Several approximations for the localization function L(E) are calculated in the case of Lorentzian distributed potential parameters. The behaviour of the mobility edges in dependence on the strength of fluctuations are studied in comparison with the shape of the density of states.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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1. INTRODUCTION

Recently[1] the electron localization in amorphous one-component systems was investigated on the basis of a tight binding model involving off-diagonal randomness (ODR). An application of this theory to amorphous covalent semi-conductors[2] requires the use of a more realistic two-band model. For this purpose the Weaire model[3-7] is suitable and, so far we know, the Mott-Anderson localization[2,8,9] due to potential fluctuations was not considered in this model.

In spite of rather idealization the Weaire model described amorphous tetrahedrally bounded semiconductors like Ge and Si in a qualitative significant way. The amorphous structure is assumed to be a random network with almost perfectly tetrahedrally coordinated atoms in the nearest-neighbour sphere. The model Hamiltonian may be written as

$$\langle ni|H|mj\rangle = V_0^{ni}\delta_{nm}\delta_{ij} + V_1^{nij}\delta_{nm} + V_2^{ni}\delta_{lj}\delta_{mn_i} . \qquad (1)$$

The sp^3-orbitals $|n\,i\rangle$ are assumed to form an orthonormal set and are labelled by the position of the atom n and the bond i. The first

term V_0^{ni} determinates the energy level of the state $|ni>$. V_1^{nij} describes the hopping between the bonds i and j at the atom n and V_2^{ni} involves the transfer from the atom n along the bond i to the neighbouring atom n_i. Caused by little variations of the bond lengths and angles the potential parameters may vary considerably. The influence of this quantitative disorder on the density of states and especially on the gap was considered in [6,10-12]. In this paper the dependence of the mobility edges E_c, which separate regions of localized states from those of extended states, upon the strength of disorder is investigated in relation to the shape of the density of states (cf. [12]). In Sect. 2 it is demonstrated that for the two-band Weaire model the localization function L(E) of the Economou and Cohen theory [9] may be reduced to corresponding one-band formulas [1] with energy-dependent diagonal and off-diagonal disorder. Two approximations for L(E) are given analytically where for the sake of simplicity the potential parameters are taken to be statistical independent variables with a Lorentzian distribution. For the one-band approximation of the Weaire model (see [11]) L(E) is also given. In Sect. 3 the results are discussed. It is found that for physically reasonable fluctuations the mobility gap for this model is enlarged as compared with the ordered case. Furthermore, because of the delocalization effect of ODR, there is, in general, no relation between the smearing out effect of the density of states and the localization tendency of states.

2. LOCALIZATION CRITERIONS FOR THE WEAIRE MODEL

Economou and Cohen (E/C) [9] have shown that an eigenstate of a tight binding Hamiltonian with eigenenergy E is localized if and only if the self-energy of the diagonal Green's function is analytic at E. The investigation of this property analogous to [9] requires a perturbation series solution for the self-energy. In principle such an approach to the electron localization is also possible for the Weaire model. Considering diagonal Green's function $G_{nn}^{ii} = <ni|(E-H)^{-1}|ni>$, a perturbation series solution is, however, too complicated for further discussions. The application of the localization theory of E/C becomes, on the other hand, easy if we consider the behaviour of the s- and p-part of Green's function $\tilde{G}$. Introducing zero Green's function $\tilde{G}^\circ$ which belongs to the case $V_1^{nij} = 0$, $\tilde{G}$ obeys the operator equation

$$\tilde{G} = \tilde{G}^\circ + \tilde{G}^\circ \tilde{V}_1 \tilde{G} = \tilde{G}^\circ + \tilde{G}^\circ \tilde{\tau} \tilde{G}^\circ,$$

where

$$\tilde{\tau} = \tilde{V}_1 + \tilde{V}_1 \tilde{G}^\circ \tilde{\tau} . \qquad (2)$$

$\tilde{G}^\circ$ and $\tilde{V}_1$ have the following matrix elements

$$<ni|\tilde{G}^\circ|mj> = G_{nn}^{\circ i} \delta_{nm}\delta_{ij} + G_{nn_i}^{\circ i} \delta_{mn_i} \delta_{ij} ,$$

$$G_{nn}^{\circ i} = E/(E^2 - V_2^{ni\,2}), \quad G_{nn_i}^{\circ i} = V_2^{ni}/(E^2 - V_2^{ni\,2}), \qquad (3)$$

$$<ni|\tilde{V}_1|mj> = V_1^{nij} \delta_{nm} .$$

As the bond angle variation in the tetrahedrally bonded semiconductors is supposed to be small, the V_l^{nij} may be assumed independent of the bonds i,j and different only for atoms of various kinds. Therefore $\tilde{V}_l$ becomes diagonal for s-states $|ns\rangle = 1/2 \sum_i |ni\rangle$. Because of that the $\tilde{\tau}$ -matrix is entirely s -like, i.e., only $\langle ns|\tilde{\tau}|ms\rangle \neq 0$. As $\tilde{G}^\circ$ describes completely localized states, it follows from (2) that only the existence of s -states can cause delocalized states for the whole system. Consequently, for detecting localized states it is sufficient to consider merely the s-part of $\tilde{G}$ which is given by

$$G^s_{nm} = \sum_j G^{\circ j}_{nm}(\delta_{nm} + \delta_{n_j m}) + \sum_j G^{\circ j}_{nn} V_l^n G^s_{nm} + \sum_j G^{\circ j}_{nn_j} V_l^{n_j} G^s_{n_j m} \quad (4)$$

After some manipulations the searched diagonal element of $\tilde{G}^s$ may be written in the form

$$G^s_{nn} = \mathcal{G}_{nn} + \sum_m \mathcal{G}_{nm} V_{mn} / V_l^n \,. \quad (5)$$

Green's function $\mathcal{G}_{nm}$ obeys an equation which is similar to that in the one-band case (Eq. (11) in /1/)

$$\mathcal{G}_{nm} = g_n \delta_{nm} + g_n \sum_{m'} V_{nm'} \mathcal{G}_{m'm} \,. \quad (6)$$

Here we have used the abbrevation

$$g_n = (\omega_n - V_l^n)^{-1}, \quad \omega_n^{-1} = \sum_j G^{\circ j}_{nn} \,, \quad (7)$$

and

$$V_{nm} = \omega_n G^{\circ j}_{nn_j} V_l^{n_j} \delta_{mn_j} \,.$$

Using analogous arguments as in /1/ it can be shown that the analyticity of the self-energy for G^s_{nn} follows from the analytic behaviour of the self-energy for $\mathcal{G}_{nn}$. This quantity has a perturbation series solution which is formally equivalent to that solution in the one band case. Because of the clear analytic behaviour of g_n the analyticity of this self-energy can be obtained by the convergence of the perturbation series - as demonstrated by E/C. Hence a localization function L(E) for the two-band Weaire model can be got by corresponding formulas of the one-band case. Here we want to consider the same approximations for L(E) as discussed in /1/. Numerical estimations are performed for the simplified case where the potential parameters V_l^n and V_2^{ni} fluctuate statistical independently according to a Lorentzian distribution. Furthermore we assume that deviations of local energy levels V_0^{ni} are strong coupled to the variations of the distances between the atoms along the bond i, i.e., in the first approximation we express V_0^{ni} by V_2^{ni} (cf. /1/)

$$V_0^{ni} = a V_2^{ni} + b \,. \quad (8)$$

The averaging over the Lorentzian distribution for the potentials may be carried out by contour integration in the same way as in /9,12,13/.

In detail we cite the two criteria L_0 and L_3 which are defined in /1/ and have the following form

$$L(E) \approx L_0(E) = |4V_1V_2/(E'^2 - V_2^2 - 4E'V_1)| \qquad (9)$$

and

$$L(E) \approx L_3(E) = |EZ \mp (EZ^2 - 3)^{1/2}| \quad (\mathrm{Re}\,EZ \gtrless 0), \qquad (10)$$

where $EZ = (E'^2 - V_2^2 - 4E'V_1)/2V_1V_2$.

The quantities V_1, V_2, and E' are defined by

$$V_1 = V_1^\circ - i\Gamma_1 \ , \quad V_2 = V_2^\circ - i\Gamma_2\,\mathrm{sign}(a), \qquad (11)$$

$$E' = E - V_0^\circ + i\Gamma_0 \ ,$$

where V_0°, V_1° and V_2° are the mean values and $\Gamma_0 = |a|\Gamma_2$, Γ_1, and Γ_2 the half-width of the Lorentzian distributed V_0^{ni}, V_1^n, and V_2^{ni}. The L_3-criterion is valid only for $|a| \geq 1$ (cf. [12]).

One can get an approximated expression for $L(E)$ neglecting the interaction between bonding and antibonding states, so that the Hamiltonian (1) is reduced to two separated one-band Hamiltonians (cf. [11]). $\tilde{V}_0$ and $\tilde{V}_2$ are diagonal for bonding $|a\rangle = 1/\sqrt{2}(|ni\rangle + |n_i i\rangle)$ and antibonding states $|\beta\rangle = 1/\sqrt{2}(|ni\rangle - |n_i i\rangle)$. Cancelling the transfer element of $\tilde{V}_1$ for this states the equation of motion for Green's function becomes

$$(E - V_1^\circ)G^{\beta\beta'}_{aa'} = \delta^{\beta\beta'}_{aa'} + ((V_0^{ni} + V_0^{n_i i})/2 \mp V_2^{ni})\, G^{\beta\beta'}_{aa'} + \sum_{\substack{\beta'' \\ a''}} V_1^\circ/2\, G^{\beta''\beta'}_{a''a'} \ . \qquad (12)$$

For the sake of simplicity we have chosen $V_1^n = V_1^\circ$; the sum in (12) runs over all nearest-neighbour bonds $a''(\beta'')$ of the $a(\beta)$-bond. The corresponding L_0-criterion is then given by (cf. Eq. (19) in [1])

$$L_0^{\beta}{}_{a}(E) = 2V_1^\circ/((E - 2V_1^\circ - V_0^\circ \pm V_2^\circ)^2 + (a \mp 1)^2\Gamma_2^2)^{1/2}. \qquad (13)$$

3. RESULTS AND DISCUSSIONS

At the beginning, we remind of several exact results for the density of states (DS) in that case where V_0^{ni} , V_1^n , and V_2^{ni} do not fluctuate. In Fig. 1 the DS for a Bethe lattice is shown. There are a valence band and a conduction one separated by a gap. It is seen that the valence band persists mostly bonding and s-states. The s-character of the states becomes smaller for increasing energy of both the bands. The delta functions at the top of both the bands are entirely p-like. All these features are structure independent [3-6], i.e., hold also for topological disorder.

Now let us consider the influence of quantitative disorder on the mobility edges E_c which are defined by $L(E_c) = 1$. All numerical examples refer to a Bethe lattice structure with potential parameters $V_0^\circ = 0$, $V_1^\circ = -1$, and $V_2^\circ = -4$.

In Figs. 2 and 3 only the $\tilde{V}_0$-fluctuations are taken into account ($\Gamma_1 = 0$, $\Gamma_2 \to 0$, $\Gamma_0 \neq 0$). Since $\tilde{V}_0$ acts as diagonal disorder for all states, it is well to understand that the positions of the mobility edges with respect to the band centre are the same for the valence and the conduction band (Fig. 2).

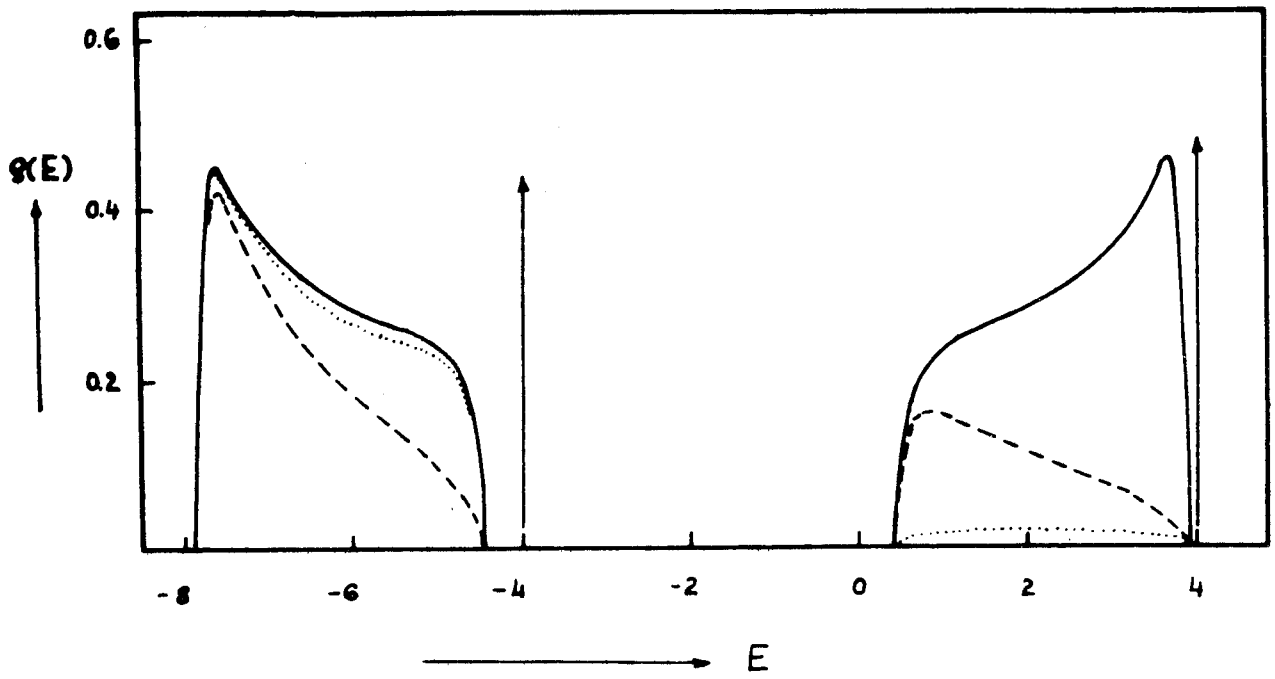

Fig. 1. The total density of states $\rho(E)$ (——), the s-part of $\rho(E)$ (---), and $\rho(E)$ of the bonding states (....) for a Bethe lattice. $V_0^\circ = 0$, $V_1^\circ = -1$, $V_2^\circ = -4$, $\Gamma_1 = \Gamma_2 = \Gamma_0 = 0$.

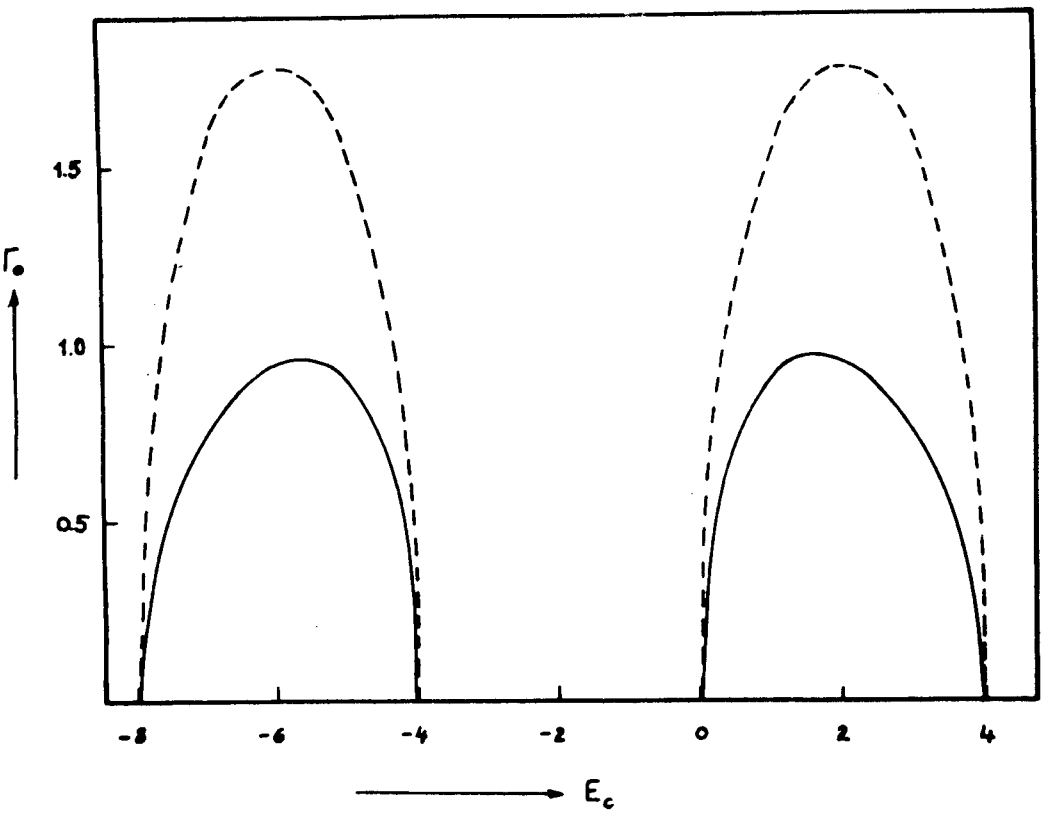

Fig. 2. Mobility edges E_c in dependence on $\Gamma_0 = |a|\Gamma_2 (\Gamma_2 \to 0, \ \Gamma_1 = 0)$. Dashed lines, E_c for L_0-criterion; solid lines, E_c for L_3-criterion.

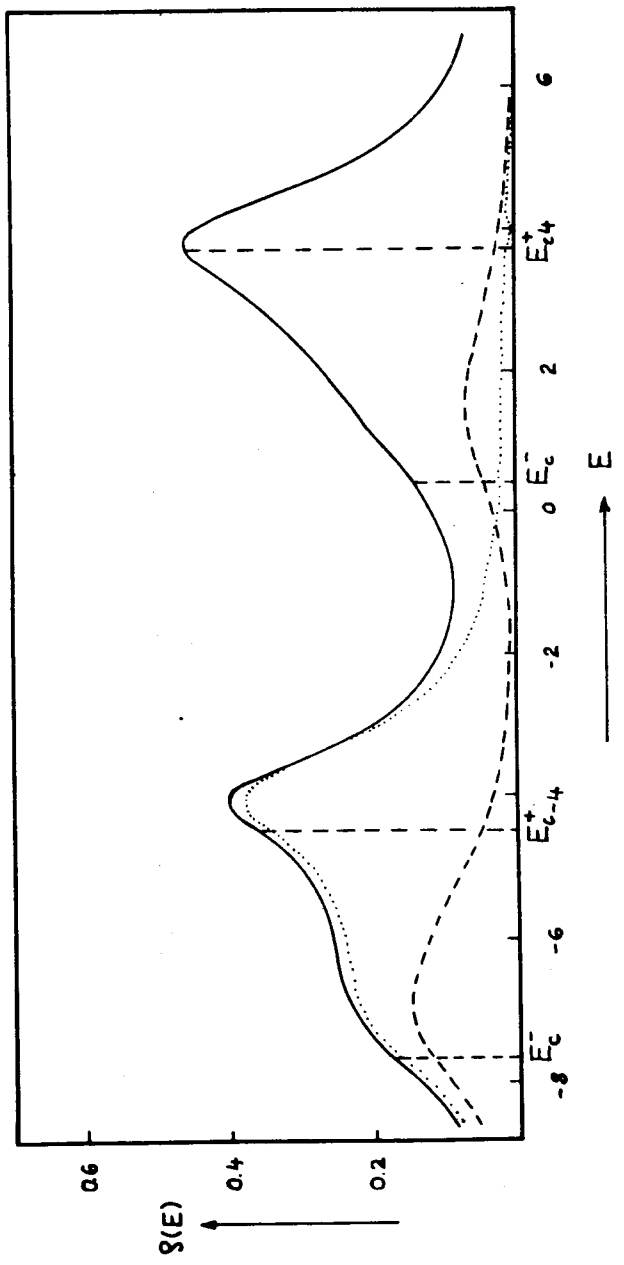

Fig. 3. Density of states $\rho(E)$ for $\Gamma_0 = 1.0$ ($\Gamma_2 \to 0$, $\Gamma_1 = 0$) see Fig. 1. The L_3-criterion yields only localized states; $E_c^{\pm}$ are the mobility edges of the L_0-criterion.

In contrast to that, the DS is not symmetrically changed by V_0-fluctuations (Fig.3). This is caused by a superposition of the smeared out δ-peaks - symmetric to $E=0$ - and the broad bands - symmetric to $E=-2$.

We note yet that the critical value Γ_0 / B(bandwidth $B = 4V_1^2$), at which an Anderson transition takes place, is smaller than the corresponding value in the one band case -1/2 for L_0- and 1/4 for the L_3 - criterion (cf. /1/).

The fluctuations of $\tilde{V}_1$ influence the diagonal and the off-diagonal randomness for Green's function $\mathcal{G}_{nm}$ (Eq. (6)). However, in regions, where the s-states dominate, the effect of off-diagonal disorder is small since for pure s-states $\tilde{V}_1$ is diagonal. On the other hand, the diagonal disorder can be neglected in the vicinity of $E \simeq 0$ (see Eq. (6) and (7)). Regarding these properties and the qualitative different influence of diagonal and off-diagonal disorder (cf. /1/), we can in principle understand the behaviour shown in Fig. 4 and 5. As for the derivation of the L_0-criterion the self-energy is neglected, this criterion cannot be responsible to the percentage of s-states. Therefore the delocalization effect can dominate all over in the region $|E| \leq |V_2^0|$.

In contrast to that the L_3-criterion takes into consideration that for small Γ_1 almost only s-states occur at the lower band edge of the conduction band. Hence states at $E \geq 0$ may become localized in this case. If Γ_1 increases, the relative percentage of s-states decreases (Fig. 5), consequently, the delocalization effect due to V_{nm}-fluctuations increases and in

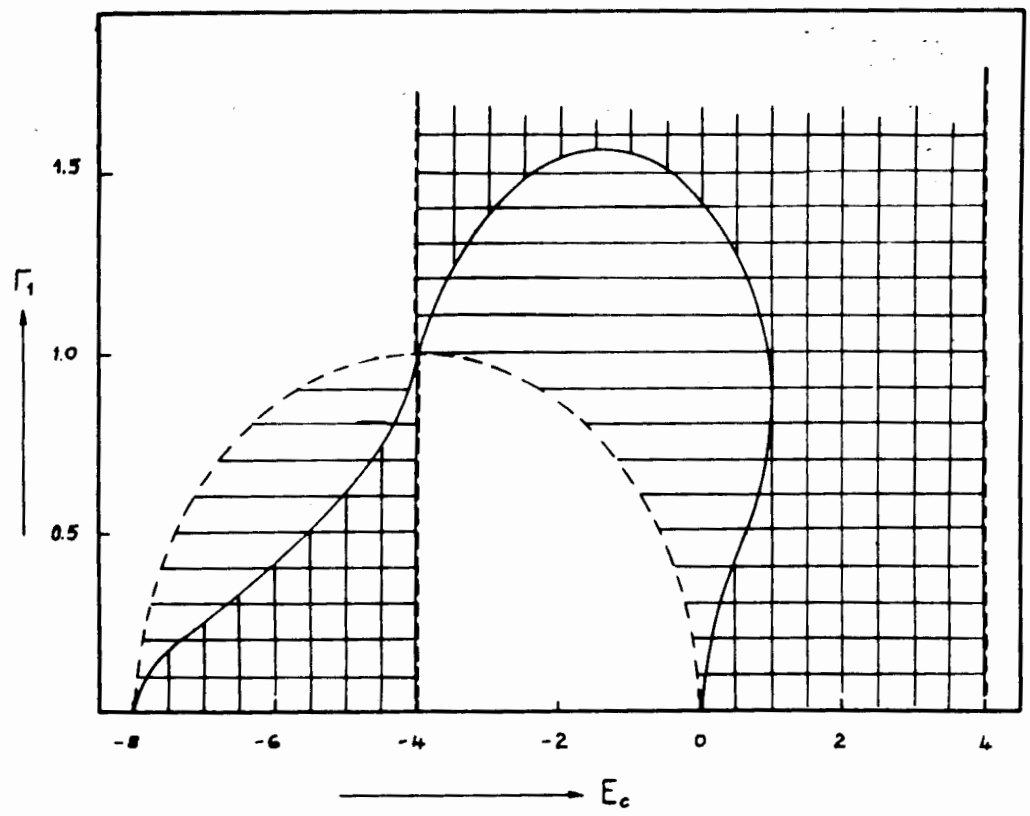

Fig. 4. Dependence of the mobility edges E_c upon Γ_1 ($\Gamma_2 = 0$, $\Gamma_0 = 0$). Regions of extended states for the L_0-criterion are single hatched, and those for the L_3-criterion are cross hatched.

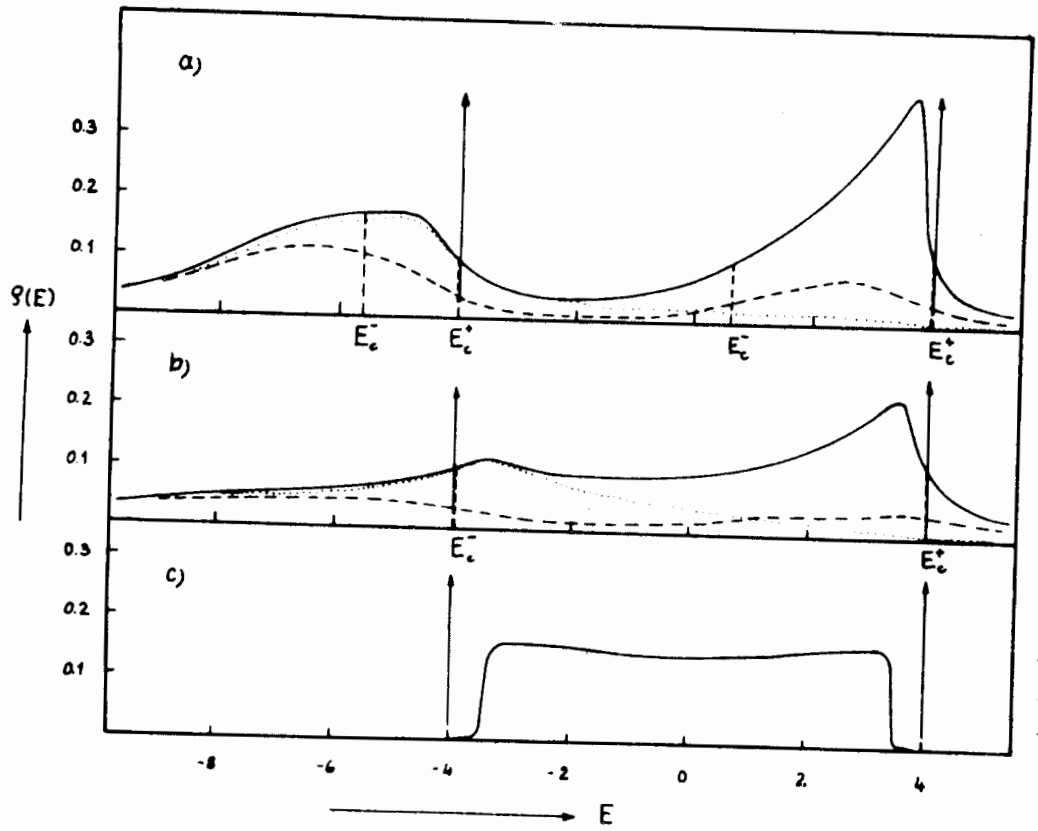

Fig. 5. The total density of states $\rho(E)$ (————), the s-part of $\rho(E)$ (- - - -), and $\rho(E)$ of the bonding states (...) for a) $\Gamma_1 = 0.5$, b) $\Gamma_1 = 1.7$ and c) $\Gamma_1 = 99$ ($\Gamma_2 = 0$, $\Gamma_0 = 0$). The mobility edges E_c belongs to the L_3 -criterion.

the region $|E| \leq |V_2^\circ|$ only delocalized states remain for sufficiently large Γ_1 - values. Then also the DS changes their shape characteristically. The s-states become damped out throughout the whole energy range, but for $\Gamma_1 \to \infty$ it remains an undamped band of p-states - symmetrical to $E = 0$ (Fig. 5).

The results for coupled fluctuations of $\tilde{V}_0$ and $\tilde{V}_2$ are shown in Figs. 6 and 7. Here the valence and the conduction band are oppositely influenced by disorder and in the physically relevant case $a < 0$, $V_2^\circ = -4$, and $V_1^\circ = -1$ the off-diagonal disorder (V_2 - fluctuations) yields an additional delocalization of states in the valence band and a localization in the conduction band. In this case we compare the results for the full two band model (Eq. (9)) with these for the one band approximation of the Weaire model (Eq. (13)). The relatively good agreement of the corresponding mobility edges (Fig.6) is sufficient, since the DS results imply that the error in the approximated one band model must be small (see[11]).

Regarding the change of DS and the change of the mobility edges, we can make the following conclusion. If the effect of diagonal disorder is predominating, localized states first appear in such energy regions where the DS is strong smeared out (Figs.2,3 and 6,7). In contrast to that off-diagonal disorder causes a marked change of the DS, but lead in these regions to a delocalization of states (Figs. 4,5). As the relative influence of diagonal and off-diagonal disorder is energy dependent (cf. Eqs. (4),(6) and (7)), it is therefore, in general, impossible to detect anything about localization from the DS results.

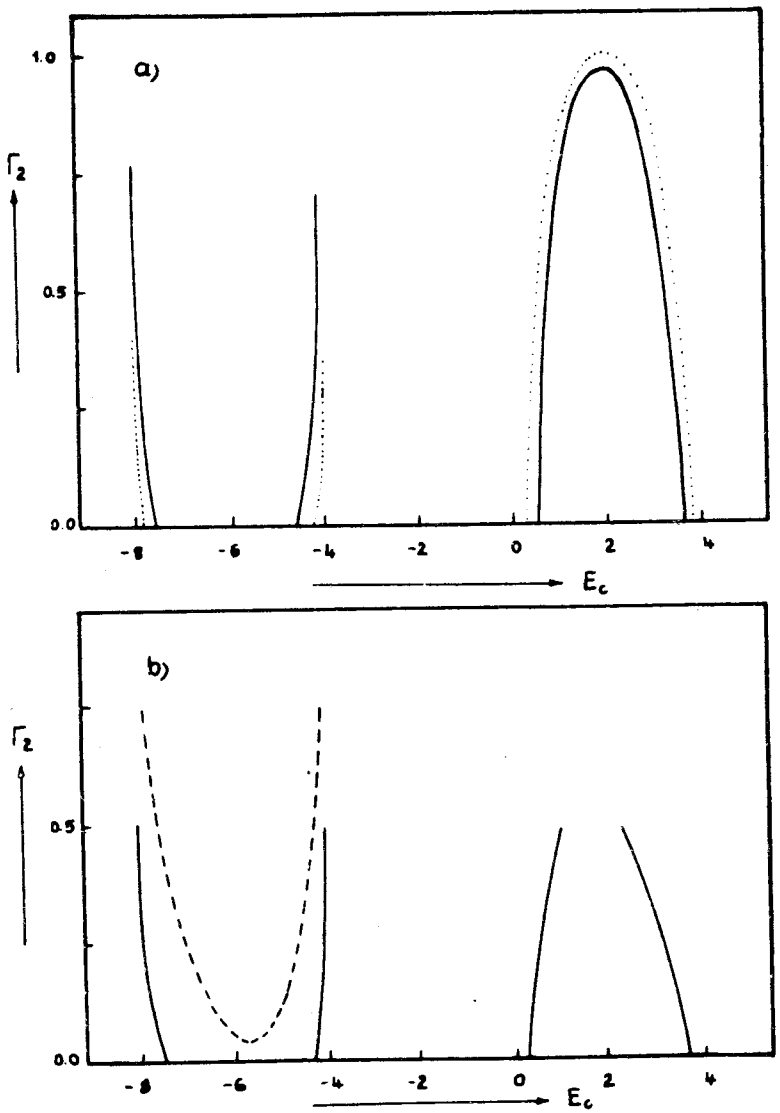

Fig. 6. Dependence of the mobility edges E_c upon Γ_2 for constant Γ_0 ($\Gamma_1 = 0$). a) Full line, E_c for L_0-criterion (Eq.(9)); dotted line, E_c for L_0-criterion of the one-band approximation of the Weaire model (Eq.(13)). b) E_c for the L_3-criterion (—— $\Gamma_0 = 0.5$, - - - $\Gamma_0 = 1.0$).

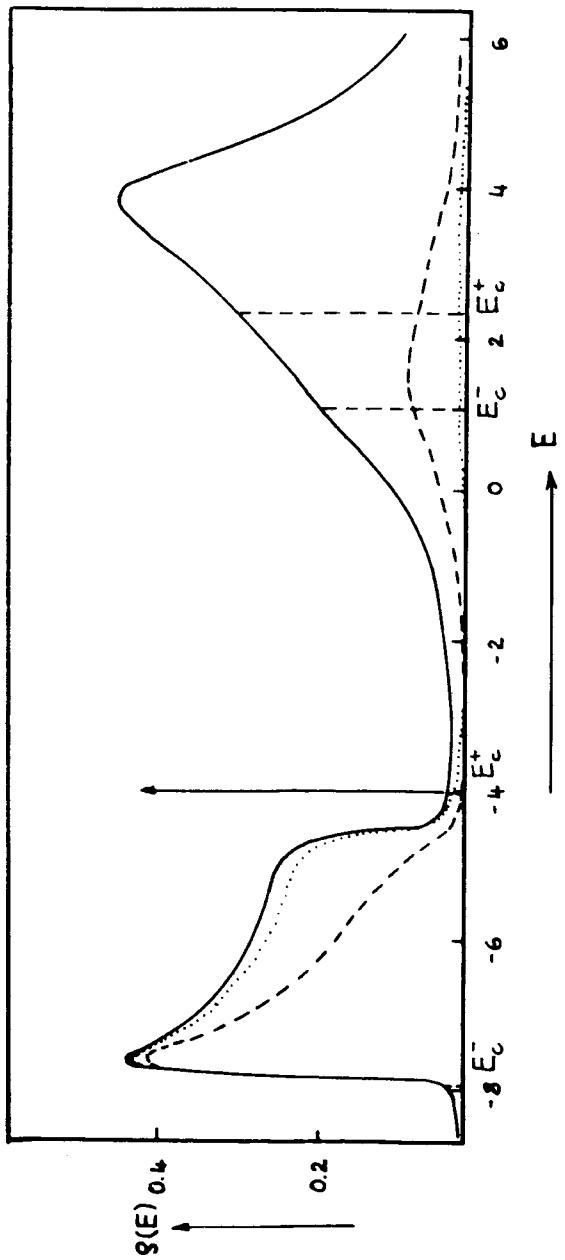

Fig. 7. The total density of states $\rho(E)$(——), the s-part of $\rho(E)$(- - -), and $\rho(E)$ of the bonding states(...) for $\Gamma_2=\Gamma_0=0.5$, $a=-1$, and $\Gamma_1=0$. $E_c^{\pm}$ belong to the L_3-criterion.

Comparing DS results of our theory with those of experiments (cf. [6.7]) we may suppose that the fluctuations of $\tilde{V}_0$, $\tilde{V}_1$, and V_2 are not very large in amorphous semiconductors. Therefore the obtained results for localization of electrons in the Weaire model suggest that the mobility gap in amorphous semiconductors is probably greater than in the corresponding ordered systems.

Recently, there have been found experimental confirmations of the "Mott-Anderson localization" in two-dimensional Si inversion layers[14]. Choosing an adequate set of parameters V_0°, V_1°, V_2°, Γ_0, Γ_1, and Γ_2 it is, maybe, possible to explain more quantitatively some experimental results. However, one must keep in mind that, first, the used Lorentzian distribution is rather fictive and, second, the Weaire model has only a qualitative significance. Because of that here we have discussed only the qualitative characteristics of electron localization in the Weaire model.

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