The second part of this work deals with the effects of elevated temperatures upon the thermal resistivity of complex crystals. Theoretically, it is understood that a locus will participate in the summation over reciprocal-lattice vector only when its thickness does not exceed its size. Practically, however, this effect is not dramatic owing to the fact that the summation over reciprocal-lattice vectors can be replaced by an integral which diverges like b^5. Consequently, if the lower limit of integration is replaced by $b_{\min}$ defined by $A\omega^2 T/v$ instead of zero, no net effect will be observed.

Early work by Eucken[3,14] pointed towards a departure from the $1/T$ dependence of the thermal conductivity at elevated temperatures. We conclude that this should not be an intrinsic effect. For example, experimental thermal-conductivity curves of naphthalene by Lees[15] showed a weak temperature dependence, not inconsistent with $\kappa \propto T^{-1/2}$. However, recent work on naphthalene,[16] as well as an earlier measurement,[3] shows that the thermal resistivity is directly proportional to temperature. The weak temperature dependence observed by Lees is now believed to be due to defects. We now expect that in structurally perfect crystals the $1/T$ dependence should hold until the temperature is high enough so that the phonon mean free path is short enough to approach interatomic distances. At those temperatures, however, the melting point has been exceeded in most cases.[7]

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Electron Localization and Atomic Correlation in One-Dimensional Disordered Systems*†

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The author reports fairly extensive new investigations of the electronic structure of one-dimensional disordered systems. A formalism is developed in the tight-binding approximation that includes nearest-neighbor correlation. This formalism is used to calculate density of states and two kinds of localization lengths for several model systems. In the uncorrelated binary alloy good agreement is found with Monte Carlo calculations performed recently by Bush. The results in the study of the disorder-induced metal-nonmetal transition confirm the model of Cohen and Sak.

I. INTRODUCTION

One-dimensional disordered systems have been extensively studied for the last two decades. The propagation of phonons as well as electrons in one-dimensional random chains and lattices have occupied many researchers, such as Dyson, Mott, Borland, and Hori *et al.*[1,2] In almost all cases, the problem was treated in the framework of a single-particle Hamiltonian with random potential. The problem has been of relatively little physical interest, because many of the results were true only for one dimension, and therefore were of little use for real physical systems. Recently, however, the problem acquired considerable physical importance after the discovery and experimental study of a number of very interesting solids.[3,4] These solids consist of long conducting stacks of planar organic or metallo-organic ions. These stacks interact very weakly with each other. The propagation of electrons is thus largely confined to individual stacks and is nearly one dimensional. Many of these solids also contain an element of randomness in their structure, affecting the electronic motion.[5] Thus the conduction electrons in these materials effectively move in a one-dimensional random potential, making the previous theoretical work on such systems of greater physical interest and raising the question of whether further work is required.

The solution of the problem requires, in principle, the explicit knowledge of the Hamiltonian of the system. In the present case, the potential is random and therefore varies from system to system. The only knowledge we can possibly have of it is that the potential is a member of a statistical ensemble of potentials. Given the properties of the ensemble, we are interested either in quantities that are sharply distributed and therefore independent of the particular member of the ensemble, or in ensemble averages of others not sharply distributed. An example of a sharply distributed quantity is the density of states of the infinitely long system. In a tight-binding representation, the density of states per site $\rho_N(E)$, of a system of N sites, is expressed as $-(1/\pi)\sum_l (1/N)\,\mathrm{Im}\langle l \mid G(E) \mid l\rangle$. By letting the system become infinitely long ($N\to\infty$), we sample all possible configurations contributing to $\langle l \mid G(E) \mid l\rangle$, and therefore at that limit the expression $(1/N)\sum_l \langle l \mid G(E) \mid l\rangle$ is sharply distributed around the value $\langle\langle i \mid G(E) \mid i\rangle\rangle_{\mathrm{av}}$, i.e., the ensemble average of one of its terms, implying directly the sharp distribution of $\rho_\infty(E)$. There are two methods of calculation for the sharply distributed quantities. The first method makes explicit use of the fact that the quantity is independent of the specific member of the ensemble, and calculates the quantity in a particular member of the ensemble, generated in the computer. The other method is the probabilistic approach which applies equally well for quantities sharply or not sharply distributed. This method uses statistical techniques to derive tractable equations for ensemble averages and the width of distribution of different quantities. We use the latter to calculate the density of states and characteristics of the eigenfunctions of the infinitely long disordered system.

At this point the notion of localization of eigenfunctions is introduced. The definition of the term localization has been discussed by many authors. It was conjectured in 1961 by Mott and Twose[6] and was rigorously proved subsequently by Borland[7] that in a one-dimensional random system all eigenfunctions are exponentially localized. This means that each eigenfunction is appreciable in some region of space, associated with a particular potential fluctuation there, and that its envelope decays exponentially far away from the potential fluctuation. The rate of decay in the tails of an eigenfunction is of great interest, especially in the case of phonon-assisted dc conductivity. Therefore that rate of decay must be studied and its statistical behavior determined. We call $L_d(E)$ the characteristic length entering the expression $e^{-X/L_d(E)}$ that describes the asymptotic decay of the envelope, and we shall prove that it is sharply distributed in the infinite system. The length over which the eigenfunction remains appreciable before it starts decaying to zero is another quantity of interest. Probabilistic considerations indicate that this length is not sharply distributed unless special dynamical correlations are present.[8] We call this length l_e, and we shall calculate its ensemble average $L_e(E)$.

As mentioned in the beginning, a considerable amount of work has been done concerning one-dimensional random systems. Review articles such as Ref. 9 and books such as Refs. 1 and 2 have collected this work for the interested. Nevertheless, the literature is inadequate in the following respects: (a) No work has been reported on $L_e(E)$ or has included effects of short-range order. (b) Very little work has been done on $L_d(E)$ and numerical procedures, and results are not sufficiently detailed or accurate even for the density of states. (c) Finally, the difference between one-dimensional disordered systems (all states localized for any degree of disorder[7]), and two and three dimensions (all states localized for disorder greater than a certain degree[10]) may have been overemphasized. Strong parallels remain, as pointed out by Economou and Cohen,[11] and we can exploit these to learn, *inter alia,* about the disorder-induced metal-nonmetal transition.

Accordingly, in the present paper fairly extensive new investigations of the electronic structure of one-dimensional disordered systems is reported. In Sec. II, a formalism is presented which is, in its first part, an extension of the Economou-Cohen theory.[12] In Sec. III, explicit solutions of the equations for several model systems, for the density of states, and for both localization lengths are presented and interpreted. For the uncorrelated binary-alloy case (Sec. III C), good agreement is found with the Monte Carlo calculations performed recently by Bush.[13] The results in the correlated binary-alloy case (Sec. III E) confirm the model of Cohen and Sak[14] for metal-semiconductor transitions in liquid and amorphous alloys.

II. FORMALISM

In the present section, the mathematical formalism developed for this problem is presented. In order to maintain generality throughtout the analysis, we specify only those properties of the system that are necessary for the definition of the model. This way, we can treat the widest possible class of physical systems to which this formalism can be applied. We thus consider a set of sites located on an infinite non-self-intersecting curve (the one-dimensional periodic array being a special case). We label these sites sequentially with integers, and define the Hamiltonian H in a Wannier-like representation. Its matrix elements i and j are $H_{ij} = \epsilon_i \delta_{ij} + V_{ij}$, where ϵ_i and V_{ij} are all real. We further restrict the elements V_{ij} to nearest neighbors:

$$V_{ij} = V(\epsilon_i, \epsilon_j)(\delta_{i,j+1} + \delta_{i,j-1}), \tag{2.1}$$

where $V(\epsilon_i, \epsilon_j)$ is a function of the values of ϵ_i and ϵ_j and obeys the relation

$$V(\epsilon_i, \epsilon_j) = V(\epsilon_j, \epsilon_i) \tag{2.2}$$

in order to maintain the Hermiticity of H, i.e., $H_{ij} = H_{ji}$ for eal H_{ij}. The model Hamiltonian is then

$$H_{ij} = \epsilon_i \delta_{ij} + V(\epsilon_i, \epsilon_j)(\delta_{i,j+1} + \delta_{i,j-1}) . \tag{2.3}$$

Following Economou and Cohen[12] we use a Green's-function approach. The Green's function $G(Z)$ has its poles on the real axis, the poles being the eigenvalues E_n of H, and has matrix elements $G_{ij}(Z) = [(Z - H)^{-1}]_{ij}$. Its diagonal elements $G_{ii}(Z)$ define a set of functions $\Delta_i(Z)$ through the relation

$$G_{ii}(Z) = [Z - \epsilon_i - \Delta_i(Z)]^{-1} , \tag{2.4}$$

each associated with the corresponding site i, usually called "the self-energy of i." One can write a renormalized perturbation expansion (RPE) for $\Delta_i(Z)$[10,12] when the Hamiltonian is defined as in (2.3). Terms in the RPE are the contributions from all self-avoiding paths starting from and ending at site i and only connecting nearest neighbors (because in it only nearest neighbors interact). A factor V_{ij} [see (2.1)] corresponds to each step from site i to site j, and a factor $G_{ii}^{n;\cdots}(Z)$ corresponds to each site $i \neq n$. [$G_{ii}^{n;\cdots}(Z)$ represents the i-i matrix element of the Green's function corresponding to a Hamiltonian differing from (2.2) in that $\epsilon_k = \infty$, k denoting every site preceding i in the particular path under consideration.] Applying the above rule for $\Delta_i(Z)$, one sees that there are only two self-avoiding paths starting from and ending at site i for nearest neighbor V_{ij} (see Fig. 1) and, therefore only two terms in its RPE. We have

$$\Delta_i(Z) = V_{i,i+1} G^{i}_{i+1,i+1}(Z) V_{i+1,i} + V_{i,i-1} G^{i}_{i-1,i-1}(Z) V_{i-1,i} , \tag{2.5}$$

which we write as

$$\Delta_i(Z) = t_i^{+}(Z) + t_i^{-}(Z) , \tag{2.6}$$

where [using (2.5) and (2.2)]

$$t_i^{\pm}(Z) = V^2_{i,i\pm1} G^{i}_{i\pm1,i\pm1}(Z) . \tag{2.7}$$

Following Economou and Cohen[12] we write (2.7) as a continued fraction

$$t_i^{\pm}(Z) = \frac{V^2_{i,i\pm1}}{Z - \epsilon_{i\pm1} - V^2_{i\pm1,i\pm2}/(Z - \epsilon_{i\pm2} - \cdots)} , \tag{2.8}$$

from which the relation

$$t_i^{\pm}(Z) = \frac{V^2_{i,i\pm1}}{Z - \epsilon_{i\pm1} - t^{\pm}_{i\pm1}(Z)} \tag{2.8$'$}$$

follows immediately.

From the above analysis it is obvious that the set $\{\epsilon_i\}$ of the diagonal elements of our Hamiltonian, plus the functional form of $V(\epsilon_i, \epsilon_j)$ are sufficient to determine H and, therefore, the whole problem. It is only at this point that we introduce randomness by requiring the $\{\epsilon_i\}$ to be a set of random variables and by assuming their joint probability distribution $P(\{\epsilon_i\})$ to be known. As mentioned in the Introduction, the quantities of interest are averages over the ensemble of $\{\epsilon_i\}$, and for their evaluation one needs certain probability distribution functions. The joint probability distribution $P(\{\epsilon_i\})$ and the functional form of $V(\epsilon_i, \epsilon_j)$ should be the only input for the evaluation of those other probability distributions required. Certain assumptions about the form of $P(\{\epsilon_i\})$ are necessary to make the solution of the problem feasible. Economou and Cohen[12] treated the first part of our problem in the case of $\{\epsilon_i\}$ independent random variables. We generalize their work to $\{\epsilon_i\}$ such that nearest neighbors are statistically correlated, and such that the joint probability distribution $P(\epsilon_i, \epsilon_{i+1})$ of two nearest neighbors does not depend on the position i and, moreover that it is symmetric in them, i.e., $P(\epsilon_i, \epsilon_{i+1}) = P(\epsilon_{i+1}, \epsilon_i)$. Then one easily sees that

$$P(\epsilon_i) = \int_{-\infty}^{+\infty} P(\epsilon_i, \epsilon)\, d\epsilon , \tag{2.9}$$

and that

$$P(\epsilon_i, \epsilon_{i+1}) = P(\epsilon_i) P_c(\epsilon_{i+1}/\epsilon_i) = P(\epsilon_{i+1}) P(\epsilon_i/\epsilon_{i+1}) , \tag{2.10}$$

where $P_c(\epsilon_k/\epsilon_l)$ is the probability density of ϵ_k, under the condition that at site l we have a fixed ϵ_l. Under the above assumptions, the probability density $P(\epsilon_{i-k}, \epsilon_{i-k+1}, \ldots, \epsilon_{i-1}, \epsilon_i)$ of successive neighbors from sites $i-k$ to i can be expressed as $P(\epsilon_i) P_c(\epsilon_{i-1}/\epsilon_i) P_c(\epsilon_{i-2}/\epsilon_{i-1}) \cdots P_c(\epsilon_{i-k}/\epsilon_{i-k+1})$, and so the entire $P(\{\epsilon_i\})$ can be expressed this way. We shall need, in addition, the joint probability distribution $f(\epsilon_i, t_i; Z)$ of ϵ_i and t_i for given

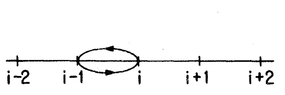

FIG. 1. Two diagrams for the RPE of the self-energy $\Delta_i(E)$, when only nearest-neighbor coupling is present.

energy Z, where t_i is t_i^+ or t_i^-, the functional form being the same in both cases as shown below. In (2.8′) we have $t_i^\pm$ expressed in terms of ϵ_i, $\epsilon_{i\pm1}$, and $t_{i\pm1}^\pm$. Using standard mathematical techniques, we write

$$f(\epsilon_i, t_i^\pm; Z) = \int_{-\infty}^{+\infty} \delta\left(t_i^\pm - \frac{V^2(\epsilon_i', \epsilon_{i\pm1})}{Z - \epsilon_{i\pm1} - t_{i\pm1}^\pm}\right) \times \delta(\epsilon_i' - \epsilon_i) f(\epsilon_{i\pm1}, t_{i\pm1}^\pm; Z) \times P_c(\epsilon_i'/\epsilon_{i\pm1})\, d\epsilon_i'\, d\epsilon_{i\pm1}\, dt_{i\pm1}^\pm, \tag{2.11}$$

where $t_{i\pm1}^\pm$ does not enter the conditional probability for ϵ_i' because the latter is independent of it [see (2.8)]. Using the translational invariance of $P(\epsilon_i, \epsilon_{i+1})$ and its symmetry in ϵ_i and ϵ_{i+1}, we easily see that $P_c(\epsilon_i/\epsilon_{i+1}) = P_c(\epsilon_i/\epsilon_{i-1})$ when $\epsilon_{i+1} = \epsilon_{i-1}$; or in other words, the two conditional probability densities have the same functional dependence on ϵ_i. Because of that, it follows from (2.11) that $f(\epsilon_i, t_i^+; Z)$ and $f(\epsilon_i, t_i^-; Z)$ have the same functional dependence on their t_i's. To simplify notation, we shall call "t_i" the t_i^+ and deal with the (+) case without any loss of generality. Integrating trivially over ϵ_i' in (2.11), we get

$$f(\epsilon_i, t_i; Z) = \int_{-\infty}^{+\infty} \delta\left(t_i - \frac{V^2(\epsilon_i, \epsilon_{i+1})}{Z - \epsilon_{i+1} - t_{i+1}}\right) \times f(\epsilon_{i+1}, t_{i+1}; Z) P_c(\epsilon_i/\epsilon_{i+1})\, d\epsilon_{i+1}\, dt_{i+1}. \tag{2.12}$$

Equation (2.12), as stated before, is an extension of the Economou–Cohen theory. Here, too, one easily sees, after performing integrations over $d\epsilon_{i+1}$ and dt_{i+1} in both sides of (2.12), that

$$\int_{-\infty}^{+\infty} f(\epsilon_i, t_i; Z)\, d\epsilon_i\, dt_i = \int_{-\infty}^{+\infty} f(\epsilon_{i+1}, t_{i+1}; Z)\, d\epsilon_{i+1}\, dt_{i+1},$$

which means that the kernel of the integral equation has indeed the eigenvalue 1, as implied by (2.12). From here on, $f(\epsilon_i, t_i; Z)$ will be considered known, as given by the solution of (2.12) normalized to 1, i.e.,

$$\int_{-\infty}^{+\infty} f(\epsilon_i, t_i; Z)\, d\epsilon_i\, dt_i = 1. \tag{2.13}$$

Here we start the evaluation of quantities of interest. We deal first with the average density of states per site, $\rho(E)$, which is given by

$$\rho(E) = -(1/\pi)\, \mathrm{Im}[(1/N)\, \mathrm{Tr}\, G_N(E)],$$

for a system of N sites and one state per site. The ensemble average for the infinite ($N \to \infty$) random system is given by

$$\rho(E) = -(1/\pi)\, \mathrm{Im}\langle G_{ii}(E)\rangle_{\mathrm{av}}, \tag{2.14}$$

where $\langle\ \rangle_{\mathrm{av}}$ denotes average over all configurations. In (2.14) we identify $\lim_{N\to\infty}(1/N)\,\mathrm{Tr}\,G_N(E)$, the average over sites, with the ensemble average for a site. Using (2.4) and (2.6) we write

$$\rho(E) = -(1/\pi)\, \mathrm{Im}\langle [E - \epsilon_i - t_i^+(E) - t_i^-(E)]^{-1}\rangle_{\mathrm{av}}$$

or, explicitly,

$$\rho(E) = -\frac{1}{\pi}\, \mathrm{Im} \int_{-\infty}^{+\infty} \frac{P(\epsilon_i, t_i^+, t_i^-)\, d\epsilon_i\, dt_i^+\, dt_i^-}{E - \epsilon_i - t_i^+ - t_i^-}, \tag{2.15}$$

where $P(\epsilon_i, t_i^+, t_i^-)$ is the joint probability distribution of ϵ_i, t_i^+, and t_i^-. Using the Cauchy identity in (2.15), we write

$$\rho(E) = \int_{-\infty}^{+\infty} \delta(E - \epsilon_i - t_i^+ - t_i^-)\, P(\epsilon_i, t_i^+, t_i^-)\, d\epsilon_i\, dt_i^+\, dt_i^-. \tag{2.15′}$$

$P(\epsilon_i, t_i^+, t_i^-)$ is identically written

$$P(\epsilon_i, t_i^+, t_i^-) = f(\epsilon_i, t_i^+; E)\, f_c(t_i^-/\epsilon_i, t_i^+; E), \tag{2.16}$$

$f_c(t_i^-/\epsilon_i, t_i^+; E)$ being again a conditional probability for t_i^-. From (2.8′) one sees that t_i^- depends only on the t^-'s, and so it is independent of t_i^+, which means

$$f_c(t_i^-/\epsilon_i, t_i^+; E) = f_c(t_i^-/\epsilon_i; E). \tag{2.17}$$

Combining (2.16) and (2.17) with the identity

$$f(\epsilon_i, t_i^-; E) = P(\epsilon_i)\, f_c(t_i^-/\epsilon_i; E), \tag{2.18}$$

where $P(\epsilon_i)$ is given by (2.9), we get the final expression for $P(\epsilon_i, t_i^+, t_i^-)$:

$$P(\epsilon_i, t_i^+, t_i^-) = f(\epsilon_i, t_i^+; E)\, f(\epsilon_i, t_i^-; E)\, P^{-1}(\epsilon_i), \tag{2.19}$$

and therefore (2.15′) becomes

$$\rho(E) = \int_{-\infty}^{+\infty} \delta(E - \epsilon_i - t_i^+ - t_i^-)\, f(\epsilon_i, t_i^+; E) \times f(\epsilon_i, t_i^-; E)\, P^{-1}(\epsilon_i)\, d\epsilon_i\, dt_i^+\, dt_i^-. \tag{2.20}$$

One can easily check the condition

$$\int_{-\infty}^{+\infty} \rho(E)\, dE = 1 \tag{2.21}$$

(because we assumed one state per site). Indeed using (2.13), (2.18), and (2.20), one verifies (2.21). Finally we shall see that (2.20) simplifies considerably in certain special cases.

In Sec. I the concepts of two localization lengths $L_d(E)$ and $L_e(E)$ were introduced. $L_d(E)$ was introduced to describe the rate of decay of the envelope of a state, far away from the fluctuation with which it is associated. $L_e(E)$ was introduced to describe the average length of the potential fluctuations associated with states around a given energy E, or in other words, the average length over which the envelope of a state remains roughly unchanged before it starts decaying quasiexponentially to zero. In order to put these quantities into mathematical terms, one must return to the Green's-function formalism. Following Anderson, one can use a perturbation expansion for $G_{l0}(Z)$ expressed as the contributions of all paths starting from site 0 and ending at site l. One then has

$$G_{l0}(Z)=G_{00}(Z)V_{0,1}G^{0}_{1,1}(Z) \times V_{1,2}G^{0,1}_{2,2}(Z)V_{2,3}\cdots V_{l-1,l}G^{0,1,\ldots,l-1}_{ll}(Z) . \qquad (2.\,22)$$

We observe that

$$G^{0,1,\ldots,i-1}_{ii}(Z)=G^{i-1}_{ii}(Z) . \qquad (2.\,22')$$

One easily verifies the above by writing each side of (2. 22′) in terms of the corresponding self-energy $\{G^{0,1,\ldots,i-1}_{ii}(Z)=[Z-\epsilon_i-\Delta^{0,1,\ldots,i-1}_i(Z)]^{-1}$, $G^{i-1}_{ii}(Z)=[Z-\epsilon_i-\Delta^{i-1}_i(Z)]^{-1}\}$ and observing that in both cases the self-energy is expressed as a continued fraction (2. 8), and thus $\Delta^{0,1,\ldots,i-1}_i(Z)=\Delta^{i-1}_i(Z)$. Using (2. 1) and (2. 7) in the form

$$V_{i,i+1}G^{i}_{i+1,i+1}(Z)=t^{+}_i(Z)/V_{i,i+1} , \qquad (2.\,23)$$

and (2. 22′), we have

$$G_{l0}(Z)=G_{00}(Z)\prod_{i=0}^{l-1}\frac{t^{+}_i(Z)}{V(\epsilon_i,\epsilon_{i+1})} , \quad l\geqslant 1 . \qquad (2.\,24)$$

We now express G in terms of the eigenstates $|E_n)$ of the Hamiltonian

$$G(Z)=\sum_n\frac{|E_n)(E_n|}{Z-E_n} . \qquad (2.\,25)$$

Hence we have [denoting by $\psi_i(E_n)$ the overlap of $|E_n)$ with site i]

$$G_{00}(Z)=\sum_n\frac{\psi_0(E_n)\psi^*_0(E_n)}{Z-E_n} , \qquad (2.\,26)$$

$$G_{l0}(Z)=\sum_n\frac{\psi_l(E_n)\psi^*_0(E_n)}{Z-E_n} . \qquad (2.\,27)$$

In order to simplify notation, we write (2. 24) in the form

$$G_{l0}(Z)=G_{00}(Z)F_{l0}(Z) , \qquad (2.\,28)$$

where [using (2. 24)]

$$F_{l0}(Z)=\prod_{i=0}^{l-1}\frac{t^{+}_i(Z)}{V(\epsilon_i,\epsilon_{i+1})} , \quad l\geqslant 1 . \qquad (2.\,29)$$

Combining (2. 26)–(2. 28) we get

$$\sum_n\frac{\psi_l(E_n)\psi_0(E_n)}{Z-E_n}=\sum_n\frac{F_{l0}(Z)\psi_0(E_n)\psi^*_0(E_n)}{Z-E_n} . \qquad (2.\,30)$$

We observe that $F_{l0}(Z)$ has no common poles with $G_{l0}(Z)$ and $G_{00}(Z)$, and that $G_{l0}(Z)$ and $G_{00}(Z)$ have exactly the same poles, the eigenenergies of H. Equating the residues of each pole in (2. 30), one gets

$$\psi_l(E_n)\psi^*_0(E_n)=F_{l0}(E_n)\psi_0(E_n)\psi^*_0(E_n) . \qquad (2.\,31)$$

At this point one can argue that the probability of having $\psi_0(E_n)=0$ for an eigenstate E_n is zero. This means that $\psi_0(E_n)\neq 0$ for all configurations $\{\epsilon_n\}$, apart from some of measure zero. We can then write (2. 3) in a form that holds with probability 1:

$$F_{l0}(E)=\psi_l(E_n)/\psi_0(E_n) \qquad (2.\,32)$$

and $E=E_n$. Next we rewrite (2. 30) in the form

$$F_{l0}(E)=\sum_n\frac{\psi_l(E_n)\psi^*_0(E_n)}{E-E_n}\Bigg/\sum_n\frac{\psi_0(E_n)\psi^*_0(E_n)}{E-E_n} . \qquad (2.\,33)$$

Relation (2. 32) simply says that when $E=E_n$, the term $\psi_l(E_n)\psi^*_0(E_n)/(E-E_n)$ dominates completely over all the other terms in the numerator of (2. 33), and similarly the term $\psi_0(E_n)\psi^*_0(E_n)/(E-E_n)$ dominates completely in the denominator. The same relation (2. 32) holds approximately for $F_{l0}(E)$ when E is different from E_n, but in a sufficiently narrow neighborhood of width $2\Delta E_n$ around the pole E_n [i. e., $E\in(E_n-\Delta E_n, E_n+\Delta E_n)$]. The width $2\Delta E_n$ and, consequently, the statistical weight of the pole E_n decreases exponentially as $e^{-2l_p/L_d(E_n)}$ when the corresponding eigenstate is peaked around site l_p outside the interval $[0, l]$. When the pole E_n corresponds to such a remote state, the probability that the energy E lies outside the exponentially narrow interval is high. For E outside that interval, the terms that dominate in the expression (2. 33) for $F_{l0}(E)$ come from eigenstates that are peaked around site 0 (in the denominator) or, at most, in the interval $(0,l)$ (in the numerator), and have eigenenergy E_n closest to E. Since eigenstates neighboring in energy are widely separated in space, expression (2. 33) is dominated by only one eigenstate for small l's, and $F_{l0}(E)$ is still given by (2. 32), where $\psi(E_n)$ is now the dominant eigenstate which is peaked around zero and of energy closest to E.

Now we consider the probability distribution of the values of $F_{l0}(E)$ for the different systems, members of the ensemble. The above analysis demonstrated that the probability distribution of $F_{l0}(E)$ is dominated by the behavior of eigenstates of energy around E that are peaked around site zero or, at most, in the interval $(0, l)$. Our purpose is to study the ensemble average behavior of the *envelope* of an eigenstate of energy around E. Therefore we introduce the statistical quantity $\tau_l(E)$, defined by the relation

$$\tau_l(E)=|F_{l0}(E)|=\prod_{i=0}^{l-1}\left|\frac{t^{+}_i(E)}{V(\epsilon_i,\epsilon_{i+1})}\right| , \quad l\geqslant 1 . \qquad (2.\,34)$$

For each member of the ensemble, τ_l obeys the relation

$$\tau_l(E)=|\psi_l(E_n)/\psi_0(E_n)| \qquad (2.\,34')$$

[see (2. 32)]. The above analysis convinces us that $\tau_l(E)$ is the proper statistical quantity for our study of the localization lengths.

We start with $L_d(E)$. For that, we need to know the behavior of $\tau_l(E)$ as $l\rightarrow\infty$. We shall prove that $\tau_l(E)$ is sharply distributed around the value $e^{-l/L_d(E)}$ as $l\rightarrow\infty$. For that purpose we study the variable $T_l(E)$ given by the relation

$$T_l(E) \equiv (1/l)\ln\tau_l(E) . \qquad (2.35)$$

Combining this with (2.34) we have

$$T_l(E) = \frac{1}{l}\sum_{i=0}^{l-1}\left[\ln\left|t_i^+(E)\right| - \ln\left|V(\epsilon_i, \epsilon_{i+1})\right|\right] . \qquad (2.36)$$

Applying again standard mathematical techniques, we can express the probability distribution of τ_l as

$$P(T_l) = \int_{-\infty}^{+\infty} \delta\left(T_l - \frac{1}{l}\sum_{i=0}^{l-1}\left[\ln\left|t_i^+\right| - \ln\left|V(\epsilon_i, \epsilon_{i+1})\right|\right]\right) P(\{\epsilon_i\}, \{t_i^+\})\, d\epsilon_l \prod_{i=0}^{l-1} d\epsilon_i\, dt_i^+ , \qquad (2.37)$$

where $P(\{\epsilon_i\}, \{l_i^+\})$ is the joint probability distribution of all the random variables involved in (2.37) except T_l. Starting from (2.37) we may compute moments of the distribution. We have

$$\langle T_l\rangle_{\text{av}} = \int_{-\infty}^{+\infty} T_l P(T_l)\, dT_l = \int_{-\infty}^{+\infty} \frac{1}{l}\sum_{i=0}^{l-1}\left[\ln\left|t_i^+\right| - \ln\left|V(\epsilon_i, \epsilon_{i+1})\right|\right] P(\{\epsilon_i\}, \{t_i^+\})\, d\epsilon \prod_{i=0}^{l-1} d\epsilon_i\, dt_i^+ , \qquad (2.38)$$

$$\langle T_l^2\rangle_{\text{av}} = \int_{-\infty}^{+\infty} T_l^2 P(T_l)\, dT_l = \int_{-\infty}^{+\infty} \left(\frac{1}{l}\sum_{i=0}^{l-1}\left[\ln\left|t_i^+\right| - \ln\left|V(\epsilon_i, \epsilon_{i+1})\right|\right]\right)^2 P(\{\epsilon_i\}, \{t_i^+\})\, d\epsilon_l \prod_{i=0}^{l-1} d\epsilon_i\, dt_i^+ . \qquad (2.39)$$

Working on (2.38) first, we have

$$\langle T_l\rangle_{\text{av}} = \frac{1}{l}\sum_{i=0}^{l-1} \int_{-\infty}^{+\infty} \ln\left|t_i^+\right| P(\{\epsilon_i\}, \{t_i^+\})\, d\epsilon_l \prod_{i=0}^{l-1} d\epsilon_i\, dt_i^+ - \frac{1}{l}\sum_{i=0}^{l-1} \int_{-\infty}^{+\infty} \ln\left|V(\epsilon_i, \epsilon_{i+1})\right| P(\{\epsilon_i\}, \{t_i^+\})\, d\epsilon_l \prod_{i=0}^{l-1} d\epsilon_i\, dt_i^+ .$$

In each term of the sum, the integrals over all variables but t_i^+, ϵ_i, and ϵ_{i+1} are straightforward, and the above relation simplifies to

$$\langle T_l(E)\rangle_{\text{av}} = \frac{1}{l}\sum_{i=0}^{l-1} \int_{-\infty}^{+\infty} \ln\left|t_i^+\right| f(t_i; E)\, dt_i^+ - \frac{1}{l}\sum_{i=0}^{l-1} \int_{-\infty}^{+\infty} \ln\left|V(\epsilon_i, \epsilon_{i+1})\right| P(\epsilon_i, \epsilon_{i+1})\, d\epsilon_i\, d\epsilon_{i+1} , \qquad (2.40)$$

where

$$f(t_i^+; E) = \int_{-\infty}^{+\infty} f(\epsilon_i, t_i^+; E)\, d\epsilon_i \qquad (2.41)$$

and $f(\epsilon_i, t_i^+; E)$ and $P(\epsilon_i, \epsilon_{i+1})$ are as defined previously. Since $f(t_i^+; E)$ is obviously independent of i, each of the integrals in (2.40) is independent of i and (2.40) simplifies to

$$\langle T_l(E)\rangle_{\text{av}} = \int_{-\infty}^{+\infty} \ln|t|\, f(t; E)\, dt - \int_{-\infty}^{+\infty} \ln\left|V(\epsilon', \epsilon'')\right| P(\epsilon', \epsilon'')\, d\epsilon'\, d\epsilon'' . \qquad (2.40')$$

We observe that $\langle T_l(E)\rangle_{\text{av}}$ does not depend on l. Therefore its limit trivially exists:

$$\lim_{l\to\infty}\langle T_l(E)\rangle_{\text{av}} = \langle T(E)\rangle_{\text{av}} , \qquad (2.40'')$$

where $\langle T(E)\rangle_{\text{av}}$ is given by the right-hand side of (2.40′). In order to examine the sharpness of the distribution as $l\to\infty$, we examine its variance

$$\sigma_l^2(E) = \langle T_l^2(E)\rangle_{\text{av}} - \langle T_l(E)\rangle_{\text{av}}^2 \qquad (2.42)$$

to see whether it goes to zero as $l\to\infty$. For that, we simply observe that

$$\lim_{l\to\infty}\frac{1}{l}\sum_{i=0}^{l-1}\left[\ln\left|t_i^+(E)\right| - \ln\left|V(\epsilon_i, \epsilon_{i+1})\right|\right] = \langle T(E)\rangle_{\text{av}}$$

(i.e., we identify the left-hand side of the expression with the average of its individual terms). From (2.39) we clearly see that

$$\lim_{l\to\infty}\langle T_l^2(E)\rangle_{\text{av}} = \langle T(E)\rangle_{\text{av}}^2 \int_{-\infty}^{+\infty} P(\{\epsilon_i\}, \{t_i^+\})\, d\epsilon_l \times \prod_{i=0}^{l=1} d\epsilon_i\, dt_i^+ = \langle T(E)\rangle_{\text{av}}^2 .$$

It follows that

$$\lim_{l\to\infty}\sigma_l^2(E) = 0 , \qquad (2.43)$$

and $T_l(E)$ is sharply distributed at infinity around the value $\langle T(E)\rangle_{\text{av}}$. Recalling the definition of $T_l(E)$ [see (2.35)] and the relation (2.34′) as well as the discussion given there, we have

$$\lim_{l\to\infty}\left|\frac{\psi_l(E_n)}{\psi_0(E_n)}\right| = \lim_{l\to\infty} e^{lT_l(E_n)} = e^{l\langle T(E_n)\rangle_{\text{av}}} , \qquad (2.44)$$

where E_n is an eigenenergy of the system. The characteristic decay length $L_d(E)$ obeys the relation

$$\lim_{l\to\infty}\left|\psi_l(E_n)/\psi_0(E_n)\right| = e^{-l/L_d(E_n)}$$

on an eigenenergy E_n and [using (2.40′), (2.40″), and (2.44)] is given as

$$L_d(E) = -\left[\int_{-\infty}^{+\infty} \ln|t|\, f(t;E)\, dt - \int_{-\infty}^{+\infty} \ln|V(\epsilon',\epsilon'')|\, P(\epsilon',\epsilon'')\, d\epsilon'\, d\epsilon''\right]^{-1} \quad (2.45)$$

in number of sites rather than length.

Finally we come to the study of $L_e(E)$, which we will define later on. For the time being, we return to (2.33) and (2.34) and study the probability distribution of $\tau_l(E)$, $l \geqslant 1$. As before, we now have

$$P(\tau_l(E)) = \int_{-\infty}^{+\infty} \delta\left(\tau_l(E) - \prod_{i=0}^{l-1} \left|\frac{t_i^+(E)}{V(\epsilon_i,\epsilon_{i+1})}\right|\right) \times P(\{\epsilon_i\},\{t_i^+\})\, d\epsilon_l \prod_{i=0}^{l-1} d\epsilon_i\, dt_i^+ \ . \quad (2.46)$$

The above probability distribution has a tail which extends to infinity. This tail is unrelated to the behavior of the eigenfunctions because it is due to the poles of $F_{l0}(E)$—all of which are created by zeros of $G_{00}(E)$ [see (2.28), (2.29) and (2.34)] and therefore are physically unimportant. However, this tail is responsible for the nonexistence of the positive moments of the distribution, since it causes the divergence of the integrals that compute those moments. Therefore one cannot study $P(\tau_l)$ by calculating its moments. There are several ways to overcome this difficulty. One possibility suggested by Anderson[10] is to study the most probable value of the distribution. Another approach would be to truncate $P(\tau_l)$ as to eliminate the tail and then study the behavior of the moments. The latter approach is followed in the present study. The truncation is fixed by requiring the calculated value for $L_e(E)$ to agree with the exact value in one of the limiting cases where the exact result is known (see Sec. III D). A volume of information can be obtained from the truncated $P(\tau_l)$, because it has well-defined moments that are directly related to the shape of $P(\tau_l)$ for finite τ_l and, therefore, directly related to the behavior of the eigenfunctions. We deal below with the first moments of the truncated probability distribution of $\tau_l(E)$. The truncation is implicit in the formalism and is properly taken into account in the numerical part (Sec. III D). We start with $\langle\tau_l(E)\rangle_{\text{av}}$ and $\langle\tau_l^2(E)\rangle_{\text{av}}$, which are given by

$$\langle\tau_l^n(E)\rangle_{\text{av}} = \int_{-\infty}^{+\infty} \tau_l^n(E)\, P(\tau_l(E))\, d\tau_l(E) \ , \quad n = 1, 2 \ .$$

Using (2.46) we write

$$\langle\tau_l(E)\rangle_{\text{av}} = \int_{-\infty}^{+\infty} \prod_{i=0}^{l-1} \left|\frac{t_i^+(E)}{V(\epsilon_i,\epsilon_{i+1})}\right| \times P(\{\epsilon_i\},\{t_i^+\})\, d\epsilon_l \prod_{i=0}^{l-1} d\epsilon_i\, dt_i^+ \ , \quad (2.47)$$

$$\langle\tau_l^2(E)\rangle_{\text{av}} = \int_{-\infty}^{+\infty} \prod_{i=0}^{l-1} \left|\frac{t_i^+(E)}{V(\epsilon_i,\epsilon_{i+1})}\right|^2 \times P(\{\epsilon_i\},\{t_i^+\})\, d\epsilon_l \prod_{i=0}^{l-1} d\epsilon_i\, dt_i^+ \ . \quad (2.48)$$

The final step towards an explicit expression for $\langle\tau_l(E)\rangle_{\text{av}}$ and $\langle\tau_l^2(E)\rangle_{\text{av}}$ is to express $P(\{\epsilon_i\},\{t_i^+\})$ in terms of known functions such as $P(\epsilon_i,\epsilon_{i+1})$, $f(\epsilon_i, t_i^+;E)$, or those that are derived from them [like $P(\epsilon_i)$ given by (2.9), etc.]. Writing explicitly the set of variables in $P(\{\epsilon_i\},\{t_i^+\})$, we have

$$P(\{\epsilon_i\},\{t_i^+\}) = P(\epsilon_l,\epsilon_{l-1},t_{l-1}^+,\epsilon_{l-2},t_{l-2}^+,\ldots,\epsilon_0,t_0^+) \ . \quad (2.49)$$

This can be written in our previous manner

$$P(\{\epsilon_i\},\{t_i^+\}) = P(\epsilon_l,\epsilon_{l-1},t_{l-1}^+) \times P_c(\epsilon_{l-2},t_{l-2}^+/\epsilon_{l-1},t_{l-1}^+)\cdots \times P_c(\epsilon_0,t_0^+/\epsilon_1,t_1^+) \ . \quad (2.50)$$

The reason why the conditional probabilities can be written in this fashion lies in the way we have constructed the ensemble $(\{\epsilon_i\},\{t_i^+\})$ [see (2.8′)]. That is, once a pair of values (ϵ_i,t_i^+) is fixed, the probability of the pair $(\epsilon_{i-1},t_{i-1}^+)$ depends only on these values and on nothing that comes after them. In order to derive the final form for $P(\{\epsilon_i\},\{t_i^+\})$, we have to express $P(\epsilon_l,\epsilon_{l-1},t_{l-1}^+)$ and $P_c(\epsilon_i,t_i^+/\epsilon_{i+1},t_{i+1}^+)$ explicitly. Using our previous technique, we write

$$P_c(\epsilon_i,t_i^+/\epsilon_{i+1},t_{i+1}^+) = \int_{-\infty}^{+\infty} \left(\delta\, t_i^+ - \frac{V^2(\epsilon,\epsilon_{i+1})}{E-\epsilon_{i+1}-t_{i+1}^+}\right) \times P_c(\epsilon/\epsilon_{i+1})\, d\epsilon \ . \quad (2.51)$$

Integrating trivially over ϵ we get

$$P_c(\epsilon_i,t_i^+/\epsilon_{i+1},t_{i+1}^+) = \delta\left(t_i^+ - \frac{V^2(\epsilon_i,\epsilon_{i+1})}{E-\epsilon_{i+1}-t_{i+1}^+}\right) \times P_c(\epsilon_i/\epsilon_{i+1}) \ . \quad (2.52)$$

For $P(\epsilon_l,\epsilon_{l-1},t_{l-1}^+)$ we write

$$P(\epsilon_l,\epsilon_{l-1},t_{l-1}^+) = P(\epsilon_l,\epsilon_{l-1})\, P_c(t_{l-1}^+/\epsilon_l,\epsilon_{l-1}) \ , \quad (2.53)$$

$$P_c(t_{l-1}^+/\epsilon_l,\epsilon_{l-1}) = \int_{-\infty}^{+\infty} \delta\left(t_{l-1}^+ - \frac{V^2(\epsilon_{l-1},\epsilon_l)}{E-\epsilon_l-t_l^+}\right) \times P_c(t_l^+/\epsilon_l,\epsilon_{l-1})\, dt_l^+ \ , \quad (2.54)$$

and

$$P_c(t_l^+/\epsilon_l,\epsilon_{l-1}) = P_c(t_l^+/\epsilon_l) = f(\epsilon_l,t_l^+;E)\, P^{-1}(\epsilon_l) \ , \quad (2.55)$$

because t_l^+ does not depend on things that precede it, such as ϵ_{l-1}. Combining (2.10) and (2.53)–(2.55), we have

$$P(\epsilon_l, \epsilon_{l-1}, t^+_{l-1}) = P_c(\epsilon_{l-1}/\epsilon_l) \times \int_{-\infty}^{+\infty} \delta\left(t^+_{l-1} - \frac{V^2(\epsilon_{l-1}, \epsilon_l)}{E - \epsilon_l - t^+_l}\right) \times f(\epsilon_l, t^+_l; E)\, dt^+_l \,. \tag{2.56}$$

Combining (2.50), (2.52), and (2.56), we express $P(\{\epsilon_i\}, \{t^+_i\})$ as

$$P(\{\epsilon_i\}, \{t^+_i\}) = \int_{-\infty}^{+\infty} dt^+_l f(\epsilon_l, t^+_l; E) \times \prod_{i=0}^{l-1} \delta\left(t^+_i - \frac{V^2(\epsilon_i, \epsilon_{i+1})}{E - \epsilon_{i+1} - t^+_{i+1}}\right) P_c(\epsilon_i/\epsilon_{i+1}) \;. \tag{2.57}$$

Using (2.57), the relations (2.47) and (2.48) finally become

$$\langle\tau_l(E)\rangle_{\text{av}} = \int_{-\infty}^{+\infty} f(\epsilon_l, t^+_l; E)\, d\epsilon_l\, dt^+_l \prod_{i=0}^{l-1} \left|\frac{t^+_i}{V(\epsilon_i, \epsilon_{i+1})}\right| \times \delta\left(t^+_i - \frac{V^2(\epsilon_i, \epsilon_{i+1}}{E - \epsilon_{i+1} - t^+_{i+1}}\right) P_c(\epsilon_i/\epsilon_{i+1})\, d\epsilon_i\, dt^+_i \quad , \tag{2.58}$$

and

$$\langle\tau^2_l(E)\rangle_{\text{av}} = \int_{-\infty}^{+\infty} f(\epsilon_l, t^+_l; E)\, d\epsilon_l\, dt^+_l \prod_{i=0}^{l-1} \left|\frac{t^+_i}{V(\epsilon_i, \epsilon_{i+1})}\right|^2 \times \delta\left(t^+_i - \frac{V^2(\epsilon_i, \epsilon_{i+1})}{E - \epsilon_{i+1} - t^+_{i+1}}\right) P_c(\epsilon_i/\epsilon_{i+1})\, d\epsilon_i dt^+_i \,. \tag{2.59}$$

The quantity of interest is $\langle\tau_l(E)\rangle_{\text{av}}$ as a function of l. It is obvious that $\langle\tau_0(E)\rangle_{\text{av}} = 1$. Also, the $l \to \infty$ behavior of $\langle\tau_l(E)\rangle_{\text{av}}$ is known from the analysis for $L_d(E)$, i.e., $\langle\tau_l(E)\rangle_{\text{av}} \to \exp(-l/L_d(E))$ as $l \to \infty$. Between $l = 0$ and $l = \infty$ there should be a region in which $\langle\tau_l(E)\rangle_{\text{av}}$ will be appreciable, of the order 1, before it starts decaying exponentially to zero with increasing l. We choose to define $L_e(E)$ as the effective number of sites l_c that satisfies the condition

$$\langle\tau_{l_c}(E)\rangle_{\text{av}} = 1 \;. \tag{2.60}$$

If condition (2.60) happens to be satisfied by more than one l_c, thus defining more than one $L_e(E)$, we choose to take their arithmetic average as an effective $L_e(E)$. Since $\langle\tau_l(E)\rangle_{\text{av}}$ is an average over configurations, condition (2.60) means that a large percentage of states have about equally large amplitudes at 0 and l_c, and therefore are appreciable inside an interval $(0, l_c)$, a justification for the definition [see (2.32), (2.34′), and relevant discussion there]

$$L_e(E) = l_c \tag{2.61}$$

[given, as with $L_d(E)$, as an effective number of sites]. $L_e(E)$ is, in general, not a sharply distributed quantity because its variance

$$\sigma^2_l(E) = \langle\tau^2_l(E)\rangle_{\text{av}} - \langle\tau_l(E)\rangle^2_{\text{av}}, \quad l \cong l_c \tag{2.62}$$

is in most cases much larger than zero. It is only $\lim \sigma^2_l(E)$ as $l \to \infty$ which vanishes.

In summary, three quantities of interest have been defined and given closed mathematical expressions. The formulas become simple and computationally easier in certain special cases that are solved numerically in Sec. III.

III. NUMERICAL SOLUTIONS

A. Numerical Method

The three quantities of interest given by (2.20), (2.45), and (2.58) and (2.60) are straightforward integrals over the probability distribution functions $P(\epsilon_i, \epsilon_{i+1})$ (which is the input function in our problem), $f(\epsilon_i, t_i; Z)$ [which is obtained from the solution of (2.12)], and a few others that are derived straightforwardly from those two. The main computational problem is to solve numerically the integral equation (2.12) for $f(\epsilon_i, t_i; Z)$.

For this, we first integrate over the variable ϵ_{i+1}, making use of the presence of the δ function. Thus we are left with an integral equation for the variable t_i, which is solved for different values of the variable ϵ_i as parameter. We then make a change of variables inside the integral, changing t_{i+1} to $A + B\tan\phi_{n+1}$, and so are left with an integral from $-\frac{1}{2}\pi$ to $\frac{1}{2}\pi$ instead of from $-\infty$ to $+\infty$. Next we go from a continuous to a discrete properly normalized kernel, subdividing the interval $(-\frac{1}{2}\pi, \frac{1}{2}\pi)$ into a suitable number of subdivisions. We are then left with a matrix equation of the form $K|x\rangle = |x\rangle$. This is solved by iteration, starting with an initial guess $|x_0\rangle \propto |1\rangle$ and iterating to the point $K|x_n\rangle = |x_{n+1}\rangle$, where $|x_n\rangle$, component by component, differs from $|x_{n+1}\rangle$ by less than a very small number (e.g., 10^{-5}). This iteration procedure should always converge to a solution, as Economou and Cohen proved in their work for a special case of our problem,[12] and indeed we have found it to converge. The over-all accuracy of this procedure can be very high, depending on the capabilities of the computer. We have limited ourselves to 2–4% over-all accuracy, good enough for our purposes.

B. Anderson's Distribution

In this section we give numerical results for $\rho(E)$ and $L_d(E)$ when the following conditions are satisfied: (i) Nearest neighbors on the chain are uncorrelated. (ii) The probability distribution $P(\epsilon_i)$ is continuous. (iii) The off-diagonal element is a constant $V > 0$.

Under these conditions, the formalism simplifies considerably. At first (2.8) becomes

$$t_i^{\pm}(Z)=\frac{V^2}{Z-\epsilon_{i\pm1}-t_{i\pm1}^{\pm}(Z)} \quad . \tag{3.1}$$

Also, because of condition (ii) we have

$$P_c(\epsilon_i/\epsilon_{i+1})=P_c(\epsilon_i/\epsilon_{i-1})=P(\epsilon_i). \tag{3.2}$$

From the above we see that in this case, $t_i^{\pm}$ is not correlated with ϵ_i, so that $f(\epsilon_i, t_i^{\pm}; Z)$ can be written

$$f(\epsilon_i, t_i^{\pm}; Z)=f(t_i; Z)\,P(\epsilon_i) \quad , \tag{3.3}$$

where $f(t_i^{\pm}; Z)$ coincides with the function defined by (2.41). Using (3.1)–(3.3), we simplify (2.12) as follows:

$$f(t_i; Z)=\int_{-\infty}^{+\infty}\delta\left(t_i-\frac{V^2}{Z-\epsilon_{i+1}-t_{i+1}}\right)$$

$$\times f(t_{i+1}; Z)\,P(\epsilon_{i+1})\,d\epsilon_{i+1}\,dt_{i+1} \quad . \tag{3.4}$$

Performing the integration over the δ function, we obtain

$$f(t_i; Z)=(V^2/t_i^2)\int_{-\infty}^{+\infty} P(Z-t_{i+1}-(V^2/t_i))$$

$$\times f(t_{i+1}; Z)\,d\,t_{i+1} \quad . \tag{3.5}$$

The above relation is identical to the one derived by Economou and Cohen[12] under essentially the same assumptions as above. Here too, we can use $f(t_i^{\pm};\ Z)$ to calculate quantities of interest. For $\rho(E)$ we start from (2.20) and we use (3.3) to write

$$\rho(E)=\int_{-\infty}^{+\infty}\delta(E-\epsilon_i-t_i^{+}-t_i^{-})f(t_i^{+}; E)$$

$$\times f(t_i^{-}; E)\,P(\epsilon_i)\,dt_i^{+}\,dt_i^{-} \quad . \tag{3.6}$$

Performing an integration over ϵ_i, we get

$$\rho(E)=\int_{-\infty}^{+\infty} P(E-t_i^{+}-t_i^{-})f(t_i^{+}; E)f(t_i^{-}; E)\,dt_i^{+}\,dt_i^{-} \quad , \tag{3.7}$$

and changing the variable t_i^{+} to V^2/x and using (3.5), we easily obtain

$$\rho(E)=\int_{-\infty}^{+\infty} f(x; E)f((V^2/x); E)\,dx \quad . \tag{3.8}$$

Finally $L_d(E)$, given by (2.45), reduces to[15]

$$L_d(E)=-\left[\int_{-\infty}^{+\infty}\ln|t|f(t; E)\,dt-\ln V\right]^{-1} \quad . \tag{3.9}$$

At this point we assume that $P(\epsilon_i)$ is a rectangular distribution (the so-called Anderson's distribution) given by

$$P(\epsilon)=\tfrac{1}{2}(\alpha V)^{-1} \quad \text{for } |\epsilon/V|\le\alpha$$

$$P(\epsilon)=0 \quad \text{for } |\epsilon/V|>\alpha \quad , \tag{3.10}$$

where α characterizes the degree of randomness in the system. At the limit $\alpha\to0$, the problem reduces to the periodic one. We study two cases, one with small α ($\alpha=0.4$) (Fig. 2) and one with large α ($\alpha=4.0$) (Fig. 3). In both cases, the standard features are present—like the broadening of the band and the decrease of $L_d(E)$ towards the band edges. In the present case, the rigorous band edges (Lifshitz limits) are at $E/V=\pm2.4$ (Fig. 2) and at $E/V=\pm6.0$ (Fig. 3), as given by

$$|E/V|=2+\alpha \quad . \tag{3.11}$$

It is worthwhile to note that in both cases the density of states is practically zero before the rigorous band edges—a common feature in disordered systems—which simply means that the density of states in the deep tails is negligibly small.

Also, it is very important to notice the agreement of the behavior of the present system with the predictions of the Mott-CFO model for its three-dimensional analog.[16] According to the Mott-CFO model, there are two critical energies, called mobility edges, that separate the region of extended states (in the middle of the band) from the region of localized states (at the band edges) (Fig. 4). Moreover, the region of extended states narrows with increasing randomness and vanishes at a certain value of randomness (the Anderson transition), making all states in the band localized. In one-dimensional systems, of course, all states are localized.[7] However, one can distinguish qualitatively between two kinds of localization: one very strong [$L_d(E)$ of the order of few sites], corresponding to three-dimensional localized states, and one very weak [$L_d(E)$ containing many sites], corresponding to three-dimensional extended states.

Then one clearly sees in the case $\alpha=0.4$ (Fig. 2) such a region of "pseudoextended states" in the middle of the band and a smooth transition around two "pseudomobility edges," close to the band edges, to the region of "localized states." This transition will gradually become abrupt as we approach the periodic case. Also, one sees in the case $\alpha=4.0$ (Fig. 3) that all states are "localized," which means that at that high randomness the system has

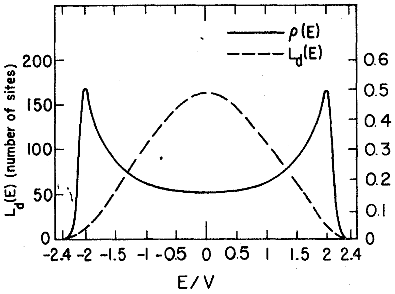

FIG. 2. Density of states $\rho(E)$ and localization length $L_d(E)$ in number of sites vs energy/V, for a rectangular distribution of width $2\alpha=0.8$.

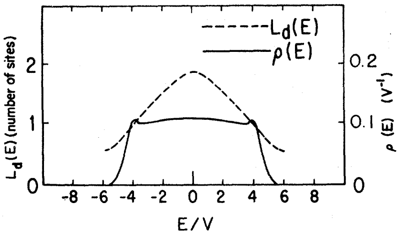

FIG. 3. Density of states $\rho(E)$ and localization length $L_d(E)$ in number of sites vs energy/V, for a rectangular distribution of width $2\alpha = 0.8$.

undergone a "pseudo-Anderson-transition." Similar remarks were made by Economou and Cohen[11] earlier, but on the basis of momentum matrix elements, a less satisfactory basis than the present calculation of localization length.

A final remark about the results is that as α increases, the shape of the probability distribution tends to dominate the shape of the density of states. This is quite clearly seen in the case $\alpha = 4.0$, and is easily understood because $\alpha \to \infty$ should be equivalent to $V \to 0$.

C. Uncorrected Binary Alloy

In this section we give numerical results for $\rho(E)$ and $L_d(E)$ when the following conditions are satisfied: (i) Nearest neighbors on the chain are uncorrelated. (ii) The probability distribution $P(\epsilon_i)$ is a binary-alloy distribution, i.e., of the form

$$P(\epsilon) = X_A\,\delta(\epsilon - \epsilon_A) + X_B\,\delta(\epsilon - \epsilon_B) \;, \tag{3.12}$$

$$X_A + X_B = 1 \;, \tag{3.13}$$

where A and B are the two types of atoms in the alloy. (iii) The off-diagonal element is a constant $V > 0$.

The above assumptions are the same as in Sec. III B, except for $P(\epsilon_i)$. The formulas for this case are trivially obtained from those of Sec. III B. Using (3.5) and (3.12) it follows that

$$f(t_i; Z) = \frac{X_A V^2}{t_i^2}\, f(Z - \epsilon_A - V^2/t; Z) + \frac{X_B V^2}{t_i^2}\, f(Z - \epsilon_B - V^2/t_i; Z) \;. \tag{3.14}$$

The quantities $\rho(E)$ and $L_d(E)$ are given by (3.8) and (3.9), respectively. To follow the usual convention for alloys, we introduce the quantity

$$\delta = (\epsilon_B - \epsilon_A)/V \;, \tag{3.15}$$

which represents the relative scattering strength and, together with the concentration X_A, constitutes a measure of the randomness in the system.

For numerical convenience we use δ as our parameter, and we put

$$\epsilon_A = -\tfrac{1}{2}\delta V, \quad \epsilon_B = \tfrac{1}{2}\delta V \;. \tag{3.16}$$

Figure 5 presents the results for a 10-at.% concentration of impurities B ($X_B = 0.1$) and $\delta = 1.0$.

The standard features of a binary alloy are exhibited. The first is the existence of an impurity subband well separated, at this value of δ, from the band of the host atom A. The second is the existence of a marked structure in the density of states $\rho(E)$ and the localization length $L_d(E)$, apparent in both the host and impurity subbands. The structure in the impurity subband as mentioned in the Introduction was first demonstrated by Dean[17] with his Monte Carlo calculations for the vibrational spectrum. Subsequent work[2,18] has confirmed the existence of this marked structure of the spectrum and has interpreted it as owing to

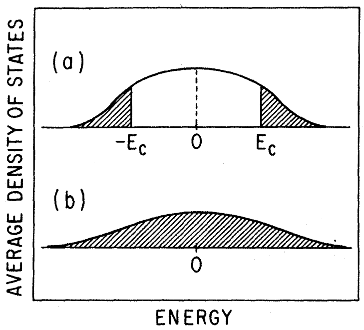

FIG. 4. Sketch of the average density of states vs energy for two different degrees of randomness. In (a), according to the Mott-CFO model for a small degree of randomness, the mobility edges E_c separate regions of localized states (shaded) from those of extended states. In (b), all states are localized for randomness larger than a critical value.

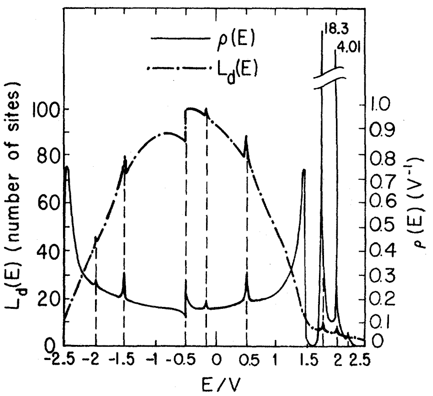

FIG. 5. Density of states $\rho(E)$ and localization length $L_d(E)$ in number of sites vs energy/V, for an uncorrelated binary alloy with $X_B = 0.1$ and $\delta = 1.0$.

impurity atom clusters. The present results not only agree, in the density of states, with those mentioned above, but they also show the existence of structure in the host band (not previously identified), as well as a similar structure in the localization length. Moreover the method presented here shows that these peaks, in certain cases, are much sharper than has been previously anticipated. This is due to the fact that this method computes the density of states directly and not its integral over energy, thus being more accurate when close to sharp peaks. The interpretation of the structure of the impurity subband is carried out following Agacy and Borland,[18] and the strong peaks around the values $E/V=1.763$, 2, and 2.1667 are attributed to states bound around clusters of the form B, BB, and BBB, respectively.

The structure inside the host cannot arise from states bound to impurity clusters embedded in an environment of host atoms A. A completely different physical origin is indicated. We studied the reflection coefficients of different $mA\,nB$ clusters, replacing A atoms in an A crystal, as functions of energy. Figure 6 shows the behavior of the reflection coefficients for the clusters BB, BAB, and BBB. The reflection coefficient for each of those clusters becomes zero at least once inside the host band. This fact, combined with the qualitative argument saying that localization is caused by successive incoherent reflections on impurities, explains why at those energies we should expect, and indeed we find (Fig. 5), a localization length larger than at neighboring energies, i.e., a peak in the localization length.

An extensive study of the reflection coefficient for several classes of clusters revealed that for each energy $E/V=-1.5$, -0.5, and 0.5, there is a different infinite set of clusters whose reflection coefficient vanishes. These are the $B(A+3nA)B$, $BB(2nA)B$, and $B(3nA)B$, $n=0, 1, 2, \ldots$, respectively, for $E/V=-1.5$, -0.5, and 0.5. This explains why at those energies the peaks are much stronger than at $E/V=-1.9812$, or -0.1889, where the $BAAB$ cluster is the only relatively probable configuration with vanishing reflection coefficient.

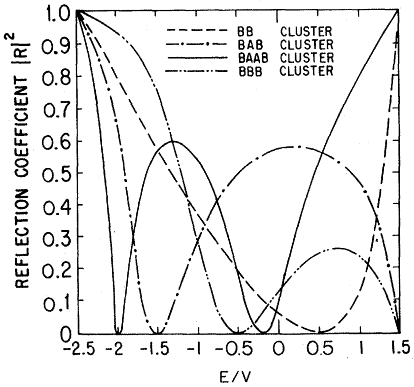

FIG. 6. Reflection coefficient $|R|^2$ vs energy/V for different clusters. The energies lie in the host-atom band of the binary alloy.

The final step needed to explain fully the structure in both $\rho(E)$ and $L_d(E)$ as well as the fact that the peaks appear at exactly the same energies in both $\rho(E)$ and $L_d(E)$ is the following: Cohen and Sak[14] have argued that the density of states at some energy is roughly proportional to the "available volume" of the corresponding wave functions, as they call it. They have successfully used this argument to explain the appearance of a mobility gap in certain metallic alloys (we will return to that in greatest detail in Sec. III E). According to this argument, we should find a peak in the density of states at every place in the spectrum where there is a peak in the degress of localization of the states there, and vice versa. The results we have obtained are in exact agreement with this argument; they are clearly understood through it and confirm it at the same time.

There is one detail in the behavior of $\rho(E)$ and $L_d(E)$ that cannot be explained through the simple picture of nonreflecting special clusters. This is a discontinuity in the localization length and, at the same time, in the density of states, which occurs exactly at the middle of the host band ($E/V=-0.5$). For its explanation, one should make an "average-reflection-coefficient" study, because the effect is due to multiple contributions from a whole class of special clusters. One calculates the average reflection coefficient $\langle |R(E)|^2\rangle$, i.e., the reflection coefficient that is obtained as the sum of the reflection coefficients of each special cluster weighted with the probability of having that cluster. The result of importance is

$$\frac{d}{dE}\langle |R(E)|^2\rangle=-\infty \quad \text{for } E/V=-0.5$$

This result is obtained by expressing $(d/dE)\langle |R(E)|^2\rangle$ in the fashion described above. We find that all members of the group $B(nA)BB$ have vanishing reflection coefficients at $E=-0.5V$, so we neglect that group. We consider the quantity

$$\Delta R_n=\frac{d}{dE}\left[|R(E)|^2_{B2nAB}+0.9\,|R(E)|^2_{B(2n+1)AB}\right] \tag{3.17}$$

for the remaining two important groups of clusters (groups with more than three B's are very unprobable). At $E=-0.5V$, ΔR_n has a negative value decreasing rapidly with increasing n (e.g., -0.4 and -0.36 for $n=0, 1$). Expressing $\langle |R(E)|^2\rangle$ in the fashion described above, we have [using

(3.17)]

$$\frac{d}{dE}\langle\,|R(E)|^2\rangle = 0.1^2 \sum_{n=0}^{\infty} 0.9^{2n}\,\Delta R_n . \qquad (3.18)$$

Observing that ΔR_n is negative and decreases rapidly with n, which means for $\Delta R_{n+1}/\Delta R_n \gg 1$, we obtain $(0.9)^2\,\Delta R_{n+1}/\Delta R_n > 1$. Consequently each term of our series is larger in absolute value than that of a diverging geometric series. Equation (3.18) therefore diverges at the center of the host band. This behavior of $\langle\,|R(E)|^2\rangle$ around $E/V = -0.5$ is shown in Fig. 7, and tells us that we should expect the reciprocal behavior for the localization length and, by the "available-volume" argument, for the density of states as well. This, we believe, completes the explanation.

D. Behavior of $L_e(E)$ for Binary Alloys

In this section numerical values of $L_e(E)$ are presented for the first time. The calculations are performed for the case of the uncorrelated binary alloy (see Sec. III C). Under the assumptions (i), (ii), and (iii) introduced in the beginning of Sec. III B, formulas (2.58) and (2.59) for $\langle\tau_l(E)\rangle_{av}$ and $\langle\tau_l^2(E)\rangle_{av}$, respectively, simplify considerably. In that case, V is a constant, independent of the ϵ's; therefore the integrations over the ϵ's can easily be performed in (2.58) and (2.59). Making use of (3.2) and (2.40), as well as (3.5), Eqs. (2.58) and (2.59) finally become

$$\langle\tau_l(E)\rangle_{av} = \int_{-\infty}^{+\infty} f(t_{l-1}^{+};\; E)\left|\frac{t_{l-1}^{+}}{V}\right| dt_{l-1}^{+}$$

$$\times\prod_{1=0}^{l-2}\left|\frac{t_i^{+}}{V}\right|\frac{V^2}{t_i^{+2}}\;P(E - t_{i+1}^{+} - V^2/t_i^{+})\,dt_i^{+}, \qquad (3.19)$$

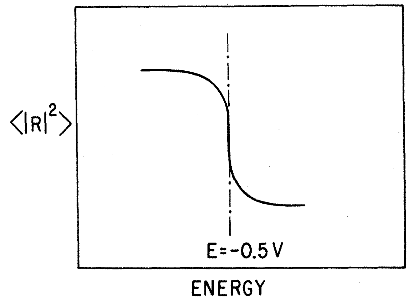

FIG. 7. Behavior of the average reflection coefficient $\langle|R|^2\rangle$ for energies around the anomaly at $-0.5V$. $L_d(E)$ should behave as $\langle|R|^2\rangle^{-1}$.

$$\langle\tau_l^2(E)\rangle_{av} = \int_{-\infty}^{+\infty} f(t_{l-1}^{+};\; E)\left|\frac{t_{l-1}^{+}}{V}\right| dt_{l-1}^{+}$$

$$\times\prod_{i=0}^{l-2}\left|\frac{t_i^{+}}{V}\right|^2 \frac{V^2}{t_j^{+2}}\;P(E - t_{i+1}^{+}\;\; V^2/t_i^{+})\,dt_i^{+} . \qquad (3.20)$$

We observe that a simple algorithm permits the calculation of successive $\langle\tau_l\rangle_{av}$'s or $\langle\tau_l^2\rangle_{av}$'s as well as any higher moment of the distribution. One can easily check and see that the following relations are equivalent to (3.19) and (3.20):

$$A_l^n \equiv \int_{-\infty}^{+\infty} |\,t/V\,|^n F_l^n(t)\,dt, \qquad (3.21)$$

$$F_l{}^n(t) \equiv (V^2/t^2)\int_{-\infty}^{+\infty} |\,t'/v\,|^n\, P(E - t' - V^2/t)$$

$$\times F_{l=1}^n(t')\,dt' , \qquad (3.22)$$

$$F_1^n(t) \equiv f(t;\; E)\,, \qquad (3.23)$$

where A^n stands for $\langle\tau_l^n(E)\rangle_{av}$. In the case of a binary alloy, $P(\epsilon)$ is given by (3.12) and (3.13), so that (3.22) becomes simply

$$F_l^n(t) = \frac{X_A V^2}{t^2}\left|\frac{E - \epsilon_A - (V^2/t)}{V}\right|^n F_{l-1}^n(E - \epsilon_A - (V^2/t)) + \frac{X_B V^2}{t^2}\left|\frac{E - \epsilon_B - (V^2/t')}{V}\right|^n F_{l-1}^n(E - \epsilon_B - (V^2/t)). \qquad (3.24)$$

Values for $\langle\tau_l(E)\rangle_{av}$ and $\langle\tau_l^2(E)\rangle_{av}/\langle\tau_l(E)\rangle_{av}^2$ are presented in Fig. 8 for $\delta = 1$, $X_B = 0.15$, and $E = -0.4V$. According to the definition for $L_e(E)$ given by (2.60) and (2.61), we obtain in this particular case a value $L_e(-0.4V) = 167$ sites.

Three important characteristics appear in Fig. 8. The first is the high value of $\langle\tau_l^2(E)\rangle_{av}/\langle\tau_l(E)\rangle_{av}^2$, of the order of 500, which proves that $\tau_l(E)$ is broadly distributed for small l's. Equivalently, this means that l_e, the length over which the amplitude remains appreciable, is also a broadly distributed quantity. Therefore our definition of $L_e(E)$, which relates only indirectly to the average of l_e over all configurations, may give only part of the information needed for the calculation of observable properties, like conductivity. The second characteristic is the presence of oscillating values of the averages in the region of small l's. These oscillations have the wavelength of a Bloch wave corresponding to the value of E used, and they are dumped to zero as l increases. The presence of these oscillations creates some ambiguity in the value of L_e in certain cases of small L_e, by passing through 1 more than once inside a narrow interval of l's. The third characteristic of the behavior of $L_e(E)$ is the exponential-like decay of the average toward zero after the initial region of oscillation. The rate of decay is not constant. For $\langle\tau_l(E)\rangle_{av}$ we find, in all cases, a rate of decay two times slower

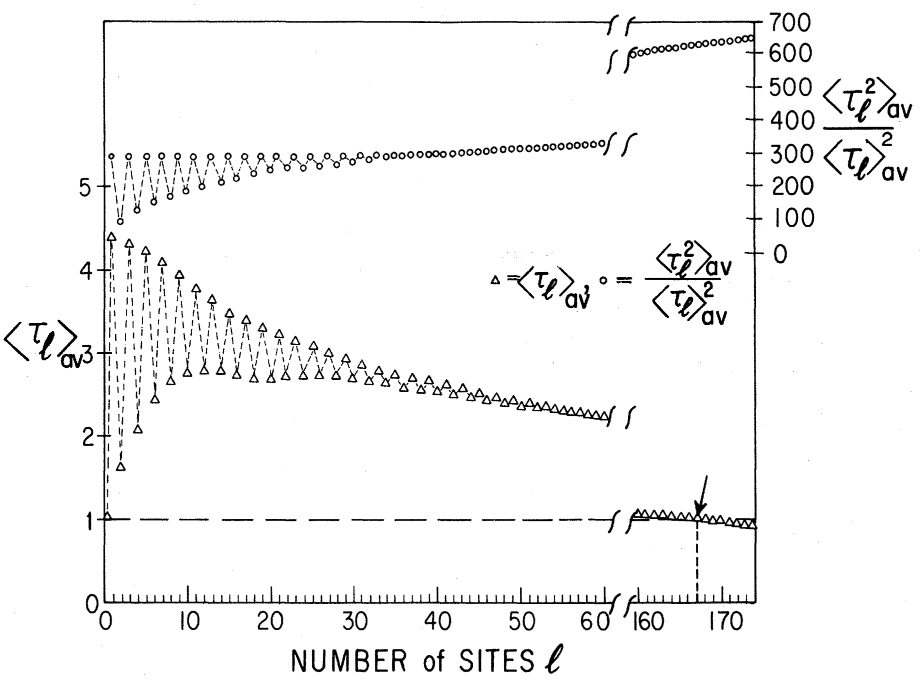

FIG. 8. Values for $\langle\tau_l\rangle_{av}$ and $\langle\tau_l^2\rangle_{av}/\langle\tau_l\rangle_{av}^2$ vs number of sites l for an uncorrelated binary alloy with $X_B=0.15$, $\delta=1.0$, and $E=-0.4\ V$. According to the definition (2.60) and (2.61), $L_e(-0.4V)$ = 167 sites.

than the one described by the corresponding asymptotic decay length $L_d(E)$.[19] This can be qualitatively understood, since the decay of $\langle\tau_l(E)\rangle_{av}$ is expected to be intermediate between that of states decaying as $e-l/L_d(E)$ and of states remaining roughly constant in that region, e.g., a decay of the form $e-l/2L_d(E)$, taking a crude average between 0 and $-1/L_d(E)$. The decay becomes faster as l increases and presumably goes to $-l/L_d(E)$ as $l\to\infty$.

This last property of $\langle\tau_l(E)\rangle_{av}$ permits the approximate calculation of $L_e(E)$ without actually having to perform the calculation of all successive $\langle\tau_l\rangle_{av}$'s to the point $\langle\tau_l\rangle_{av}=1$. Figure 8, by itself, suggests the method. The idea is that even in the region of oscillating values, $\langle\tau_l\rangle_{av}$ decays on the average. Therefore one needs, say, the average value A_{10} of the first ten $\langle\tau_l\rangle_{av}$'s and, of course, the decay length $L_d(E)$ given by (3.9). Then one says that

$$\langle\tau_l\rangle_{av}=A_{10}\exp\left(-\frac{l-5}{2L_d(E)}\right) \tag{3.25}$$

[we subtract 5 in order to incorporate the fact that with the above calculation, the decay described by (3.25) starts in between 0 and 10]. Formula (3.25) is combined with (2.60) and (2.61) to yield

$$L_e(E)=5+2L_d(E)\ln A_{10}. \tag{3.26}$$

In all cases checked, the above formula is only a few percentage points off the actual value. It even works in those cases where the presence of $\langle\tau_l\rangle_{av}$'s oscillating around 1 creats some ambiguity about the value of $L_e(E)$.

Extensive study of $L_e(E)$ has revealed another important property, shown in Fig. 9. In that figure, $L_e(E)$ is plotted versus $L_d(E)$ for a fairly random selection of parameters (energy/V, concentration X_B of impurities B, and scattering strength δ). Remarkably enough, the points all lie on a straight line passing approximately through zero for a wide range of $L_d(E)$. It is only at the limit $L_d\to 0$ that we find deviations from the above behavior. At that limit, the values of $L_e(E)$ depend on the parameters directly and not simply through

	A	B	C	D	E	F	G	H	I
δ	1.0	1.0	1.94	1.4	1.94	5.0	5.0	5.0	5.0
E/V	-0.4	-0.4	-0.85	-0.6	-0.85	-2.21	-0.6	-0.52	-0.6
X_B	0.1	0.15	0.05	0.1	0.1	0.05	0.05	0.05	0.1

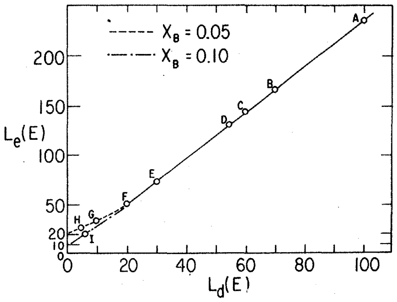

FIG. 9. $L_e(E)$ vs $L_d(E)$ (both in number of sites), for a fairly random selection of parameters δ, E/V, and X_B. The parameters for the different points $A, B, C\ldots$ are given by the associated table. Note the agreement of the behavior at $L_d\to 0$, with (3.27).

the dependence of $L_d(E)$ on them.[13] This is to be expected; it is the physically correct behavior and justifies our definition for $L_e(E)$ at the same time. One can see that by considering a binary alloy with high δ. At the limit $\delta\to\infty$, it is obvious that $L_d(E)\to 0$ and that states are localized between neighboring impurities, which at that limit act as infinitely high potential barriers. The average extent of a state is obviously the average impurity separation which goes as X_B^{-1} independently of the energy. Therefore

$$\lim_{\delta\to\infty} L_e(E) = X_B^{-1}. \qquad (3.27)$$

We have examined this limit by fixing the concentration and increasing δ. We used the case $X_B = 0.15$ in order to fix the truncation for the present calculation. The behavior of our $L_e(E)$ is in agreement with (3.27). Because of computational problems, we cannot go beyond $\delta = 5$ or below $L_d = 5$; but to that extent we obtain the correct behavior for $X_B = 0.05$ and 0.10, where we approach $L_e = 20$ and 10, respectively, as $L_d\to 0$.

In conclusion, there seems to be a simple proportionality between the two localization lengths: For binary alloys, we obtain $L_e(E) = 2.35 L_d(E)$ outside regions of strong localization. This proportionality breaks down when strong localization is present; in that limit, simple physical arguments are confirmed through our calculation.

E. Metal-Nonmetal Transition Induced by Randomness

As pointed out in Sec. III C, special configurations of atoms are responsible for many features of the electronic structure of a binary alloy. Consequently, by creating or destroying such special configurations or clusters, as we call them, one can influence certain physical properties of an alloy. Experimentally it is found[20] that some metallic alloys, like liquid Te-Tl and amorphous Mg-Bi, exhibit a strong dependence of their transport properties on composition. Specifically, their conductivity goes through a sharp minimum in a concentration range centered around a hypothetical compound composition Tl_2Te and Mg_2Bi_3, respectively. A successful explanation of the above behavior has been given through the special cluster picture.[14,21] The idea is that compound formation at these concentrations drastically affects the probability of existence of different configurations, favoring the ones that form compound clusters. The result of this short-range order[22] is a semiconductorlike density of states, with impurity states inside a gap that separates a valence from a conduction band. Cohen and Sak[14] employed this idea to present a semiclassical treatment of the transport properties of those alloys. For an electron with energy lying inside that semiconducting gap, the compound clusters were treated as excluded volumes, and the whole problem was thus reduced to a semiclassical percolation one. The main result of their analysis is that the "available volume" for a state inside the semiconducting gap is small (passing through a minimum at the compound composition) and as a result of it the state can be localized. In the same picture, one sees how the decrease of the available volume is by itself responsible for the decrease of the density of states, creating what we have called the semiconducting gap. Therefore their analysis predicts not a real gap, but rather a mobility gap or Mott pseudogap (i.e., an energy interval in which all states are localized), that appears for concentrations around the compound concentration and is responsible for the nonmetallic behavior of the system at those concentrations. The Cohen–Sak treatment of the problem seems to explain the experimental results. Nevertheless, a first-principles justification of their basic assumptions is desirable because of the potentially broad applicability of similar models to related problems, and to reveal any features wiped out by the semiclassical treatment. Our model can be applied to solve the corresponding one-dimensional problem. The results fully justify their analysis.

We present the results obtained under the following assumptions: (i) The probability distribution $P(\epsilon_i)$ is that of a binary alloy (see Sec. III C), and (ii) nearest neighbors on the chain are correlated. In the case of a binary alloy, the correlation between nearest neighbors is fully described by a single parameter. One can see this by writing (2.10) in the form

$$P(\epsilon_i,\ \epsilon_j) = X_A\,\delta(\epsilon_i - \epsilon_A)\,P_c(\epsilon_j/\epsilon_A) + X_B\,\delta(\epsilon_i - \epsilon_B)\,P_c(\epsilon_j/\epsilon_B), \qquad (3.28)$$

$$P_c(\epsilon_j/\epsilon_A) = P_{AA}\,\delta(\epsilon_j - \epsilon_A) + P_{BA}\,\delta(\epsilon_j - \epsilon_B), \qquad (3.29)$$

$$P_c(\epsilon_j/\epsilon_B) = P_{AB}\,\delta(\epsilon_j - \epsilon_A) + P_{BB}\,\delta(\epsilon_j - \epsilon_B), \qquad (3.30)$$

where the parameter P_{AB}, for example, means the probability of having a site of type A when its nearest neighbor is a site of type B. The four parameters P_{AA}, P_{AB}, P_{BB}, and P_{BB} are not independent. They obey four relations:

$$P_{AA} + P_{BA} = 1, \qquad (3.31)$$

$$P_{AB} + P_{BB} = 1; \qquad (3.32)$$

$$X_A P_{AA} + X_B P_{AB} = X_A, \qquad (3.33)$$

$$X_A P_{BA} + X_B P_{BB} = X_B. \qquad (3.34)$$

These relations hold because according to (2.9) the form of $P(\epsilon)$ must be the same, given by (3.12), whether we integrate (3.28) over ϵ_i or over ϵ_j. One sees easily that only three of those are linearly independent, because X_A and X_B obey (3.13).

Therefore, out of the four parameters that describe the correlation between nearest neighbors, only one is independent.

We now rewrite (2.12) in a form more suitable for numerical calculations. First, we observe that in the present case, the off-diagonal element $V(\epsilon_i, \epsilon_j)$ reduces to three constants V_{AA}, V_{BB}, and $V_{AB}=V_{BA}$ [because of (2.2)]. We further write

$$\begin{aligned} f(\epsilon, t; Z) &= P(\epsilon) f_c(t/\epsilon; Z) \\ &= X_A f_c(t/\epsilon_A; Z)\, \delta(\epsilon-\epsilon_A) \\ &\quad + X_B f_c(t/\epsilon_B; Z)\, \delta(\epsilon-\epsilon_B). \end{aligned} \tag{3.35}$$

For simplicity of notation, we define

$$\begin{aligned} f_c(t/\epsilon_A; Z) &\equiv f_A(t; Z), \\ f_c(t/\epsilon_B; Z) &\equiv f_B(t; Z), \end{aligned} \tag{3.36}$$

and

$$\begin{aligned} f(\epsilon, t; Z) &= X_A f_A(t; Z)\, \delta(\epsilon-\epsilon_A) \\ &\quad + X_B f_B(t; Z)\, \delta(\epsilon-\epsilon_B). \end{aligned} \tag{3.37}$$

We also write

$$\begin{aligned} P_c(\epsilon_i/\epsilon_{i+1}) &= P(\epsilon_A/\epsilon_{i+1})\, \delta(\epsilon_i-\epsilon_A) \\ &\quad + P(\epsilon_B/\epsilon_{i+1})\, \delta(\epsilon_i-\epsilon_B), \end{aligned} \tag{3.38}$$

where the coefficients $P(\epsilon_i/\epsilon_{i+1})$ are the previously introduced constants $P_{AA}, \ldots, P_{BB}$. We use (3.37) and (3.38) in (2.12), and then we perform the integrations over ϵ_{i+1} on its right-hand side. Next we integrate both sides of (2.12) over ϵ_i, first around ϵ_A and then around ϵ_B. We thus obtain a system of two equations:

$$\begin{aligned} X_A f_A(t_i; Z) &= \int_{-\infty}^{+\infty} \left[X_A P_{AA}\, \delta\!\left(t_i - \frac{V_{AA}^2}{E-\epsilon_A-t_{i+1}}\right) f_A(t_{i+1}; Z) + X_B P_{AB}\, \delta\!\left(t_i - \frac{V_{AB}^2}{E-\epsilon_B-t_{i+1}}\right) f_B(t_{i+1}; Z) \right] dt_{i+1}, \\ X_B f_B(t_i; Z) &= \int_{-\infty}^{+\infty} \left[X_B P_{BA}\, \delta\!\left(t_i - \frac{V_{BA}^2}{E-\epsilon_A-t_{i+1}}\right) f_A(t_{i+1}; Z) + X_B P_{BB}\, \delta\!\left(t_i - \frac{V_{BB}^2}{E-\epsilon_B-t_{i+1}}\right) f_B(t_{i+1}; Z) \right] dt_{i+1}. \end{aligned} \tag{3.39}$$

Integrating over t_{i+1}, we finally obtain

$$\begin{aligned} X_A f_A(t; Z) &= X_A P_{AA} \frac{V_{AA}^2}{t^2} f_A(E-\epsilon_A-(V_{AA}^2/t); Z) + X_B P_{AB} \frac{V_{AB}^2}{t^2} f_B(E-\epsilon_B(-V_{AB}^2/t); Z), \\ X_B f_B(t; Z) &= X_A P_{BA} \frac{V_{BA}^2}{t^2} f_A(E-\epsilon_A-(V_{BA}^2/t); Z) + X_B P_{BB} \frac{V_{BB}^2}{t^2} f_B(E-\epsilon_B(-V_{BB}^2/t); Z). \end{aligned} \tag{3.40}$$

The density of states $\rho(E)$ is given by (2.15′) combined with (2.16) and (2.17). Making use of (3.36) and (3.37) and integrating out the δ functions, we obtain

$$\begin{aligned} \rho(E) &= X_A \int_{-\infty}^{+\infty} f_A(t; E) f_A(E-\epsilon_A-t; E)\, dt \\ &\quad + X_B \int_{-\infty}^{+\infty} f_B(t; E) f_B(E-\epsilon_B-t; E)\, dt. \end{aligned} \tag{3.41}$$

The decay length $L_d(E)$ is given by (2.45). Using (2.41) and (3.37) for $f(t; E)$, and the expression (3.28) for $P(\epsilon', \epsilon'')$, we obtain

$$\begin{aligned} L_d(E) = -\Big[&\int_{-\infty}^{+\infty} \ln|t| [X_A f_A(t; E) + X_B f_B(t; E)]\, dt \\ &- X_A (P_{AA} \ln|V_{AA}| + P_{BA} \ln|V_{BA}|) \\ &- X_B (P_{AB} \ln|V_{AB}| P_{BB} \ln|V_{BB}|) \Big]^{-1}. \end{aligned} \tag{3.42}$$

The degree of correlation is given by parameter P_{AB}. When $P_{AB}=X_A$, we obviously have the completely uncorrelated case. When $P_{AB}>X_A$, we favor the formation of AB clusters, i.e., compound formation in the alloy. When $P_{AB}=1$ (we assume $X_A \geq X_B$), we have either $(AB)^n$ clusters embeded in a matrix of A (when $X_A > X_B$), or a periodic sequence $ABABAB\ldots$ (when $X_A = X_B$). We assume one electron per atom, i.e., a half-filled band. If $P_{AB}=1$ (full correlation), at $X_A=X_B=0.5$ we have an $ABABAB\ldots$ crystal. We know from elementary analysis that the density of states splits into two subbands of extended (Bloch type) states separated by a gap of width δV (from $E=-\frac{1}{2}\delta V$ to $E=\frac{1}{2}\delta V$). Since we assumed a half-filled band, the system is an insulator. As we change the concentration to $X_A>0.5$, we immediately introduce strongly localized impurity states in the gap, which is the one-dimensional analog of the mobility gap mentioned before. On the other hand, if $P_{AB}=X_A$ (no correlation), then for concentrations close to 0.5 the density of states in the same region of energies as before is fairly flat and the localization length L_d is fairly long, the one-dimensional analog of metallic behavior. Through our calculations, we can display the continuous change of character of our system by changing the correlation parameter P_{AB} from X_A to 1. We solve numerically the case $X_A=0.55$. For simplicity we take $V_{AA}=V_{AB}=V_{BA}=V_{BB}>0$. The results are shown in Fig. 10. One indeed sees a transition from metallic behavior for $P_{AB}=0.55$ (flat density of states around $E=0$, i.e., where the Fermi energy lies, and fairly extended states) to insulating behavior for $P_{AB}=1.0$ (low density of states inside the gap and strong localiza-

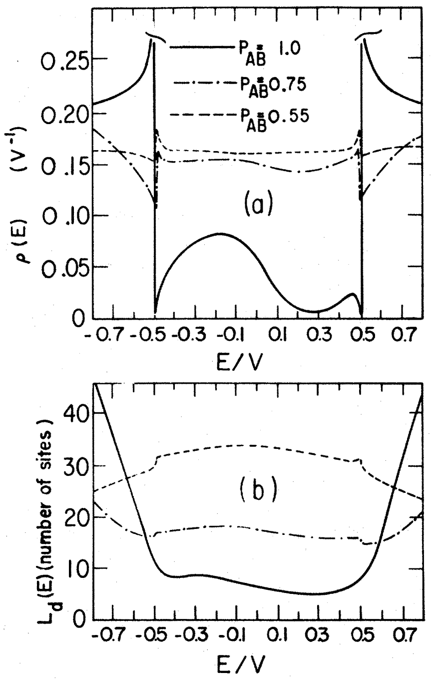

FIG. 10. Density of states $\rho(E)$, (a), and localization length $L_d(E)$ in number of sites, (b), vs energy/V for a correlated binary alloy ($X_A = 0.55$, $\delta = 1$). Increasing the short-range order (parameter P_{AB}) from complete absence ($P_{AB} = 0.55$) to complete AB compound formation ($P_{AB} = 1.0$), the behavior changes from "metallic" to "insulating." Dashed, solid, and dash-dot lines in (b) same as in (a).

tion—a mobility gap). It is interesting to note the gradual formation of the peaks as we increase P_{AB} from 0.55 to 1.0. Those peaks become very pronounced at $P_{AB} = 1.0$, approaching the square-root singularity of the periodic case, at $E/V = -0.5$ and 0.5.

In conclusion, we have demonstrated the correctness of the idea of the central role of special clusters [in this case the (AB) clusters] in the randomness-induced metal-nonmetal transition.

IV. DISCUSSION

Let us now discuss the results presented above and other cases of interest that could be treated with the present formalism as it stands, as well as indicate possible extensions of the theory in order to deal with other important physical problems. The first point that deserves some attention is the resemblance of certain aspects of the behavior of these systems to the behavior of their three-dimensional analogs. The agreement of the results with the predictions of the Mott-CFO model (Fig. 4) is apparent in the cases of Anderson's distribution (Fig. 2) of the uncorrelated binary alloy (Fig. 5, note especially the presence of a pseudo-Anderson-transition in the impurity subband), and of the mobility gap studied in Sec. III E. The standard impurity subband, present in many real binary-alloy systems, is also present here (see Sec. III C). Finally, the role of special clusters in affecting important properties of the system, and idea proposed to explain the electronic behavior in certain real alloys,[14,21] is also presented here. The second point that deserves some attention is the existence of real random systems with one-dimensional character. In all cases in which the tight-binding approximation is good, those systems can be analyzed and their randomness-dependent properties fully studied with our formalism. An example is the case of the N-methylphenazinium tetracyanoquinodimethane (NMP-TCNQ) salt.[3] A simple analysis shows that the tight-binding single-site potential has a random component with Gaussian distribution and Gaussian correlation with neighboring site. The general formulas of Sec. II would then give the expressions for $\rho(E)$, $L_d(E)$, and $L_e(E)$, although computationally it is harder than the cases calculated here. The third point is the inclusion of off-diagonal randomness in the calculation. As seen in the formulas of Sec. II, the formalism can treat a certain kind of off-diagonal randomness. Thus the off-diagonal randomness in the binary alloy and the correlated binary alloy case can be studied starting from formulas of Sec. III E and with only a minor computational complication. The fourth point is the application of the formalism to one-dimensional phonon systems. A simple change of variables[12] transforms the phonon Hamiltonian to that used in our model [Eq. (2.3)]. Therefore one can easily translate the results obtained for the electronic cases to solve the corresponding phonon problems. Finally I would like to point out the possibility that many-body effects can be treated, in the presence of randomness, with a modification of the present formalism. The formalism seems to be a covenient starting point for the study of the metal-insulator transition in the disordered Hubbard model using the method of Gaussian random fields to treat the electron-electron interaction.

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