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# Study of localization in Anderson's model for random lattices*

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Various approaches to the problem of localization within Anderson's model for random lattices are examined. A new approximate criterion based on the Economou-Cohen $L(E)$ approximation is developed. Results are presented and compared for several real lattices and for various probability distributions of the site energies. The new criterion is shown to be remarkably successful.

## I. INTRODUCTION

Any advancement to the theory of electronic transport in noncrystalline materials requires information about the nature of the eigenstates. Possibly the most important information to be acquired from the eigenstates is their localization properties, i.e., to inquire whether the electrons are essentially confined within finite volumes of the material or are allowed to escape to infinity.[1,2]

This important question has been studied theoretically within the framework of certain simplified models, most notably the so-called Anderson model for random lattices. It is widely accepted, however, that certain qualitative conclusions based on Anderson's model are of universal validity. Experimental evidence seems to support this supposition.[1,3]

Anderson's model is a tight-binding Hamiltonian in which a band is formed from atomic orbitals associated with lattice points. Randomness is introduced in the model by assuming that the site energies (i.e., the diagonal matrix elements of the Hamiltonian) are statistical variables having a given probability distribution of width $W$, which is taken as a measure of the degree of randomness.

It has been demonstrated[4-11] within Anderson's model that a critical value of $W$, $W_c$, may exist such that all eigenstates are localized for $W > W_c$. For $W < W_c$ the spectrum is separated[12] by critical energies $E_c$, termed mobility edges, into regions of extended (i.e., not localized) and localized eigenstates.[1] As $W$ approaches $W_c$ the mobility edges merge together eliminating the regions of extended eigenstates. This disappearance of extended eigenstates has been termed Anderson's transition.

Although some other models have been examined,[2,13-15] most of the theoretical attention has been focused on Anderson's model because the latter includes some of the universal properties characterizing disordered systems.[1,2] In spite of the oversimplifications present in Anderson's model various assumptions and approximations are needed to obtain solutions. Although these approximations lead to the same qualitative conclusions they differ appreciably in their quantitative results.

Until recently the quantitative discrepancies among the various approaches have been given incidental attention[6] since there existed almost no means by which to check the approximations or the results; moreover, the exact numbers were not considered very important since they were not related with observable quantities. The whole quantitative picture is presently receiving increased interest[13,16-18] due partly to the suggestion by Mott[19] of the existence of a minimum metallic conductivity at $T = 0$ when the Fermi energy $E_F$ lies at the mobility edge; Mott connects this minimum conductivity directly with $W_c$. Since the minimum metallic conductivity, if it exists, is a measurable quantity, the exact value of $W_c$ is very significant. Moreover, the theoretical results for $W_c$ can now be checked against some recent numerical work on finite systems[20,21] as well as against[17,18,22] the results on percolation theory.[23,24]

It is in this light that we systematically examine here the problem of localization within the framework of Anderson's model. In Sec. II we summarize the general theoretical formulation of the problem as developed by various authors.[4-6,8] In Sec. III the existing approximate approaches to the problem are outlined with particular emphasis on their relationship. Next, in Sec. IV, a new criterion for localization is developed which is shown to be particularly successful. In Sec. V we present and compare results (for various real lattices and probability distributions of the site energies) obtained by using the methods outlined in Sec. III and developed in Sec. IV. A discussion on the accuracy of the different methods is presented in Sec. VI. Finally, in Sec. VII, conclusions are given.

## II. GENERAL THEORY

Most of the discussion in this section is applicable to a general disordered system; however, for the sake of clarity and simplicity we consider here the specific case of Anderson's model for disordered lattices.

The Hamiltonian $\hat{H}$ in Anderson's model may be expressed by

$$\langle \vec{n}|\hat{H}|\vec{m}\rangle = \epsilon_{\vec{n}}\delta_{\vec{n}\vec{m}} + V_{\vec{n}\vec{m}}, \tag{2.1}$$

where $|\vec{n}\rangle$ is an atomic orbital associated with the site $\vec{n}$, the sites form a lattice, and $V_{\vec{n}\vec{m}}$ is taken equal to a constant $V$ for $\vec{n}$, $\vec{m}$ nearest neighbors and zero otherwise. Randomness is introduced by assuming that $\epsilon_{\vec{n}}$ are statistically independent random variables with a common probability distribution $p(\epsilon_{\vec{n}})$.

### A. Definition of localization

There are several definitions of a localized eigenfunction $\Psi(\vec{r})$ of which the most intuitive requires the existence of the integral $\int \Psi^*(\vec{r})\Psi(\vec{r})d\vec{r}$. Demanding a more stringent test one could use the existence of $\int r^2\Psi^*(\vec{r})\Psi(\vec{r})d\vec{r}$ as a criterion for localization. In cases where the wave function has been evaluated, usually in one dimension, $\Psi(\vec{r})$ is known to behave exponentially,

$$\Psi(\vec{r}) \underset{r\to\infty}{\sim} e^{-r/R_d},$$

so that one may define a decay localization length $R_d$. These statements are taken to imply a vanishing of the dc conductivity at $T=0$ which is sometimes itself used as a criterion for localization. Another useful trick used mostly in the numerical computation[9] of localization properties is the observation that changes in the boundary conditions for finite systems shift the energy levels by an amount only of order $e^{-N1/d}$ (assuming exponential decay) for localized states as opposed to $1/N$ for extended states; $d$ is the dimensionality of the system.

The method advanced by Anderson[4] considers the infinite time evolution of an electron wave function which was initially localized at a particular site or region of the system. If there are localized eigenstates in the neighborhood of the region considered, these would certainly overlap with the site in question and the particle would have a finite probability of being initially in each one of these eigenstates. Since these states localize the electron and are time independent, one would expect a finite probability $p_{\vec{0}\vec{0}}$ of rediscovering the particle at the initial region after an infinite time lapse. On the other hand, if no localized states exist in the neighborhood of the region considered, the particle will diffuse away, and the overlap with the site will approach zero as $t\to\infty$. Thus, according to this criterion, the existence or not of localized eigenstates is associated with whether or not $p_{\vec{0}\vec{0}}$ is different from zero. It seems that these definitions of localization are equivalent, although no rigorous proof exists for this statement.[9]

An eigenfunction is called extended or propagating if it is not localized.

### B. Localization of the behavior of $G(z)$

Any of the above definitions of localized eigenstates implies a basic difference in the analytic structure of the Green's function $G(z)$ for localized and extended states; here $G(z)$ is defined as $(z-\hat{H})^{-1}$, where $\hat{H}$ is the Hamiltonian of the system. As is clear from the definition, $G(z)$ is analytic at every point in the $z$ plane not belonging to the spectrum of $\hat{H}$, e.g., $\mathrm{Im}z\neq 0$. Further, it exhibits a branch cut at portions of the spectrum corresponding to extended states. Those parts of the continuum spectrum belonging to localized states (if any) are lines of singularity which are not branch cuts; they are the so-called natural boundaries at which not even the side limits, i.e., $\lim_{s\to 0^+} G(E\pm is)$, exist.

To be more specific, consider Anderson's definition of localization in which one assumes the particle initially at the site $\vec{0}$ with a wave function $|\vec{0}\rangle$. For $t>0$ the wave function can be written as

$$\Psi(t) = \sum_{\vec{n}} c_{\vec{n}}(t)|\vec{n}\rangle . \tag{2.2}$$

The quantity of interest is

$$p_{\vec{0}\vec{0}} = \lim_{t\to\infty}\frac{1}{t}\int_0^t |\, c_{\vec{0}}(t')|^2\, dt' .$$

The time average has been taken to avoid unnecessary oscillations as $t\to\infty$. $p_{\vec{0}\vec{0}}$ is the (time averaged) probability of finding the particle in the state $|\vec{0}\rangle$ at $t=\infty$, if initially ($t=0$) it was in the same state $|\vec{0}\rangle$. Thus one must find for what degree of disorder $p_{\vec{0}\vec{0}}\neq 0$, which implies the existence of localized states.

It can be shown[8] that $p_{\vec{0}\vec{0}}$ is related to an integral of the form

$$p_{\vec{0}\vec{0}} = \lim_{s\to 0^+}\frac{s}{\pi}\int_{-\infty}^{\infty} dE\, G_{\vec{0}}(E+is)G_{\vec{0}}(E-is), \tag{2.3}$$

where $G_{\vec{0}}(E)$ is the diagonal element of the Green's function in configuration space, i.e., $G_{\vec{0}}(E)=\langle\vec{0}|(E-\hat{H})^{-1}|\vec{0}\rangle$. From Eq. (2.3) it is clear that the question of localization is directly related to the analytic properties of the Green's function. To proceed with this discussion we introduce the self-energy $\Delta_{\vec{0}}(E)$ at the site $\vec{0}$, which is essentially the reciprocal of $G_{\vec{0}}$ defined implicitly by

$$G_{\vec{0}} = (E-\epsilon_{\vec{0}}-\Delta_{\vec{0}})^{-1} . \tag{2.4}$$

Here $\epsilon_{\vec{0}}$ is the value of the energy level at the site $\vec{0}$, which is a random quantity in Anderson's model. Substituting (2.4) into (2.3) we obtain

$$p_{\vec{0}\vec{0}} = \lim_{s\to 0^+}\frac{s}{\pi}\int_{-\infty}^{\infty} dE\,\frac{\mathrm{Im}G_{\vec{0}}(E-is)}{2is-[\Delta_{\vec{0}}(E+is)-\Delta_{\vec{0}}(E-is)]} . \tag{2.5}$$

Equation (2.5) shows clearly that extended eigenstates make no contribution to $p_{\vec{0}\vec{0}}$ since for those states $\Delta_{\vec{0}}(z)$ [and equivalently $G_{\vec{0}}(z)$] has a branch cut on the real $E$ axis. On the other hand, for localized states the nonexistence of the side limits of $\Delta_{\vec{0}}$ (or $G_{\vec{0}}$) persuades one to consider alternatively the $N\to\infty$ limit of a finite system. Although for

finite systems no rigorous distinction exists between localized and extended states, the peculiarities reappear in the limit $N \to \infty$.

The quantities of interest may be written

$$G_{\vec{0}}(E) = \sum_i \frac{f_i}{E - E_i} \tag{2.6}$$

and

$$\Delta_{\vec{0}}(E) = \sum_i \frac{g_i}{E - E_i^{\vec{0}}}, \tag{2.7}$$

where $E_i$ are the energy eivenvalues corresponding to the eigenfunctions $|\Psi_i\rangle$, $f_i = \langle \vec{0}|\Psi_i\rangle\langle\Psi_i|\vec{0}\rangle$ is the probability that an electron in the eigenstate $|\Psi_i\rangle$ will be on the site $\vec{0}$, and the summation extends over all the eigenfunctions; similarly $E_i^{\vec{0}}$ is the energy eigenvalue for a system with the $\vec{0}$ site missing (i.e., $\epsilon_{\vec{0}} \to \infty$). [Equation (2.7) may easily be derived from the equation $G_{\vec{0}} = \langle \vec{0}|(E - \hat{H})^{-1}|\vec{0}\rangle$ and (2.4).] The quantities $g_i$ are rather complicated functions of overlap matrix elements. The important property of $\Delta_{\vec{0}}(E)$ is that its poles coincide with $E_i^{\vec{0}}$.[8] Using Eqs. (2.3) and (2.6) we obtain

$$p_{\vec{0}\vec{0}} = \sum_i f_i^2, \tag{2.8}$$

which satisfies (since $0 < f_i < 1$ with $\sum_i f_i = 1$)

$$0 < p_{\vec{0}\vec{0}} < 1$$

for the finite system as it should.

We examine now the consequence of allowing the dimensions of the system to approach infinity. If the states are not localized, each $f_i$ should be the order of $N^{-1}$ so that $f_i^2 \sim N^{-2}$ and the sum $p_{\vec{0}\vec{0}} \sim \sum_i^N \times 1/N^2 \to 0$ as $N \to \infty$ as expected. For localized states, the residues approach some finite limit $f_{i\infty}$ as $N \to \infty$ although they vary in magnitude considerably depending on the state. In general, if the $f_i$ are arranged for each $N$ in descending magnitude, then the $n$th term behaves, for large $n$, like $f_n \sim O(1/n^{\beta})$, where $\beta > 1$ and the largest $f_i \sim 1$. Thus, for localized states $p_{\vec{0}\vec{0}} = \sum_i f_{i\infty} \neq 0$ and the distinction between localized and extended states is recovered.

The preceding remarks imply that in the case of localized states one can approximate quantities like $p_{\vec{0}\vec{0}}$ to any degree of accuracy by taking into account only a finite number of residues in Eq. (2.8); by contrast, this would not be possible for extended states since each $f_i$ in Eq. (2.8) is the same order of magnitude.

The situation is more complicated if one considers the quantity $G_{\vec{0}}(E)$ [or $\Delta_{\vec{0}}(E)$]. One cannot rigorously approximate $G_{\vec{0}}(E)$ with a finite number of terms in Eq. (2.6) because of the possibility that $E$ may lie arbitrarily close to the position of the pole of an omitted term. A probabilistic approach should be used: For $E$ randomly chosen, the probability that it lies in regions dominated by omitted terms in Eq. (2.6) is proportional to $\sum_{i>i_0} f_i$ (since each pole dominates a region proportional to its residue). For localized states $f_i < (\text{const.})i^{-\beta}$, $\beta > 1$ and consequently $\sum_{i>i_0} f_i$ approaches zero as $i_0 \to \infty$; for extended states $f_i \sim N^{-1}$ and consequently $\sum_{i>i_0} f_i$ tends to 1 as $N \to \infty$ for every $i_0$. Thus one can conclude that for extended eigenstates one cannot approximate $G_{\vec{0}}(E)$ [or $\Delta_{\vec{0}}(E)$] by a finite number of terms in Eq. (2.6); on the other hand, for localized eigenstates one can use a finite number of terms ($i < i_0$) in (2.6) and the error approaches zero with a probability which approaches 1 as $i_0 \to \infty$.

A different but equivalent way to examine the question is the following: Consider a finite system of $N$ sites. Since $\{\epsilon_i\}$ are random variables so are $E_{i,N}$, $f_{i,N}$, $E_{i,N}^{\vec{0}}$, $g_{i,N}$ and consequently $G_{\vec{0},N}$ and $\Delta_{\vec{0},N}$. Denote by $P_N(\Delta_{\vec{0},N}; E)$ the probability distribution of $\Delta_{\vec{0},N}(E)$ for $E$ belonging to the spectrum of the infinite ($N = \infty$) system. If $E$ belongs to a segment of the spectrum corresponding to localized states the limit $\lim_{N\to\infty} P_N(\Delta_{\vec{0},N}; E)$ does exist, which implies that the probability distribution of $\Delta_{\vec{0}}(E)$ [or $G_{\vec{0}}(E)$] can be approximated by the probability distribution of the sum of a finite number of terms in (2.6). On the other hand if $E$ belongs to a segment of the spectrum corresponding to extended states the limit $\lim_{N\to\infty} P_N$ does not exist.

One can also consider[2,4] the probability distribution of $\mathrm{Im}\Delta_{\vec{0},N}(E + is)$ in the limits $s \to 0^+$ and $N \to \infty$. In the case of extended states, for example, the $\lim_{s\to 0^+}\lim_{N\to\infty} P_N^{(2)}(\mathrm{Im}\Delta_{\vec{0},N}; E + is)$ does exist[4] and is a smooth function of $E$ while for localized states it is the $\lim_{s\to 0^+}\lim_{N\to\infty} \tilde{P}_N^{(2)}(\mathrm{Im}\Delta_{\vec{0},N}/s; E + is)$ which exists[4] and defines a smooth function of $E$; $P^{(2)}$ is the probability distribution of $\mathrm{Im}\Delta_{\vec{0},N}(E + is)$ while $\tilde{P}^{(2)}$ is the probability distribution of $s^{-1}\mathrm{Im}\Delta_{\vec{0},N}(E + is)$.

The question of localization can also be decided by examining the dependence of $G_{\vec{0}\vec{n}}(E) \equiv \langle \vec{0}|(E - \hat{H})^{-1}|\vec{n}\rangle$ on the distance[10] $R_{\vec{0}\vec{n}}$ as $R_{\vec{0}\vec{n}} \to \infty$. For extended eigenstates it is expected that $G_{\vec{0}\vec{n}} \sim R_{\vec{0}\vec{n}}^{-1}$ as $R_{\vec{0}\vec{n}} \to \infty$ while for localized states exhibiting exponential decay[25] $G_{\vec{0}\vec{n}} \sim e^{-R_{\vec{0}\vec{n}}/R_d}$, where $R_d$ is defined as the decay localization length. Such an approach although more direct has the disadvantage of dealing with a more complicated quantity like $G_{\vec{0}\vec{n}}$ and requires additional approximations. In this paper we restrict ourselves to a study based on the analytical properties of $G_{\vec{0}}$ or $\Delta_{\vec{0}}$.

In summary, the existence of localized eigenstates depends on the existence of the probability distribution for the self-energy $\Delta_{\vec{0}}(E)$. In order to study the properties of this distribution one would like first to express it in terms of known quantities. Unfortunately, a simple perturbative approach in terms of site energies where the hopping potential $V$ is used as the perturbation diverges for all energies belonging to the spectrum.[2,4] The problem is resolved by expressing the self-energy $\Delta_{\vec{0}}(E)$ in a

renormalized perturbation expression[26,27] (RPE) in which the site energies are modified self-consistently:

$$\Delta_{\vec{0}}(E)=\sum_{\vec{n}\neq\vec{0}} V_{\vec{0}\,\vec{n}}(E-\epsilon_{\vec{n}}-\Delta_{\vec{n}}^{\vec{0}})^{-1}V_{\vec{n}\,\vec{0}} + \sum_{\vec{n}\neq\vec{0};\,\vec{n}'\neq\vec{n},\,\vec{0}} V_{\vec{0}\,\vec{n}'}(E-\epsilon_{\vec{n}'}-\Delta_{\vec{n}'}^{\vec{0}\,\vec{n}})^{-1} \times V_{\vec{n}'\vec{n}}(E-\epsilon_{\vec{n}}-\Delta_{\vec{n}}^{\vec{0}})^{-1}V_{\vec{n}\,\vec{0}}+\cdots \quad , \qquad (2.9)$$

where, as before, the superscripts $\vec{0}$, $\vec{n},\ldots$ denote that the corresponding quantity has been calculated for $\epsilon_{\vec{0}}$, $\epsilon_{\vec{n}},\ldots=\infty$. The right-hand side of (2.9) can be represented by all paths which begin and end at $\vec{0}$ and do not visit the same site more than once. Thus repeated scattering from the same site which leads to the divergence in ordinary perturbation theory is eliminated. The relation (2.9) for $\Delta_{\vec{0}}(E)$ holds everywhere on the complex $E$ plane except along the branch cuts on the real axis. Within the RPE, however, one no longer has an explicit expression for $\Delta_{\vec{0}}$ since unknown quantities $\Delta_{\vec{n}}^{\vec{0}\,\vec{n}}$ appear on the right-hand side of Eq. (2.9). These quantities can be expressed through relations similar to (2.9) and substituted back into (2.9). Repeating this process to eliminate all the unknowns on the right-hand side of (2.9), we obtain an infinite continued-fraction-like expression in each term of the series of the form

$$\Delta_{\vec{0}}(E)=\sum_{\vec{n}=\vec{0}} V_{\vec{0}\,\vec{n}}\left(E-\epsilon_{\vec{n}}-\sum_{\vec{1}\neq\vec{0},\,\vec{n}} V_{\vec{n}\,\vec{1}}\frac{1}{E-\epsilon_{\vec{1}}-\cdots}V_{\vec{1}\,\vec{n}}+\cdots\right)^{-1} \times V_{\vec{n}\,\vec{0}}+\cdots. \qquad (2.10)$$

Equation (2.10) may be applied to a system consisting of a finite number of sites. In this case both the continued-fraction-like structure as well as the series terminate due to the self-avoiding nature of the diagrams. Thus Eq. (2.10) constitutes an explicit closed solution for the self-energy $\Delta_{\vec{0}}$ of a finite system, a property of the RPE which makes it of central importance to our problem. We may rewrite Eq. (2.10) for the finite system of $N$ sites as

$$\Delta_{\vec{0},\vec{N}}(E)=\sum_{M=2}^{N}\Delta_{\vec{0},N}^{(M)}(E), \qquad (2.11)$$

where $\Delta_{\vec{0},N}^{(M)}(E)$ is the sum of all diagrams visiting $M$ sites. In order to show that the probability distribution of $\Delta_{\vec{0},N}(E)$ converges as $N\to\infty$ for localized states one must show that both the infinite-step iteration procedure implied by (2.10) and the series itself converges in probability. More precisely, the absence of extended states implies that (a) the probability distribution of $\Delta_{\vec{0},N}^{(M)}(E)$ converges as $N\to\infty$ and (b) the contribution of all terms $|\Delta_{\vec{0}}^{(M)}(E)|$, where $M>M_0$, are negligible as $M_0\to\infty$. Clearly if both conditions (a) and (b) are satisfied, there are no extended states at $E$.

The problem could be considerably simplified if the convergence of series [renormalized perturbation series (RPS)], for example, implied the convergence of the iteration procedure or vice versa.

Economou and Cohen[8] *assumed* that the convergence of the RPS is equivalent to the convergence of the whole RPE; as a result they studied the convergence of the RPS only. On the other hand Abou-Chacra *et al.*[16,28] examined the question of the convergence of the iteration procedure only by making in addition the *approximation* of terminating the RPS after the first term. Abou-Chacra *et al.* by terminating the series, have found that the iteration procedure converges if the randomness exceeds a critical finite value; otherwise it diverges. Thus their results indicate that the convergence of the iteration procedure may be as important as the convergence of the RPS itself. As a matter of fact the numerical values they obtained for $W_c(E)$ from this procedure are very close to the numerical values obtained originally by Anderson[4] who considered the convergence of the series. Note further, however, that these numerical estimates are inconsistent with the numerical results obtained in finite systems.[20,21]

The one-dimensional (1-D) case requires some comments because it has created certain confusion.[29] Since the RPS terminates in one-dimension (with nearest neighbors coupling only) it certainly converges, and consequently whatever divergences appear are due to the divergence of the iteration procedure. It has been shown[30,16] that in this case the iteration procedure converges for any nonzero degree of randomness. Thus *both* the Economou-Cohen procedure and the Abou-Chacra *et al.* procedure yield correct results in the 1-D case. On the other hand, it would be definitely wrong to apply the $F(E)$ (or the $G^0$) criterion (see below) in the 1-D case, since the derivation of these criteria is explicitly based on the existence of a nonterminating RPS.

Another case worthwhile referring to is that of the Cayley tree.[24] In a Cayley tree a site may have $Z$ nearest neighbors (where $Z>2$ as in the 2-D or the 3-D cases) but, on the other hand, only a finite number of self-avoiding polygons is allowed, as in the 1-D case. The total number of sites increases *exponentially* with the distance from a given central site so that the "surface" sites are as numerous as the "bulk" sites. The above properties make the Cayley tree a quite special case which should be examined with extreme care. Regarding the question of localization in a Cayley tree one should specify how localization is defined in this case since the usually assumed equivalence of the various definitions of localization is probably not valid. Obviously any approach based on the convergence of

the RPS would predict always localization since the possibility of divergence of the iteration procedure has been omitted and the RPS terminates. On the other hand, the approach by Abou-Chacra *et al.* is exact in a Cayley tree, although the physical explanation of the divergence or convergence of the RPE requires further elaboration.

Results obtained in a Cayley tree with $Z$ nearest neighbors [or with connectivity $K$, where $K$ is defined as $K=\lim_{M\to\infty}(1/M)\ln C_M$ and $C_M$ is the number of self-avoiding paths of $M$ steps; in a Cayley tree $K=Z-1$] acquire practical significance if one further assumes that they are good approximations to the corresponding results in real 2-D or 3-D lattices with the same $Z$ (or $K$). Experience with the Ising model[16,28] indicates that the above assumption is reasonable for quantities that depend mainly on local properties (as, e.g., the *local* magnetic moment) while it may lead to wrong conclusions for quantities of global character (as, e.g., the total partition function). Abou-Chacra *et al.*[16,28] *assumed* that their results for the divergence or convergence of the RPA in a Cayley tree of connectivity $K$ are reasonable approximations to the problem of localization in a real lattice of the same $K$.

If one makes the assumption that the convergence of the RPE is equivalent to the convergence of the series alone (i.e., that the convergence of the series always implies the convergence of the iteration procedure) the whole problem reduces to that of finding the probability distribution of

$$\Delta_{\vec{0}}^{(M)}(E)\equiv V\sum_{\substack{\text{all diagrams}\\ \text{of order } M}}\frac{V}{e_1}\frac{V}{e_2}\cdots\frac{V}{e_M} \tag{2.12}$$

as $M\to\infty$. Here $e_{\vec{i}}\equiv E-\epsilon_{\vec{i}}-\Delta_{\vec{i}}^{\vec{0},\vec{1},\cdots,\vec{i}-1}$ are random functions possessing a distribution function and the sum extends over all $M$-step self-avoiding diagrams starting from and ending at the site $\vec{0}$. Various approximations have been used in the literature to obtain information about the probability distribution of a particular contribution to $\Delta_{\vec{0}}^{(M)}(E)$, i.e.,

$$T_j^{(M)}\equiv V^M\frac{1}{e_1}\frac{1}{e_2}\cdots\frac{1}{e_M}. \tag{2.13}$$

Here $j$ labels a specific $M$th-order diagram. Even if one knows the probability distribution of $T_j^{(M)}$, the problem is far from solved since, in order to find the distribution of $\Delta_{\vec{0}}^{(M)}$, one needs to know the degree of statistical correlation among the various $T_j^{(M)}$. It is only in the two limiting cases of no correlation[4] or extremely strong correlation[8] that one can proceed with the present analysis. It should be noted that both these limiting cases do not correspond to the real situation. There are roughly $K^M$ $T_j^{(M)}$ terms contributing to $\Delta_{\vec{0}}^{(M)}$, where $K$ is the connectivity of the lattice; there are only $M^3$ independent statistical variables involved (since the independent statistical variables are in one-to-one correspondence with the lattice points). Consequently all $T_j^{(M)}$ cannot be independent. We show in a later section that at least in one case the assumption of strong correlation is incorrect. For our purposes, by strong correlation we mean that almost all $T_j^{(M)}$ for a given $M$ are almost equal. We make this statement more precise later. The assumption of strong correlation is probably closer to reality.[31] It has the additional advantage of allowing a more sophisticated treatment by controlling whatever additional approximations are used. By contrast the assumption of no correlation requires further drastic approximations, the effects of which are unclear.

Before we close this section we mention that different approaches to the problem of localization have been attempted. Thus Haydock and Mookerjee[13] have considered a model which is similar although not identical to Anderson's model in which they propose to replace the static site disorder by a dynamical one. This technique allows the electron to have transitions at a particular site even when the hopping $V=0$ so that in this case the energy spectrum would be equivalent to the site probability distribution. The advantage of this redefinition in which the disorder is put on an equal footing with the spacial hopping is that one may, as an approximation, ignore certain matrix-element sequences to simplify the problem. Thus Haydock and Mookerjee construct a matrix Hamiltonian which has a structure in correspondence with the Cayley tree and thereby permits an analytic solution.

Lukes[11] has examined the quantity $\langle G^*G\rangle_{\text{av}}$, which is related to the static conductivity. By using an approximation essentially equivalent to that employed by Ziman[5] he studied the localization transition. He considered also the question of the localization length which was also examined by Anderson.[31]

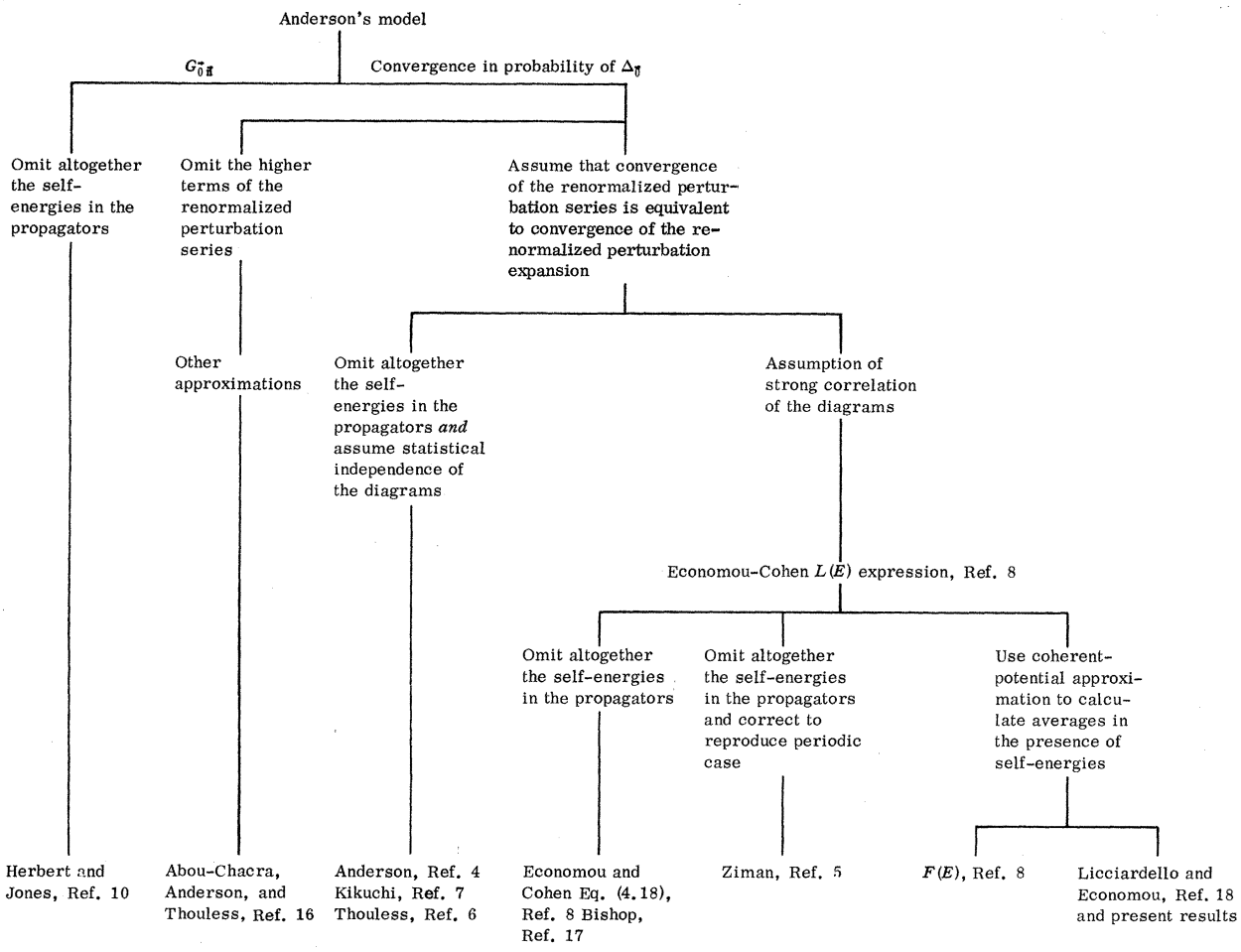
Finally, by examining an altogether different model for a disordered system, Abram and Edwards[32] provide further evidence for the basic electronic band picture described in the Introduction by reaching similar conclusions.

## III. APPROXIMATE METHODS

In this section we briefly discuss some of the existing techniques related with the present approach to the question of localization. The discussion is summarized in Table I.

The method of Herbert and Jones,[10] in which the residue of the off-diagonal propagator $G_{\vec{i}\vec{j}}$ is examined, neglects the renormalized denominators in the expansion for this residue; i.e., it replaces the denominators $e_i$ in Eq. (2.12) by $E-\epsilon_i$ and omits the self-energies $\Delta_i$ altogether. This is a

TABLE I. Approximations used in different approaches to the localization problem within Anderson's model.




very drastic approximation which eliminates the possibility of divergence of the iteration procedure but allows easy determination of the probability distribution of products of $1/e_i$ terms. Under the assumption of no correlation they obtain results identical with Anderson's[4] "upper-limit" condition. Their approach admits a procedure to include correlation effects. They argue that since the residues of the poles in the expansion for $G_{\vec{i}\vec{j}}$ are bounded by unity, the long tails in the probability distribution of $G_{\vec{i}\vec{j}}$ predicted when one assumes statistical independence is spurious and would be removed by a proper treatment of the correlations. Thus they introduce a Gaussian distribution as an approximation to the distribution of the residue to reduce the tail and they then obtain lower Anderson transitions. On the other hand, their approach treats correlations between energy levels on the *same* path and is not easily compared to the Economou-Cohen approach, which assumes strong statistical correlations among different paths of the same order. Herbert and Jones's approach using a rectangular distribution of total width $W$ for the site energies predicts

$$2e^{2.3} < W_c/V < 2e^{1.5}K \tag{3.1}$$

for the critical disorder. The above result gives the critical disorder at which the eigenstates at the center of the band ($E=0$) become localized. It was assumed that the last states to become localized are those at the center of the band.

Anderson in his classic paper[4] calculated the probability distribution of $T_j^{(M)}$ by assuming also that $e_i \approx E - \epsilon_i$, i.e., by neglecting altogether the self-energies except for a cutoff to prevent the

denominators $e_i$ from vanishing. He further assumed that the quantities $T_j^{(M)}$ are statistically independent. He thus obtains values of $W_c/V$ for $E=0$. Thouless[6] presented a critical and clarifying discussion of Anderson's method. He also extended Anderson's method to the case where the site energies possess a binary-alloy type of distribution. Generalizations[7] of Anderson's theory to $E\neq 0$ are unfortunately limited to a range of $E$ within the distribution of the site energies. This is due to the use of a theorem which depends on the uncorrelated signs of the $T_j^{(M)}$ which is true only for these limited values of $E$. Thus, for example, if one expects the range of localized states to be confined to the band tails, such states would be inaccessible within Anderson's theory. Moreover, study of the mobility edges as a function of the disorder parameter would be difficult. In spite of these limitations Kikuchi, using similar approximations to that of Anderson, derived[7] the following expression for $W_c(E)$:

$$\frac{2K}{1-4W_c^2(E)/V^2}\ln\{\tfrac{1}{2}[W_c(E)/V]n(E)\}=\tfrac{1}{2}W_c(E)/V,$$

where (3.2)

$$n(E)=\{1-[2E/W_c(E)]^2\}^{1/4},\quad 0<|E|<W/2$$

which reduces to Anderson's "best estimate" for $E=0$. $W_c(E)$ is the critical value of the randomness in which the eigenstates at energy $E$ become localized. This expression includes Anderson's cutoff in the energy denominators $e_i$ generalized for $E\neq 0$.

The $L(E)$ theory of Economou and Cohen[8] clearly delineates between the basic assumptions and any further approximation. Assuming that (a) the convergence of the RPE is equivalent to the convergence of the renormalized perturbation series and (b) the $T_j^{(M)}$ are strongly correlated as $M\to\infty$, one can show[8] that the probability

$$\mathcal{P}[L^{M-M^q}(E)<|\Delta_{\vec{0}}^{(M)}(E)|<L^{M+M^q}(E)]\underset{M\to\infty}{\longrightarrow}1, \qquad (3.3)$$

where $q<1$. Thus if $L(E)<1$ ($>1$) the RPS converges (diverges) in probability. $L(E)$ defines a localization function: Those parts of the spectrum for which $L(E)<1$ correspond to localized eigenstates whereas those eigenstates for which $L(E)>1$ are extended and the energies satisfying $L(E_c)=1$ define the so-called mobility edges $E_c$ which separate the two regions. $L(E)$ is given by

$$L(E)=\lim_{M\to\infty}\left(V^{M+1}\sum{}'\tilde{G}_{\vec{n}_1}^{\vec{0}}\tilde{G}_{\vec{n}_2}^{\vec{0}\vec{n}_1}\cdots\tilde{G}_{\vec{n}_M}^{\vec{0}\vec{n}_1\cdots\vec{n}_{M-1}}\right)^{1/M}, \qquad (3.4)$$

where the $\sum'$ in (3.4) indicates summation over all indices $\vec{n}_1\vec{n}_2\cdots\vec{n}_M$ with the restrictions corresponding to all self-avoiding paths of order $M$ starting and ending at the site $\vec{0}$. The quantities $\tilde{G}_{\vec{n}_i}^{\vec{0}\vec{n}_1\cdots\vec{n}_{i-1}}$ are defined by

$$\ln\tilde{G}_{\vec{n}_i}^{\vec{0}\vec{n}_1\cdots\vec{n}_{i-1}}=\langle\ln|G_{\vec{n}_i}^{\vec{0}\vec{n}_1\cdots\vec{n}_{i-1}}|\rangle_{\rm av}=\left\langle\ln\left|\frac{1}{E-\epsilon_{\vec{n}_i}-\Delta_{\vec{n}_i}^{\vec{0}\cdots\vec{n}_{i-1}}(E)}\right|\right\rangle_{\rm av}. \qquad (3.5)$$

It should be noted that besides the original assumption (a) and (b) no further approximation was used to arrive at Eqs. (3.4) and (3.5). On the other hand, the $L(E)$ given by (3.4) is too complicated for practical calculations. Nevertheless, as will be shown below, one can control the level and sophistication of any further approximation. In addition, the general expression (3.4) exhibits the correct behavior in the limiting cases of zero disorder and infinite disorder.[8]

Within the $L(E)$ approach one can make the further approximation of neglecting altogether the self-energies $\Delta_{\vec{n}_i}^{\vec{0}\cdots\vec{n}_{i-1}}$. This approximation was used from the very beginning in Anderson's zero-correlation treatment. Then the quantities $\tilde{G}_{\vec{n}_i}^{\vec{0}\cdots\vec{n}_{i-1}}$ can be easily evaluated and the result for $L(E)$ is

$$L(E)\approx L_0(E)=KV\,e^{-\langle\ln|E-\epsilon_{\vec{n}_i}|\rangle_{\rm av}}. \qquad (3.6)$$

Equation (3.6) is the expression within the strong-correlation approach which corresponds to Anderson's approximation. Note that both $L_0(E)$ as well as Anderson's results do not reproduce correctly the periodic limit (i.e., zero randomness) due to the omission of the self-energies.

One can partly remedy this defect by multiplying $L_0(E)$ by a constant correction factor to be determined from the condition that in the periodic limit the mobility edges coincide with the band edges. Thus, one obtains

$$L(E)\approx L_z(E)=ZV\,e^{-\langle\ln|E-\epsilon_{\vec{n}_i}|\rangle_{\rm av}}, \qquad (3.7)$$

where $Z$ is the number of nearest neighbors. $L_z(E)$ was first obtained by Ziman.[5]

Economou and Cohen[8] have obtained within the framework of an effective-medium theory[33] and for symmetrical bands a more sophisticated approximation to $L(E)$ which retains the self-energies $\Delta_{\vec{n}_i}^{\vec{0}\cdots\vec{n}_{i-1}}$ in Eq. (3.5). Their approximate localization function, denoted by $F(E)$, has in addition the property that

$$F(E)<1\rightarrow L(E)<1, \qquad (3.8)$$

and therefore is an exact underestimate of the region of localized eigenstates within the premises of $L(E)$ and the effective-medium approximation. $F(E)$ is given by

$$F(E)=ZV/|E-\Sigma(E)|, \qquad (3.9)$$

where $\Sigma(E)$ is the effective-medium site energy.

Before discussing the implications of the preceding localization criteria for various lattices and site distributions it is worthwhile to clear up some confusion apparent in the literature with respect to using effective-medium approximations in the theory of localization. It is obvious that any direct use of the effective medium to predict the nature of eigenstates would be nonsensical since for any $H_{\text{eff}}$ all the eigenstates are extended. Similarly, use of any effective-medium theory to directly calculate $\langle G^*G\rangle$ would yield results which would imply no existence of localized states. On the other hand, $L(E)$ has been derived from a first-principles theory of localization which in its final form contains averages of the type $\langle \ln|G|\rangle$. It is at this point that the effective-medium concept is applied to estimate these quantities $\langle \ln|G|\rangle$; the localization information is still predicted from $L(E)$ itself. The point is better illustrated by observing that in deriving the Ziman criterion (3.7), the omitting of the self-energies is equivalent to Ziman or Anderson considering propagators of the type $1/(E-\epsilon_i)$, which considered by themselves would only predict localized states. But at the level at which Ziman or Anderson used this approximation to obtain their results the final criterion does indeed contain information about localization transition. Thus as long as one does not ask for information about localization directly from quantities like $\langle G\rangle$, or approximate calculations of quantities like $\langle G^*G\rangle$, the coherent-potential approximation[31] (CPA) and similar approaches may be used effectively to approximate averaged quantities on which properly derived localization criteria may depend.

## IV. NEW CRITERIA BASED ON THE $L(E)$ METHOD

In this section, starting from the general expression for $L(E)$ [Eqs. (3.4) and (3.5)], we attempt to obtain more-sophisticated approximations to $L(E)$ and at the same time estimate the errors thereby introduced.

One has first to calculate the average in Eq. (3.5). This can be done exactly only for the case of Lorentzian distribution of the site energies; in all other cases some approximation must be used. A general scheme for evaluating such averages is to introduce an effective Hamiltonian $\hat{\mathcal{K}}$ satisfying the relation

$$\ln\tilde{G}^{\vec{0}\cdots\vec{n}_{i-1}}_{\vec{n}_i}(E)\equiv\langle\ln|\langle\vec{n}_i|(E-\hat{H}^{\vec{0}\cdots\vec{n}_{i-1}})^{-1}|\vec{n}_i\rangle|\rangle_{\text{av}}$$
$$\approx\ln|\langle\vec{n}_i|(E-\hat{\mathcal{K}}^{\vec{0}\cdots\vec{n}_{i-1}})^{-1}|\vec{n}_i\rangle|\,. \qquad (4.1)$$

where the superscript $\vec{0}\cdots\vec{n}_{i-1}$ denotes that $\epsilon_{\vec{0}}=\cdots=\epsilon_{\vec{n}_{i-1}}=\infty$. $\hat{\mathcal{K}}^{\vec{0}\cdots\vec{n}_{i-1}}$ is in general a *non-Hermitian* operator having the symmetry properties[33] of $\langle\hat{H}^{\vec{0}\cdots\vec{n}_{i-1}}\rangle_{\text{av}}$. One then requires that $\hat{\mathcal{K}}^{\vec{0}\cdots\vec{n}_{i-1}}$ obey certain equations which will make the approximation (4.1) as good as possible. The most successful such scheme is the coherent-potential approximation (CPA) and its extensions,[34] which in the simplest form introduces an $\hat{\mathcal{K}}$ such that the diagonal matrix elements are all equal to a complex quantity $\Sigma(E)$ which is determined self-consistently.[33,35]

Introducing

$$\mathcal{G}^{\vec{0}\cdots\vec{n}_{i-1}}_{\vec{n}_i}\equiv\langle\vec{n}_i|(E-\hat{\mathcal{K}}^{\vec{0}\cdots\vec{n}_{i-1}})^{-1}|\vec{n}_i\rangle$$

we can write Eq. (4.1) as

$$\tilde{G}^{\vec{0}\cdots\vec{n}_{i-1}}_{\vec{n}_i}=|\mathcal{G}^{\vec{0}\cdots\vec{n}_{i-1}}_{\vec{n}_i}(E;\mathcal{K}^{\vec{0}\cdots\vec{n}_{i-1}}(E))|\,. \qquad (4.2)$$

Since $\hat{\mathcal{K}}^{\vec{0}\cdots\vec{n}_{i-1}}$ has the symmetry properties of $\langle\hat{H}^{\vec{0}\cdots\vec{n}_{i-1}}\rangle_{\text{av}}$, $\mathcal{G}^{\vec{0}\cdots\vec{n}_{i-1}}_{\vec{n}_i}$ is a Green's operator matrix element corresponding to a non-Hermitian *periodic* (apart from the missing sites $\vec{0}\cdots\vec{n}_{i-1}$) Hamiltonian. Thus $\mathcal{G}^{\vec{0}\cdots\vec{n}_{i-1}}_{\vec{n}_i}$ should exhibit branch cuts and possibly isolated simple poles (associated with the missing sites) in the complex energy plane. Since $\mathcal{G}^{\vec{0}\cdots\vec{n}_{i-1}}$ is not Hermitian these singularities will not coincide with the real axis. If one replaces each $\tilde{G}^{\vec{0}\cdots\vec{n}_{i-1}}_{\vec{n}_i}$ in Eq. (3.4) according to (4.2) and defines

$$|g^M(E,\mathcal{K}(E))|\equiv|\mathcal{G}^{\vec{0}}_{\vec{n}_i}\mathcal{G}^{\vec{0}\vec{n}_1}_{\vec{n}_2}\cdots\mathcal{G}^{\vec{0}\cdots\vec{n}_{M-1}}_{\vec{n}_M}|\,, \qquad (4.3)$$

one can obtain an effective-medium localization criterion $L_e(E)$:

$$L^M(E)\simeq L^M_e(E)\equiv V^{M+1}\sum|g^M(E)|=V^{M+1}K^M|g^M| \qquad (4.4)$$

and hence

$$L_e(E)=KV|g(E)|\,. \qquad (4.5)$$

The simplification in Eq. (4.5) is less than substantial, however, since $g(E)$ is defined through the complicated Eq. (4.3). On the other hand, note that all the $\mathcal{G}$'s entering the right-hand side of (4.3) have the same branch cuts, which are therefore branch cuts of $g(E)$. If $\hat{\mathcal{K}}$ corresponds to a single branch cut (one band) this branch cut is the only singularity of $g(E)$. If, however, $\hat{\mathcal{K}}$ corresponds to two or more nonoverlapping bands then $g^M(E)$ has poles which coincide with the poles of $\mathcal{G}^{\vec{0}}_{\vec{n}_i}$ and zeros which coincide[8] with the zeros of $\mathcal{G}^{\vec{0}\cdots\vec{n}_{M-1}}_{\vec{n}_M}$. Therefore $g(E)$ may develop additional singularities which complicate the study. Note also that $g(E)$ as defined in (4.3) is, strictly speaking, path dependent. It is reasonable, however, to assume that there is a particular path $j_0$ as $M\to\infty$ such that $K^MV^M|g_{j_0}|^M=V^M\sum_j|g_j|^M$ to exponential order.

If one knows where the branch cuts of $g(E)$ are as well as the discontinuity of $g(E)$ at the branch cuts, one can determine $g(E)$ for any complex or real value of $E$. A rigorous analogy exists between the behavior of a Green's function $G(E)$ in the complex $E$ plane with a branch cut and the two-dimensional electrostatic field problem of a line charge. In particular, if we consider the discontinuity across the cut to be proportional to a line-charge density occupying the same position in the plane, then the real and imaginary parts of the Green's

function will be proportional, respectively, to the $x$ and $y$ components of the corresponding electric field due to the line charge. When one is seeking approximations this analogy is very useful because it provides a simple vivid illustration of the behavior of $g(E)$. Using this analogy we can say that the localization function is essentially given by the magnitude of the corresponding electric field evaluated at the $x$ axis, the latter corresponding to the real $E$ axis. It is worthwhile to point out that the total charge determines the behavior at infinity which is known, namely, $g(E)_{E\sim\infty} 1/E$. Thus the total charge of the equivalent electric problem is equal to 1. Another condition that the charge distribution should satisfy stems from the fact that the localization function in the periodic case (no randomness) should be equal to 1 at the band edges, which implies that $|g(E=E_b)|_{W=0}=(KV)^{-1}$. Note that for the periodic case $\hat{\mathcal{H}}=\hat{H}_{\rm per}$ and that the branch cuts of $\mathcal{G}$ coincide with the bands of $\hat{H}_{\rm per}$, which, of course, all lie on the real $E$ axis. As the randomness increases from zero the branch cuts of $g(E)$ move away from the real axis.

In what follows, whenever concrete results are sought, we use the single-site[33] CPA according to which $\hat{\mathcal{H}}$ is determined by a single effective site energy $\Sigma(E)$ so that

$$\tilde{G}^{\vec{0}\cdots\vec{n}_{i-1}}_{\vec{n}_i}(E)=\left|\mathcal{G}^{\vec{0}\cdots\vec{n}_{i-1}}_{\vec{n}_i}(E-\Sigma(E))\right|, \tag{4.6}$$

where

$$\mathcal{G}^{\vec{m}\cdots}_{\vec{n}_i}(E)\equiv\langle\vec{n}_i|\,(E-\hat{H}^{\vec{m}\cdots}_{\rm per})^{-1}\,|\vec{n}_i\rangle \tag{4.7}$$

and $\hat{H}^{\vec{m}\cdots}_{\rm per}=\sum_{\vec{n}\vec{l}}V_{\vec{n}\vec{l}}\,|\vec{n}\rangle\langle\vec{l}|$ with the sites $\vec{m}\cdots$ excluded. In this case the only singularity of $g(E)$ is a branch cut along the line determined by the equation

$$z-\Sigma(z)=x,\quad x \text{ real and } -ZV\le x\le ZV. \tag{4.8}$$

The quantity $\Sigma(z)$ is determined by standard CPA techniques.[33]

It should be noted that usually $\Sigma(E)$ is introduced through the relation $\langle G_{\vec{n}}(E)\rangle_{\rm av}\simeq\mathcal{G}_{\vec{n}}(E-\Sigma(E))$ while in the present case a logarithmic partial average is involved. It can be easily shown that to first order in $t_{\vec{n}}\equiv(\epsilon_{\vec{n}}-\Sigma)/[1-\epsilon_{\vec{n}}-\Sigma)\mathcal{G}_{\vec{n}}]$ the logarithmic and the direct average provide the same value of $\Sigma$. On the other hand the partial averaging (due to the excluded sites having fixed, i.e., infinite, values) requires in general a more sophisticated effective medium and consequently extension of the simple CPA method. Because of the numerical complexity of the CPA extensions and in view of the discussion given in Sec. VI below, we decided to use the simple CPA throughout the present work.

We examine first the case of a single band, where a highly accurate approximate technique has been developed. Then we discuss briefly some less accurate but more general techniques which can be used in more complicated cases.

### A. $G^{\vec{0}}$ criterion

Assume for the moment that for any factor in the right-hand side of (4.3) one can write approximately

$$\mathcal{G}^{\vec{0}\cdots\vec{n}_{i-1}}_{\vec{n}_i}\approx\mathcal{G}^{\vec{m}_1\cdots\vec{m}_{Z'}}_{\vec{n}_i}, \tag{4.9}$$

where $\vec{m}_1\cdots\vec{m}_{Z'}$ are the nearest-neighbor sites of $n_i$ *belonging* to the sequence $\vec{0}\cdots\vec{n}_{i-1}$. Obviously $Z'\le Z-1$ in order to permit the diagram to "escape." Using (4.9), the expression for $g(E)$ becomes

$$g(E)=(\mathcal{G}^{\vec{m}_1}_{\vec{n}})^{v_1}(\mathcal{G}^{\vec{m}_1\vec{m}_2}_{\vec{n}})^{v_2}\cdots(\mathcal{G}^{\vec{m}_1\vec{m}_2\cdots\vec{m}_{Z'}}_{\vec{n}})^{v_{Z'}}, \tag{4.10}$$

where the $v_j$ are defined as the number of times a factor $\mathcal{G}$ with $j$ neighbors excluded occurs in a given diagram of order $M$ divided by $M$. Note that only a small finite number of the various $\mathcal{G}$'s enter in (4.10) since the $\vec{m}_i$'s are nearest neighbors of $\vec{n}$. Symmetry considerations further reduce the number of different $\mathcal{G}$ entering (4.10). For example, for a diamond lattice Eq. (4.10) becomes

$$g(E)=(\mathcal{G}^{\vec{m}_1}_{\vec{n}})^{v_1}(\mathcal{G}^{\vec{m}_1\vec{m}_2}_{\vec{n}})^{v_2}(\mathcal{G}^{\vec{m}_1\vec{m}_2\vec{m}_3}_{\vec{n}})^{v_3}. \tag{4.10a}$$

For a square lattice

$$g(E)=(\mathcal{G}^{\vec{m}_1}_{\vec{n}})^{v_1}(\mathcal{G}^{\vec{m}_1\vec{m}_2}_{\vec{n}})^{v_2}(\mathcal{G}^{\vec{m}_1\vec{m}_3}_{\vec{n}})^{v_2'}(\mathcal{G}^{\vec{m}_1\vec{m}_2\vec{m}_3}_{\vec{n}})^{v_3}. \tag{4.10b}$$

For a simple-cubic lattice the expression is slightly more complicated. Using the very definition of $g(E)$ and Eq. (4.9) it is easy to see that

$$\sum_j v_j=1. \tag{4.11}$$

For a diamond lattice (4.11) means that $v_1+v_2+v_3=1$ and for a square lattice $v_1+v_2+v_2'+v_3=1$, and so on.

Thus if the decoupling implied by Eq. (4.9) is true, the Green's function at any site along a diagram path may (i) only include nearest-neighbor-excluded sites and (ii) may not include more than $Z-1$ neighboring sites in order to permit the diagram to escape. This result is particularly promising since the quantities $\mathcal{G}^{\vec{m}_1\vec{m}_2\cdots\vec{m}_i}_{\vec{n}}$, $i\le Z-1$, may be calculated without much difficulty. The only indeterminacy remaining is the quantities $v_j$ which measure the "distortion" of the typical diagram of order $M$ as $M\to\infty$. For example, those diagrams which are bubblelike or inflated should satisfy $v_1\gg v_2\gg v_3\cdots$; those which are heavily contorted should weigh more heavily those $\mathcal{G}$ with many neighbors excluded. It is in general exceedingly difficult to predict $\{v_j\}$ for a given lattice since $L(E)$ is ultimately defined for $M\to\infty$. However, the expression (4.10) is a weighted logarithmic average of the quantities $|\mathcal{G}^{\vec{m}_1\vec{m}_2\cdots\vec{m}_i}_{\vec{n}}|$ for which the numbers $v_i$ represent the "weights." Thus in those cases where the $|\mathcal{G}^{\vec{m}_1\vec{m}_2\cdots\vec{m}_i}_{\vec{n}}|$ are not very different for

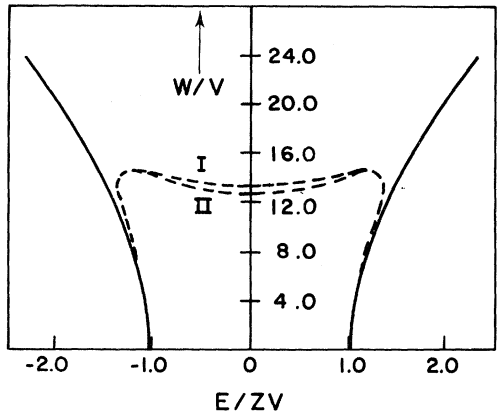



FIG. 1. Mobility edge trajectories $E_c(W)$ (dashed lines) for the simple-cubic lattice with a rectangular distribution of site energies of width $W$ demonstrating the approximation described by Eq. (4.9). I is predicted by Eq. (4.12) and II by Eq. (4.13). Solid lines denote the CPA band-edge trajectories.

various $i$, the weights will have little significance.

To illustrate the technique, we have applied the criterion (4.10) to various lattices within the CPA. In particular, the approximation (4.9) was found to be an excellent one for every case we considered. In Fig. 1 we demonstrate the mobility edge trajectory (rectangular or Anderson distribution of site energies or width $W$) for the simple-cubic lattice using the criterion

$$L_e^{\mathrm{I}}(E) = KV\left|\mathcal{G}_{\vec{n}}^{\vec{m}}(E-\Sigma)\right| \tag{4.12}$$

and

$$L_e^{\mathrm{II}}(E) = KV\left|\mathcal{G}_{\vec{n}}^{\vec{m}\,\vec{l}}(E-\Sigma)\right|, \tag{4.13}$$

where $\vec{m}$ is a neighbor of $\vec{n}$, and $\vec{l}$ is a next nearest neighbor of $\vec{n}$. We have used the approximation $v_j = 0$, $j \neq 1$, for convenience only in illustrating this point. We observe from the figure that the next-nearest-neighbor-excluded site has a negligible effect on the mobility edge trajectory. The solid line in the figure is the CPA band edge. There is some arbitrariness in choosing the next nearest neighbor in relationship to the site $\vec{n}$ but we have found this result invariant for all possibilities. Thus we conclude that the decoupling approximation (4.9) is a good one (typical errors of the order of 3% or less).

We have next examined the cases of diamond or square lattices where $g(E)$ is given by Eqs. (4.10a) and (4.10b), respectively. An important check of the success of any new criterion for localization is its behavior in the periodic limit. We should have

$$\left|g(E)\right|_{W=0} \xrightarrow[E\to E_b]{} (KV)^{-1}, \tag{4.14}$$

which stems from the condition

$$L(E)_{W=0} \xrightarrow[E\to E_b]{} 1,$$

where $E_b$ is the band edge for the periodic case ($W=0$). We have calculated the limits

$$\lim_{E\to E_b}\left|\mathcal{G}_{\vec{n}}^{\vec{m}_1}(E)\right|, \quad \lim_{E\to E_b}\left|\mathcal{G}_{\vec{n}}^{\vec{m}_1\vec{m}_2}(E)\right|,$$

and

$$\lim_{E\to E_b}\left|\mathcal{G}_{\vec{n}}^{\vec{m}_1\vec{m}_2\vec{m}_3}(E)\right|,$$

where

$$\mathcal{G}_{\vec{n}}^{\vec{m}_1} = \mathcal{G}_{\vec{n}} - \mathcal{G}_{\vec{m}_1\vec{n}}\mathcal{G}_{\vec{n}\,\vec{m}_1}/\mathcal{G}_{\vec{n}}, \tag{4.15}$$

$$\mathcal{G}_{\vec{n}}^{\vec{m}_1\vec{m}_2} = \mathcal{G}_{\vec{n}}^{\vec{m}_1} - \mathcal{G}_{\vec{n}\,\vec{m}_2}^{\vec{m}_1}\mathcal{G}_{\vec{m}_2\vec{n}}^{\vec{m}_1}/\mathcal{G}_{\vec{n}}^{\vec{m}_1}, \tag{4.16}$$

$$\mathcal{G}_{\vec{n}}^{\vec{m}_1\vec{m}_2\vec{m}_3} = \mathcal{G}_{\vec{n}}^{\vec{m}_1\vec{m}_2} - \mathcal{G}_{\vec{n}\,\vec{m}_3}^{\vec{m}_1\vec{m}_2}\mathcal{G}_{\vec{m}_3\vec{n}}^{\vec{m}_1\vec{m}_2}/\mathcal{G}_{\vec{n}}^{\vec{m}_1\vec{m}_2}. \tag{4.17}$$

Here we employ the relations[36]

$$\mathcal{G}_{\vec{n}\,\vec{m}_i}(E) = \left[E\mathcal{G}_{\vec{n}}(E) - 1\right], \tag{4.18}$$

$$\mathcal{G}_{\vec{m}_i\vec{m}_j}(E) = \tfrac{4}{3}\left[E\mathcal{G}_{\vec{n}\,\vec{m}_i}(E) - \tfrac{1}{4}\mathcal{G}_{\vec{n}}(E)\right]. \tag{4.19}$$

The values for the periodic limits of (4.15)–(4.17) are given in Table II as well as what they imply for the periodic limit of $L_e(E)$ in the case $v_1 = v_2 = v_3$. The importance of these results is as follows: (i) The narrow distribution of the periodic values of the $\mathcal{G}$'s about the exact $g(E) = 1/KV$ implies that the localization function $L_e(E)$ is insensitive to the only remaining adjustable parameters, i.e., the set $\{v_j\}$. Indeed the choice of an equal-weight logarithmic average yields values within 10% of the exact periodic limit for $L_e$ at the band edge. (ii) it is to be understood that the requirement $L(E_b) = 1$ for no randomness gives another constraint on the set of $\{v_j\}$. Note that in the cases we studied (Table II) there always exist values of $\{v_j\}$ to satisfy the requirement (4.14). From Table II it appears that "kinks" in the diagrams contributing terms of

TABLE II. Values of different approximations to the quantity $g(E)$ for the preiodic case at the band edge $E_b$. The quantity $g(E)$ determines the localization function $L(E) = KV\,|g(E)|$

| Lattice \ Approximation | $\lvert g(E_b)\rvert \approx \lvert\mathcal{G}_{\vec{n}}^{\vec{m}_1}(E_b)\rvert$ | $\lvert g(E_b)\rvert \approx \lvert\mathcal{G}_{\vec{n}}^{\vec{m}_1\vec{m}_2}(E_b)\rvert$ | $\lvert g(E_b)\rvert \approx \lvert\mathcal{G}_{\vec{n}}^{\vec{m}_1\vec{m}_2\vec{m}_3}(E_b)\rvert$ | Equal weight logarithmic average $v_1 = v_2 = v_3$ | Exact $\lvert g(E_b)\rvert = (KV)^{-1}$ |
|---|---|---|---|---|---|
| Square | 2.00 | 1.33 | 1.11 | 1.44 | 1.51 |
| Diamond | 1.44 | 1.23 | 1.01 | 1.25 | 1.39 |

the type $\mathcal{G}_{\vec{n}}^{\vec{m}_1\vec{m}_2}$ are more important for the square lattice, whereas for the diamond lattice the $\mathcal{G}_{\vec{n}}^{\vec{m}_1}$ vertices are more abundant. This kind of behavior is consistent with what one expects from dimensionality arguments, since a self-avoiding diagram would try to cross itself more frequently in the 2-D square lattice and less frequently in the 3-D diamond lattice. As is expected, in both cases three excluded site vertices appear very infrequently (i.e., requires the least weight to predict the periodic limit).

The most important information, of course, is the behavior for large disorder where the Anderson transition occurs. Fortunately, $L(E)$ is least sensitive to the parameters $\{v_j\}$ in this case and the $\mathcal{G}$'s become essentially degenerate. Thus, the localization criterion corresponding to $v_1=1$, $v_j=0$, $j\neq 1$, in Eq. (4.10) and given explicitly by

$$L_e(E)=KV\left|\mathcal{G}_{\vec{n}}(E-\Sigma(E))-\frac{\mathcal{G}_{\vec{n}\vec{m}_i}(E-\Sigma(E))\mathcal{G}_{\vec{m}_i\vec{n}}(E-\Sigma(E))}{\mathcal{G}_{\vec{n}}(E-\Sigma(E))}\right| \tag{4.20}$$

should yield good results. The subscript $e$ in $L_e$ denotes the use of effective-medium theory. We refer to the localization function (4.20) as the $G^{\vec{0}}$ approach (since one site is excluded).

To summarize this subsection the localization function defined by (4.20) is expected to be a definite improvement over old localization criteria. For low degrees of disorder the $L_e$ given in (4.20) can be further improved by using Eqs. (4.5) and (4.10), where $\{v_j\}$ satisfy (4.11) and (4.14); complete determination of the $\{v_j\}$ requires further information about the shape of the self-avoiding polygons in the lattice under study.

### B. Other techniques

Within the framework of any effective theory $\hat{\mathcal{C}}$ is known and consequently the position of the branch cuts of $g(E)$ is also known. What is not known is the discontinuity across the branch cuts, i.e., the charge distribution of the equivalent electrostatic problem. As in electrostatics one can try a moment expansion which in the simple CPA case can be written as

$$g(E)=\frac{A_1}{E-\Sigma(E)}+\frac{A_3}{[E-\Sigma(E)]^3}+\cdots. \tag{4.21}$$

Even-power terms are absent in the present simple case because $\mathcal{G}(E)=\mathcal{G}(-E)$. As was discussed before $A_1=1$. One more coefficient can be determined from the condition (4.14). Determination of the other coefficients requires elaborate numerical Monte Carlo techniques, a rather impractical approach. It is not in general possible to decide whether or not a truncated moment expansion is a good approximation to $g(E)$ for $E\approx E_c$.

We have mentioned the moment expansion (4.21) only as an interesting possibility in the evaluation of $L_e$ in difficult cases. The approximation $F(E)$ can easily be derived within this framework. Consider the first term only in (4.21). Then

$$L_e(E)\simeq KVA_1/|E-\Sigma|. \tag{4.22}$$

Now we cannot satisfy both the correct behavior at infinity and Eq. (4.14). If we choose to satisfy (4.14) we have $A_1=Z/K$. Thus we obtain

$$L_e(E)\simeq ZV/|E-\Sigma(E)|\equiv F(E). \tag{4.23}$$

As was done in deriving the Ziman criterion (3.7), we have used the one arbitrary parameter available, in this case $A_1$, to satisfy the periodic boundary condition. For a small degree of disorder the mobility edges will be close to the band edge so that it is important to satisfy this limiting condition. Further, as the disorder is increased so does $|\Sigma(E)|$ and as the mobility edges move inward the quantity $|E-\Sigma(E)|$ does not vanish. Thus $F(E)$ in this region remains a reasonable approximation to $L_e(E)$. The incorrect behavior at $E\to\infty$ again is not important for a description of the position of the mobility edge at least within this approximation; note that as $E\to\infty$, $\Sigma(E)\to 0$ and again the pole is never a problem. Since in the periodic limit $F(E)\to ZV/E$, $F(E)$ is termed a single-pole approximation to the localization function.

The pole approximation to $L_e(E)$ can be generalized to include several poles. This is equivalent to replacing a continuous distribution of charge by some properly placed point charges. This allows added degrees of freedom from the pole residues and positions by which more limiting conditions may be satisfied. Further, in cases of generalizations of the CPA in which clusters and short-range correlations[37] are included, the use of more than one pole is necessary since other techniques fail. A localization theory developed for such an extension[37] using only two poles yields results in striking agreement with what is expected from a semiclassical approach to the same problem. To proceed with a proper generalization, the following remarks are useful. It is clear that the branch cut along the real $E$ axis in $g(E)$ for the periodic case is displaced and distorted in the complex $E$ plane when $E$ is replaced by the complex $E-\Sigma(E)$ in the single-site CPA. Thus in approaching the mobility edge along the real $E$ axis to examine the behavior of $L(E)$ one observes that we are not too close to the cut, especially for large disorders. Thus it is not unreasonable to suppose (in the electrostatic language) that one could approximate the line charge by a few point charges which would approximately reproduce the field as long as we are not close to the source. Equivalently, we replace the branch cut in $g(E)$, whose corresponding dis-

continuity is extremely difficult to calculate, by a few poles. This procedure is indispensable in more complicated cases,[37] but can also be used in the simple CPA case. For the present one-band case, a two-pole approximation is not good for small degrees of disorder since it erroneously produces very small values of $|g(E)|$ for $E$ lying between the poles. Thus the simplest reasonable generalization of the simple pole approximation is the three-pole approximation (3P) which gives for $L(E)$

$$L(E)=KV\left|\frac{q}{E-\Sigma(E)}+\frac{q'}{E-\Sigma(E)+E_{q'}}+\frac{q'}{E-\Sigma(E)-E_{q'}}\right|, \tag{4.24}$$

where $q+2q'=1$, and (4.14) should be satisfied. These two equations do not determine $q$, $q'$, $E_{q'}$ uniquely and one is forced either to use elaborate numerical techniques to eliminate the uncertainty or to use $E_{q'}$, for example, as a free parameter. Although (4.24) is an improvement over $F(E)$ it is definitely worse than (4.20).

## V. RESULTS

In this section we present specific results based upon the theories of localization outlined in Sec. III and developed in Sec. IV.

We work within the framework of Anderson's model. Thus the input of our study are the following: (i) The lattice structure; quantities associated with the lattice structure are the number of nearest neighbors $Z$, and the connectivity $K$,[24] the band structure $E(\vec{k})$ associated with the periodic Hamiltonian $\hat{H}_{\rm per}=\sum'_{\vec{n}\vec{m}}V_{\vec{n}\vec{m}}|\vec{n}\rangle\langle\vec{m}|$, where $V_{\vec{n}\vec{m}}$ is a constant $V$ for $\vec{n}$ and $\vec{m}$ nearest neighbors and zero otherwise, the Green's function matrix element $\langle\vec{0}|(E-\hat{H}_{\rm per})^{-1}|\vec{0}\rangle$, and the $\vec{0}$-site contribution to the density of states $\rho_{\vec{0},\rm per}(E)=-(1/\pi)\,{\rm Im}\langle\vec{0}|(E^{+}-\hat{H}_{\rm per})^{-1}|\vec{0}\rangle$. We consider here three lattices: simple cubic ($Z=6$, $K=4.68$), diamond ($Z=4$, $K=2.88$), and square ($Z=4$, $K=2.64$). Sometimes one considers a semicircular $\rho_{0,\rm per}(E)$ (Hubbard density of states) which corresponds to no lattice but simplifies the computational work. (ii) The probability distribution of the site energies $p_0(\epsilon_i)$. We consider here the case of a binary-alloy type where $p_0(\epsilon_i)=x\delta(\epsilon_i-\epsilon_A)+(1-x)\delta(\epsilon_i-\epsilon_B)$. This probability distribution is essentially characterized by two parameters: $x$, the "concentration" of $A$ atoms, i.e., the probability that a given site will be $\epsilon_A$, and $\delta\equiv|\epsilon_A-\epsilon_B|/ZV$, which can be considered as determining the degree of disorder. We examine also the rectangular distribution where $p_0(\epsilon_i)=1/W$ for $-W/2\le\epsilon_i\le W/2$ and zero otherwise; the single parameter $W$ characterizes the degrees of disorder. Finally we consider the Lorentzian distribution where $p_0(\epsilon_i)=(1/\pi)[\Gamma/(\epsilon_i^2+\Gamma^2)]$, with the single parameter $\Gamma$ measuring the degree of disorder; the Lorentzian distribution plays a unique role because it allows an exact calculation of all the averages involved in the various theories and, consequently, no effective-field approximation is necessary.

For all distributions considered, the single-site[33] CPA has been used to evaluate the averages employing the effective site energy $\Sigma(E)$, which is in general a complex quantity. $\Sigma(E)$ has been calculated by numerically solving the basic CPA equation. It should be noted that the CPA produces the exact[8,17] result for the Lorentzian distribution. Also, the probability distribution $p_0(\epsilon_i)=(2/\pi W^2)\times(W^2-\epsilon_i^2)^{1/2}\Theta(W^2-\epsilon_i^2)$ has been used in the literature[38,17] (in addition to the more common ones previously referred) because it considerably simplifies the CPA equation from which $\Sigma(E)$ is determined.

We have used various theories of localization to obtain results; thus we are able to compare various theories among themselves. It is more important to compare the results of these theories with independent reliable results. Unfortunately the latter are not abundant. A case of importance is the binary-alloy distribution when $\delta\to\infty$. In this case, the only way an electron being initially at an $A$ ($B$) site may propagate to infinity, is to find a path consisting entirely of $A$ ($B$) sites and extending to infinity. Percolation theory[23,24] examines exactly this problem, i.e., the probability $P(x)$ of finding such an exclusively $A$ path. It turns out that this theory predicts a critical concentration $x_c$ such that $P(x)=0$ for $x<x_c$ and $P(x)>0$ for $x>x_c$, where $x_c$ depends on the particular lattice. The value of $x_c$ for various lattices has been tabulated.[24] According to these remarks, the percentage of extended states in the $A$ subband as $\delta\to\infty$ should be equal[39] to $P(x)$ and the percentage of extended states in the $B$ subband should be equal to $P(1-x)$. This may be used to check theories of localization especially with respect to whether or not they predict a critical value $x_c$ at which an Anderson transition takes place in the impurity subband and how close this value is to the one obtained from percolation theory.

The localization theories can also be tested against numerical results based on finite samples.[20,21] It seems that these results are rather reliable for the 2-D square lattice.[40] Results for 3-D lattices such as the diamond and simple-cubic lattices have been obtained in small samples and should be taken with extreme caution.

Typical results are shown in Fig. 2 for the case of a binary-alloy distribution. The average density of states per site is plotted as a function of energy for given values of $x$ and $\delta$ and for three lattices. Localized eigenstates [according to the $F(E)$ method] are shown as shaded areas and the mobility edges (arrows) separate the regions of localized eigenstates (shaded areas) from the regions of extended eigenstates (white areas). Note the signifi-

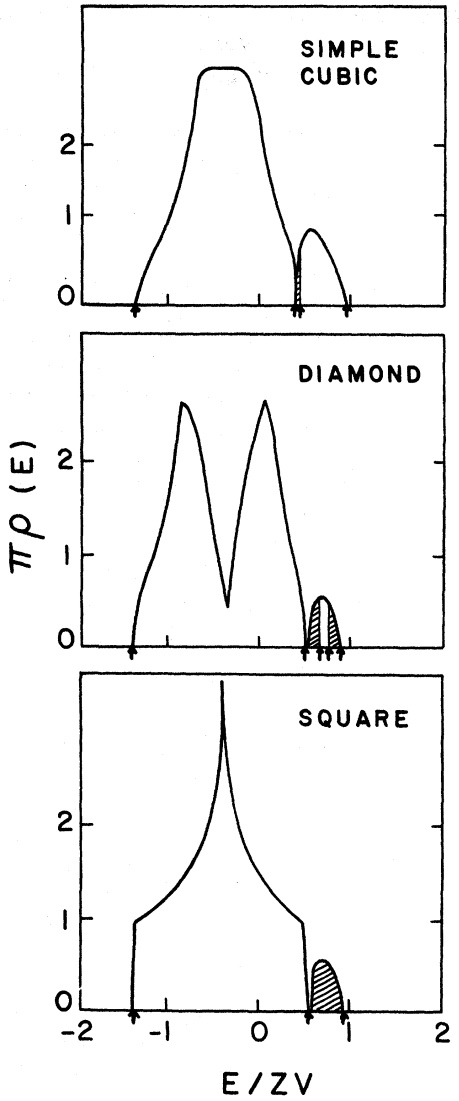



FIG. 2. Density of states per site $\rho(E)$ [in units $(ZV)^{-1}$] for a binary-alloy distribution of the site energies with $\delta = 0.8$ and $x = 0.10$ using the CPA. Shaded regions denote localized eigenstates and arrows indicate the positions of the mobility edges according to the $F(E)$ method.

cant lattice dependence of these results. It is increasingly more difficult to localized eigenstates as one moves from the square lattice to the diamond and finally to the simple-cubic lattice, in agreement with what one expects intuitively.

A more condensed and efficient way to present our results is through the so called $V$ diagrams, where one draws the trajectories of the band and mobility edges in the $E$-$R$ plane; $R$ stands for the degree of randomness. ($R = \delta$, $W/ZV$, $\Gamma/ZV$ for the binary-alloy, rectangular, and Lorentzian cases, respectively.) Cutting such diagrams with $R = \text{const.}$ lines one obtains immediate information about the localization of the energy spectrum, the portions which correspond to localized eigenstates and the portions which correspond to extended eigenstates. We classify our results mainly according to the form of the probability distribution $p_0(\epsilon_i)$.

### A. Binary-alloy distribution

We observe that the Ziman criterion (3.7) applied to the binary-alloy (BA) case[5] becomes

$$L_z^{BA}(E) = Z \exp\left(x \ln \frac{V}{|(E-\epsilon^A)|} + (1-x)\ln \frac{V}{|E-\epsilon^B|}\right), \tag{5.1}$$

which predicts no Anderson transition in either band since for $E$ arbitrarily close to the site energies $L_z^{BA} > 1$.

The argument of Anderson's theory applied to the binary-alloy case has been treated by Thouless.[6] In this case, the probability of finding conductive ($A$) sites on a particular $L$-site path is given by the binomial distribution. Assuming, according to Anderson, statistical independence of the $K^L$ paths and choosing the path with the largest number of $A$ sites one obtains[6,41] for small $x$

$$\eta = |\ln x| / \ln K, \tag{5.2}$$

where $\eta$ is the average number of steps between $A$ sites on this particular path. However, this estimate, as Thouless points out, is much too small since there can be no more than $L/x^{1/3}$ $A$-type sites on a path of length $L$. Nevertheless, this theory predicts a band of extended states within the impurity subband in the region

$$\frac{\delta}{2} - \frac{1}{Z\delta} - \left(\frac{1}{Z\delta}\right)^{\eta} < E < \frac{\delta}{2} - \frac{1}{Z\delta} + \left(\frac{1}{Z\delta}\right)^{\eta}. \tag{5.3}$$

Thus from (5.3), the Anderson-Thouless (AT) binary-alloy theory also does not allow a critical $x_c$ since it predicts an Anderson transition for $\delta \to \infty$ at any concentration. On the other hand, the recent self-consistent approach of Abou-Chacra *et al.*[16,28] predicts a critical $x_c$, where $x_c = 1/K$. This transition is predicted[28] to occur as $\delta \to \infty$.

Economou *et al.* have also shown[22] that $F(E)$ predicts a critical concentration $x_c(F)$ below which the impurity band exhibits an Anderson transition as $\delta$ increases. Furthermore, they show that for concentrations larger than the critical value, $F(E)$ predicts a persistence of extended states in the impurity band even as $\delta \to \infty$. We demonstrate here that $x_c(F)$ exhibits considerable lattice sensitivity and, further, that for each lattice $x_c(F)$ has a value less than that predicted from percolation theory consistent with the underestimate implied in Eq. (3.8). The validity and limitations of these remarkable successes will be discussed in Sec. VI.

For the sake of quantitative comparison, in Fig.

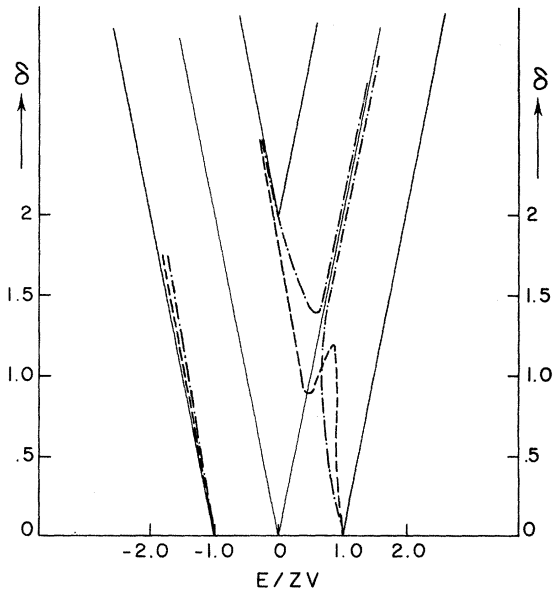



FIG. 3. Comparison of the $F(E)$ (dashed line) and the Ziman (dashed-dot line) mobility trajectories for the binary alloy (diamond lattice, $x = 0.10$) including the exact band-edge trajectories (heavy solid lines) in the $E$-$\delta$ plane. The Ziman mobility trajectory predicts no Anderson transition in the impurity subband even as $\delta \to \infty$. The light solid line denotes the site energies $\epsilon_A(E > 0)$ and $\epsilon_B(E < 0)$.

3 the trajectories of the band and mobility edges in the $E$-$\delta$ plane for the binary-alloy case are shown. The heavy solid lines describe the band edges and the light solid lines define the site energies ($\epsilon_A > 0$, $\epsilon_B < 0$). The mobility edges are calculated for $F(E)$ (dashed line) in the single-site CPA for the diamond lattice at $x = 0.10$. The mobility edge trajectory predicted from the localization criteria of Ziman is also shown (dashed-dotted line). We note that at $x = 0.10$ for diamond we are well below the critical site-percolation concentration [$x_c$(perc) = 0.42] and one observes an Anderson transition in the impurity subband ($E > 0$) predicted by the $F(E)$ criterion.

A curious feature of $F(E)$ is that it predicts the Anderson transition[22] at a finite $\delta_c$, whereas the AT mobility edge (not shown) closes only in the limit $\delta \to \infty$. [$L_Z(E)$ has no transition.] We should point out that the AT mobility edges are only valid for $\delta \gg 1$.

To demonstrate the clear lattice dependence which $F(E)$ exhibits in the binary-alloy case, the band and mobility trajectories for the diamond, simple-cubic, and square lattices are displayed in Fig. 4 for $x = 0.10$. The most obvious qualitative feature is the sharp dependence of the critical $\delta_c$ for the Anderson transition on the lattice. Although the diamond and square lattices have similar $K$ values (2.88 and 2.64, respectively) and identical values of $Z = 4$, we note in Figs. 4(a) and 4(b) a significant difference in the shape of the mobility edge trajectory. On the other hand, the $L_Z(E)$ or the AT criteria have no lattice dependence other than through $K$ and would therefore demonstrate little distinction. Indeed, $L_Z(E)$ which depends on $Z$ only would yield identical results for the diamond and square lattices.

In general, $F(E)$ predicts higher values of $\delta_c$ for the transition for larger $K$ and for larger concentrations. Further, the general behavior of the mobility edges as one increases the concentration above $x_c$ is in qualitative agreement with those predicted from percolation theory. This may be seen in Fig. 5, where we plot the percentage of extended states in the impurity band for large $\delta$ as a function of the concentration in the three lattices. As we mentioned previously, $F(E)$ predicts a critical concentration,

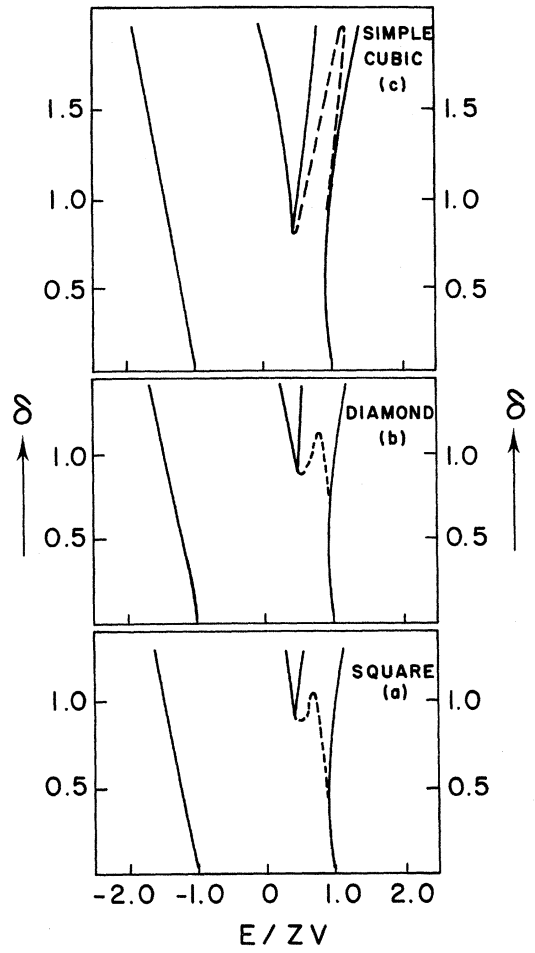



FIG. 4. Mobility edge trajectories $E_c(W)$ (dashed line) predicted by the $F(E)$ theory for the (a) square, (b) diamond, and (c) simple-cubic lattices for the binary alloy distribution with $x = 0.10$, demonstrating the lattice sensitivity of this localization criterion. The solid lines represent the CPA band-edge trajectories in the $E$-$\delta$ plane.

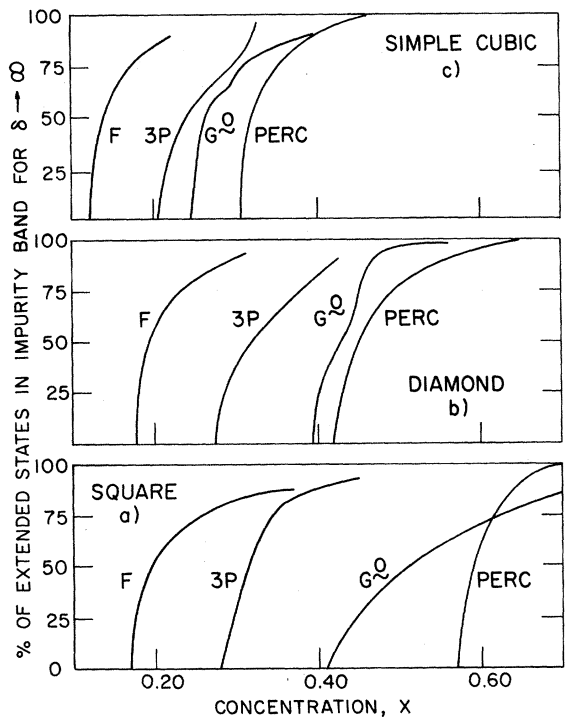



FIG. 5. Percentage of extended eigenstates in the $A$ subband for the binary-alloy distribution in the limit $\delta \to \infty$. Curves based on the $F(E)$ method ($F$), the three-pole approximation (3P), the $G^{\vec{0}}$ approach ($G^{\vec{0}}$), and the percolation theory (PERC.) are presented for three lattices.

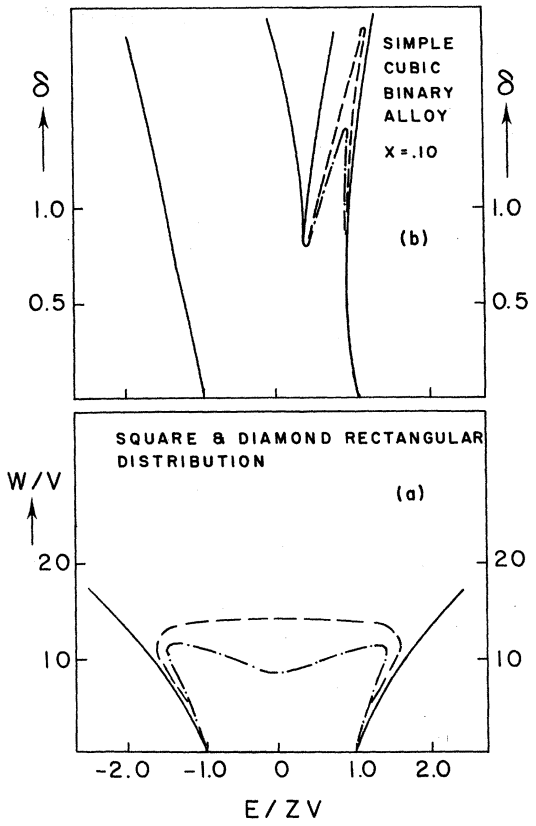



FIG. 6 Comparison of the mobility edge trajectories $E_c(W)$ predicted by the three-pole approximation (dashed-dot line) with the $F(E)$ method (dashed) for (a) square or diamond lattice with a rectangular distribution of site energies of width $W$ and (b) simple-cubic lattice with a binary-alloy distribution of site energies with $x = 0.10$. Solid lines denote the CPA band-edge trajectories.

below which the entire subband is localized for $\delta > \delta_c$. We compare in the same figure the corresponding result from percolation theory. Notice in Fig. 5 the remarkable similarity between the two curves although $x_c(F) < x_c(\text{perc})$. However, since $F(E)$ underestimates the region of localized states it therefore should predict the onset of extended states at a lower concentration than the percolation result. As may be seen from Table III (as well), this is generally true for all lattices we considered and further changes in $x_c(F)$ from lattice to lattice are in such a direction to be generally consistent with the lattice coordination, implying likely correlation to the percolative limit. Thus the $F(E)$ approximation to $L(E)$ is seen to be in qualitative and even semiquantitative agreement with what is expected in the classical limit of the binary site distribution. Moreover, this method has been applied to some real systems[42,43] with considerable success.

TABLE III. Comparison of the critical concentrations $x_c$ for a random binary alloy (see text), predicted by various theories.

| Lattice \ Theory | Other theories | Abou-Chacra *et al.* (Refs. 16 and 28) | $F(E)$ | 3P | $G^{\vec{0}}$ | Percolation (Ref. 24) |
|---|---|---|---|---|---|---|
| Square | No other theory | 0.38 | 0.17 | 0.27 | 0.42 | 0.59 |
| Diamond | predicts a | 0.35 | 0.18 | 0.28 | 0.40 | 0.42 |
| Simple cubic | critical concentration $x_c$ | 0.21 | 0.12 | 0.21 | 0.25 | 0.31 |

In Fig. 5 we have also summarized results based on the three-pole approach and on the $G^{\vec{0}}$ approach developed in Sec. IV. This figure shows clearly that the 3P approach is an improvement over the $F(E)$ method and that the $G^{\vec{0}}$ method is the best of all criteria, yielding results remarkably close to the percolative predictions at least for the 3-D cases. The $G^{\vec{0}}$ results shown in Fig. 5 as well as those in Table III have been based on Eq. (4.20). It should be noted that $x_c$ shows some sensitivity on the choice of $\{v_j\}$. For example, for the diamond lattice $0.35 < x_c < 0.40$ for all choices of the set $\{v_j\}$. It is not clear why the square lattice shows the largest deviation between the $G^{\vec{0}}$ method and the percolative predictions; however, the lower dimen-

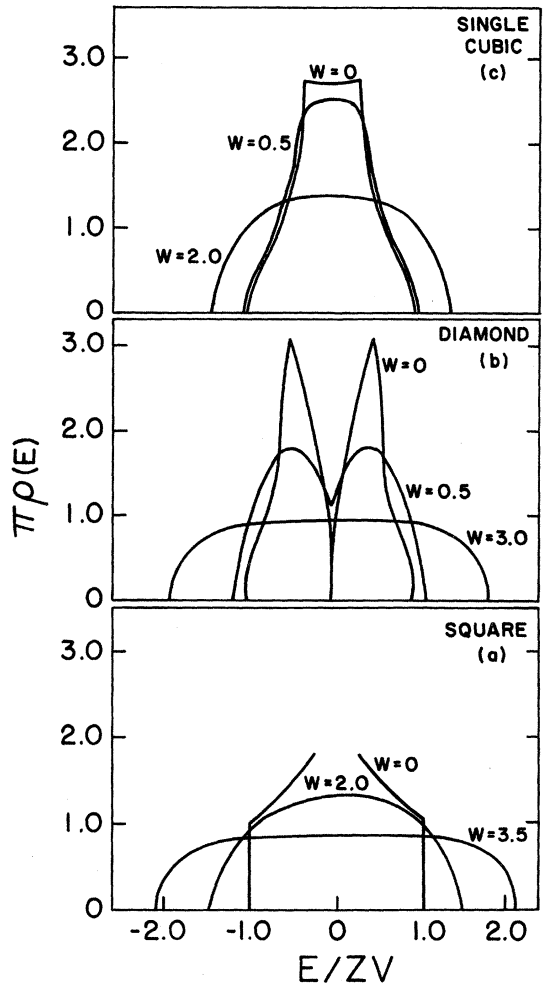



FIG. 7. Effect of rectangular site disorder on the density of states per site $\rho(E)$ of (a) square, (b) diamond, and (c) simple-cubic lattices for various widths $W$ of the disorder.

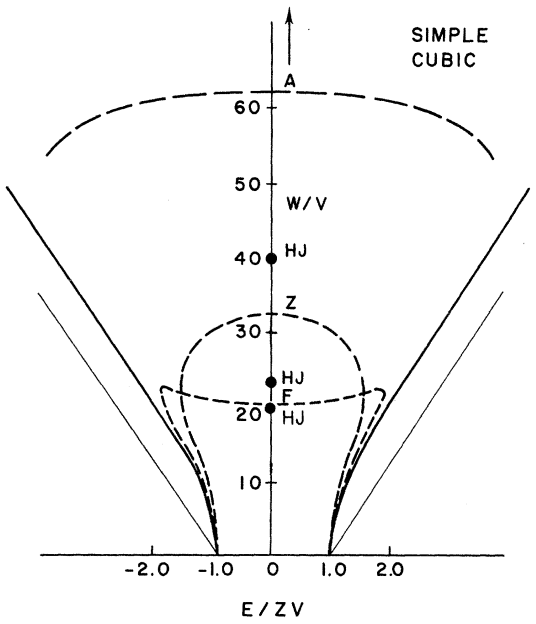



FIG. 8. Mobility edge (dashed lines) and the CPA band-edge trajectories (heavy solid line) in the $W$-$E$ plane for a rectangular distribution of site energies of width $W$. The localization results correspond to the Anderson (A), Ziman (Z), and $F(E)$ criteria for the simple-cubic lattice. The dots refer to the $W_c$ predicted by Herbert and Jones for three different approximations. The light solid line is the exact band edge trajectory.

sionality and the peculiar band-edge singularities (see Fig. 2) are suspect.

Finally, in Fig. 6(b) we compare the three-pole with the single-pole [i.e., $F(E)$] approximation for the simple-cubic lattice at $x = 0.10$. The effect of the extra poles is to lower the transition significantly. The dot-dashed trajectory corresponds to three poles, dashed to $F(E)$.

### B. Rectangular distribution

Results for the rectangular distribution are shown in Figs. 6(a) and 7–10 and in Table IV. The rectangular distribution, the one originally studied by Anderson in his famous localization paper, [4] has the additional interest that it has been examined numerically for real, finite systems[20,21] and therefore gives some reasonable handle on what is to be expected. Unfortunately, however, for this case there is no classical analog as in the binary alloy distribution.

Before we proceed to describe the localization

TABLE IV. Comparison of $W_c/V$ predicted from various theories for a rectangular distribution of site energies within the Anderson model.

| Lattice \ Theory | Anderson | Ziman | Herbert and Jones | $F(E)$ | $3P$ | $G^{\vec{0}}$ | Numerical estimates: Ref. 20 | Ref. 21 |
|---|---|---|---|---|---|---|---|---|
| Square | 28 | 22 | ••• | 14 | 11.6 | 7.2 | 5–6 | <11.2 |
| Diamond | 32 | 22 | ••• | 14 | 11.6 | 8.2 | ~15? | ••• |
| Simple cubic | 62 | 32.4 | 40,24,20 | 22 | 19.8 | 14.5 | ••• | <24 |

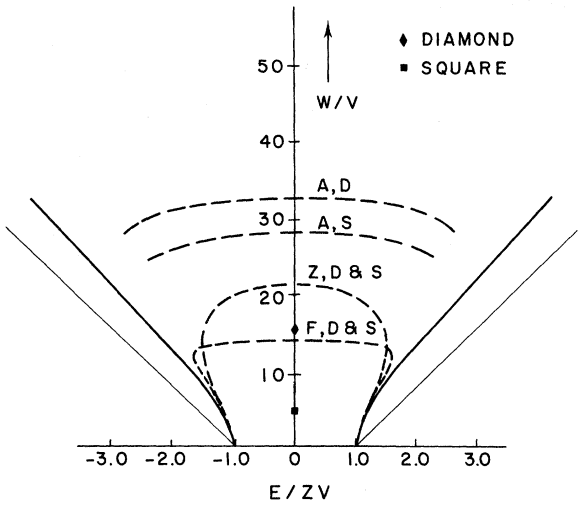



FIG. 9 Mobility edge (dashed lines) and CPA band-edge trajectories in the $W$–$E$ plane for a rectangular distribution of site energies of width $W$. The localization results correspond to the Anderson (A), Ziman (Z), and $F(E)$ criteria for the diamond (D) and square (S) lattices. The CPA (heavy solid line) and exact (light solid line) band-edge trajectories are also shown. The numerical estimates of Edwards and Thouless (Ref. 10) for the critical $W_c/V$ are indicated.

results for this case, it is worthwhile to describe the effect disorder of the present rectangular type has on the density of states. In general, large fluctuations in the site energies distributed continuously tends to broaden the spectrum and to smooth out critical points in the unperturbed density of states.[44] Thus as the disorder becomes extremely large, the spectrum tends to assume a shape very similar to the shape of the distribution itself. Figure 7 shows this phenomena quite clearly for the (a) square (b) diamond and (c) simple-cubic spectra calculated within the single-site CPA. Notice that for large widths $W$ of the site distribution, all the lattice-dependent structure is wiped out and only a rectangularlike spectra remain. Bishop has derived[17] an analytic expression for the band edge within the CPA approximation.

The band and mobility trajectories are displayed in Fig. 8 for the simple-cubic lattice ($Z=6$) and in Fig. 9 for the diamond (D) and square (S) lattices ($Z=4$). The localization results for the Ziman (Z), Anderson (A), Herbert and Jones (HJ) ($Z=6$ and $E=0$ only), and $F(E)$ are presented. The most obvious feature of the theories is their significant lack of agreement (with each other), although the Anderson (best) estimate predicts a considerably higher transition than the others. It is interesting to note that $F(E)$ and Anderson's theory show a sharp transition whereas the cruder but more straightforward approach of Ziman leads to a more gradual transition. Further it is observed that the $F(E)$ theory comes the closest to the results from numerical analysis on small finite systems.[20,21] It should be mentioned that the value of the critical $(W/V)_c$ for these lattices is still not certain since the numerical work on finite systems is inconclusive.

We also note that $F(E)$ fails to produce any distinction between the square and diamond lattices. This occurs because the large disorder at which the transition takes place wipes out any lattice dependence of the effective medium $\Sigma(E)$, as shown in Fig. 7. Similarly no distinction certainly occurs in $L_z(E)$ where $Z=4$ for both lattices and a not so significant amount for the Anderson theory ($K_S \approx K_D$). The close similarity of the mobility edge and CPA band-edge trajectories in the limit $W \to 0$ is a consistent property of all the criteria presented here; although the CPA band edge has no inherent importance, it is expected that those states neglected by the CPA are localized. On the other hand, as we shall see, the results of the new criteria based on $L(E)$ show a marked distinction in the region $W \gtrsim 0$.

Finally we point out that the Anderson transition for the simple-cubic lattice shown in Fig. 8 occurs at $E \neq 0$ within the $F(E)$ result. This result is a unique property of the Economou-Cohen localization theory and it would be extremely interesting if one could check this point numerically.

In Fig. 6(a) results for the square and the diamond lattices are shown based on the 3P approach. For comparison the single-pole $F(E)$ results are also reproduced. The shape of the mobility trajectory is altered also so that the transition is no longer at $E=0$. We remark that the position of the extra poles $E_{q'}$ [see Eq. (4.24)] has little effect on these results as long as $E_{q'} \ll ZV$ is satisfied.

Although the transition is lowered in better agreement with the square-lattice numerical results, this approximation does not break the $Z=4$ degeneracy. Thus we obtain the same lowering in both the diamond and square cases. In view of the $G^{\vec{0}}$ results (see below) for this case we think that the lowering of the mobility edge trajectory around the $E=0$ region is a spurious artifact of the three-pole approximation.

In Figs. 10 and 11 we present results based on the new $G^{\vec{0}}$ approach. This method predicts $(W/V)_c = 8.2$ for the diamond, $(W/V)_c = 7.2$ for the square, and $(W/V)_c = 14.5$ for the simple-cubic lattice (again for $E \neq 0$). The result for the square lattice is in rather good agreement with the Thouless and Edwards numerical results for that case and further is consistent with the recent upper limits evaluated by Schönhammer and Brenig. Thus far these predictions represent the only known theoretical consistency with these estimates. The theory again

does not produce any large difference between $(W/V)_c$ for the two $Z=4$ lattices. On the other hand, the present approach produces a marked distinction in the shape of the mobility trajectory near the band tails for the diamond and the square lattice. The square band seems to favor more localization in the tail for $W < W_c$ than the diamond [Fig. 10(b)]. One notices that for small disorder the shape of the mobility edge trajectories are similar according to their dimensionality (e.g., D, SC) whereas for large disorder the ones with corresponding coordination number are similar (D, S). This is, of course, what one might expect from first-principles considerations. Thus, the first such distinction for these lattices is suggested and a real new possibility to check the underlying assumption of $L(E)$ is available. Note that, similarly to the $F$ criterion, the new $\vec{G}^0$ method predicts for the simple-cubic lattice that the Anderson transition occurs for nonzero values of $E$, i.e., not at the center of the band. We were unable to locate the physical origin of such a behavior and as a consequence we do not know whether or not it is spurious. We mark in passing that using the single-site self-energy predicted from the CPA does not influence the Anderson transitions given here and as Bishop points out, [17] better approximations to the self-energy $\Sigma(E)$ than produced by the CPA have little effect on this class of localization functions. The results for the rectangular distribution are summarized in Table IV.

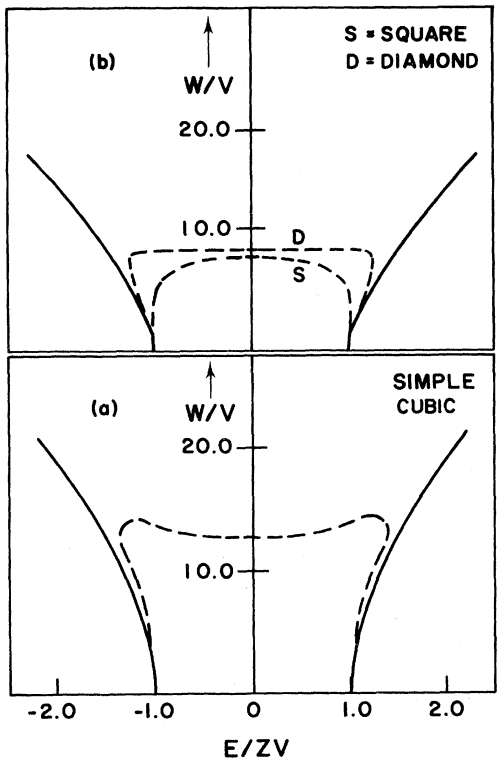



FIG. 10. Mobility edge trajectories (dashed lines) for three lattices with a rectangular distribution of site energies of width $W$ using the localization criterion $L_e(E)$ given by Eq. (4.20). Solid lines correspond to the CPA band-edge trajectories.

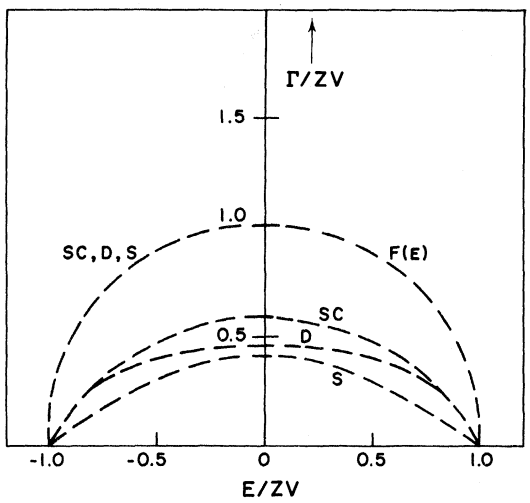



FIG. 11. Mobility edge trajectories (dashed lines) predicted by the $L_e(E)$ criterion [Eq. (4.20)] for the square (S), diamond (D), and simple cubic (SC) lattices for a Lorentzian distribution of site energies. Also shown is the trajectory predicted by the $F(E)$ method (top curve).

### C. Lorentzian distribution

Results for the Lorentzian distribution are given in Fig. 11, where the trajectories of the mobility edges are presented for the three lattices; these results are based upon the $\vec{G}^0$ method. For comparison the results based on the $F(E)$ approach are also given. The critical values of $\Gamma_c$ are $\Gamma_c/V = 1.64$ for the square, $\Gamma_c/V = 1.84$ for the diamond, and $\Gamma_c/V = 3.48$ for the simple cubic. In order to compare with the rectangular distribution we should take into account that[8] $4\Gamma \leftrightarrow W$ and consequently the critical values $4\Gamma/V$ are $4\Gamma_c/V = 6.56$ (square), $4\Gamma_c/V = 7.36$ (diamond), $4\Gamma_c/V = 13.92$ (simple cubic), values that are very close and systematically just below the corresponding values for the rectangular distribution. The feature of Fig. 11 worthwhile mentioning is the behavior of the mobility edge trajectory for the diamond lattice: For small values of disorder it behaves almost like the simple cubic. As the disorder increases diamond tends to behave more like the 2-D square lattice. Again, the possible explanation of such a behavior is that for high disorder only the immediate environment of each site is important while for small disorder longer-range features are influencing the results.

The Lorentzian distribution is important because the averages can be calculated exactly and thus no

effective-medium approximation is involved. The only remaining source of significant error is the basic assumption of strong correlation. If one assumes that correlations always overestimate the results of randomness then the values of $\Gamma_c$ obtained are essentially rigorous lower limits to the exact values of $\Gamma_c$. We are not able though to estimate the magnitude of this expected overestimation for the case of the Lorentzian distribution and thus we do not know how much (if at all) below the exact value for $\Gamma_c$ our result is. The approach based on the convergence of the iteration procedure[16,28] yields results for $\Gamma_c$ that are by a factor of 4 or 5 larger than the ones shown in Fig. 11. Another characteristic of the Abou-Chacra *et al.* approach[16,28] is that the mobility edges move first outwards from the center of the band and then inwards. This particular feature has been recently attributed[45] to a breakdown of the additional approximations employed in Refs. 16 and 28; an approximate solution was obtained[45] which shows that the mobility edges move inwards into the band for small values of $\Gamma$ for a Cayley tree. For large values of $\Gamma$ the results in Refs. 16 and 28 are almost[45,46] exact for the Lorentzian distribution and for Cayley trees. This does not imply, however, that those results are good approximations to the exact values in a *real* lattice of the same connectivity as the Cayley tree. Unfortunately no independent data are available for the Lorentzian case to serve as checks of the results discussed above.

Before we conclude this section we shall mention a recent work by Bishop, [46] who started with Eqs. (4.5) and (4.10) for $L(E)$. *At this point* he approximated the real lattice under consideration by a Cayley tree of the same connectivity $K$. We stress again that, if this approximation was done at the beginning of our theory, the result would be wrong, namely, all eigenstates would be predicted localized. On the other hand, the point at which Bishop introduced his approximation allowed him to obtain reasonable results because the quantities approximated, namely, $G_{\vec{n}}^{\vec{m}_1\vec{m}_2\cdots}$, are mainly dependent on the local environment. Bishop's approach[46] allows explicit analytical results for $L(E)$ as a function of the lattice connectivity $K$. These results show that the $G^{\vec{0}}$ method is extremely successful qualitatively.

## VI. DISCUSSION

We have seen that the $L(E)$ method coupled with effective-medium theories for evaluating averages is by far more successful than other approaches in all cases where independent checks exist. It should be pointed out that there remain essentially two sources of possible significant error in the new improved $G^{\vec{0}}$ method: (i) The assumption of strong correlation, which was used to derive the general expression for $L(E)$, and (ii) the use of effective-medium theories (usually the CPA) to calculate the averages involved in the expression for $L(E)$.

We discuss in this section these two points. It has been shown[8] that the probability distribution of $\ln|T_j^{(M)}|$ approaches a Gaussian one with a mean value $\langle x_j^{(M)}\rangle = Ma_j$ and a standard deviation $\sigma_j^{(M)} = \beta_j M^{1/2}$. This implies that the probability

$$\mathcal{P}\left[e^{Ma_j - M^q\beta_j} < |T_j^{(M)}| < e^{Ma_j + M^q\beta_j}\right] \xrightarrow[M\to\infty]{} 1,$$

where $\frac{1}{2} < q < 1$. Thus one can write $|T_j^{(M)}| \sim e^{Ma_j}$. The assumption of strong correlation demands that essentially all $T_j^{(M)}$ have about the same value so that $\sum_j |T_j^{(M)}| \sim \sum_j e^{Ma_j}$. Remember, however, that the probability distribution of $T_j^{(M)}$ has long tails, and, consequently, there will always be some diagrams (their percentage is negligible) with values of $|T_j^{(M)}|$ much larger than $e^{Ma_j}$. The contribution of these diagrams to the sum $\sum_j e^{Ma_j}$ is neglected when one makes the assumption of strong correlation. There is one case, however, when the contribution of these "tail" diagrams may be important: if $a_j \to -\infty$, $\sum_j e^{Ma_j}$ becomes so small that the tail contribution may dominate. The most favorable case for tail domination is when the probability distribution of $\epsilon_i$ consists of two widely separated peaks, since then one can easily see from the definition[8] of $a_j$ that $a_j \to -\infty$ and there is a negligibly small fraction of diagrams making a significant contribution, each in such a way that they dominate the sum $\sum_j T_j^{(M)}$. We consider below a specific example of this.

According to our remarks there are probability distributions $p_0(\epsilon_i)$ such that the assumption of strong correlation is inadequate. For such $p_0(\epsilon_i)$ the CPA approximation for calculating the quantity $a_j$ fails too. The reason is that $a_j$ involves[8] *logarithmic* averages which approach zero for the $p_0(\epsilon_i)$ we consider; on the other hand CPA reduces logarithmic averages to ordinary averages which remain finite for the $p_0(\epsilon_i)$ we consider. Thus we can conclude that there are $p_0(\epsilon_i)$ such that both the assumption of strong correlation and the CPA fail. For these $p_0(\epsilon_i)$ the assumption of strong correlation severely *underestimates* the $\sum_j T_j^{(M)}$, while the CPA severely *overestimates* $\sum T_j^{(M)}$. There is consequently a tendency for cancellation of the mistakes which probably explains the success of the present approach. As a matter of fact in the extremely unfavorable case of a binary-alloy distribution with $\delta \to \infty$ the cancellation of the errors is almost complete as is shown below.

In the limit $\delta \to \infty$ the only way for an electron, being initially in an $A$ site, to propagate is by finding paths of exclusively $A$ sites. Thus in this case the diagrams that contribute to $\Delta_{\vec{0}}^{(M)}$ are diagrams passing exclusively through $A$ sites. Hence the true localization function should be of the form

$$L(E\approx\epsilon_A)=[\Lambda_M V^M|\, g_A^M(E\approx\epsilon_A)|\,]^{1/M}, \tag{6.1}$$

where $g_A(E\approx\epsilon_A)$ denotes a quantity like that defined in Eq. (4.3) but with the average being a conditional one; namely, all the sites $\vec{n}_1, \vec{n}_2, \ldots, \vec{n}_M$ should be $A$ sites and $\Lambda_M$ is the number of $M$-step self-avoiding polygons passing through $A$ sites only. Further, if $K^M$ is the total number of $M$-step self-avoiding closed diagrams and $x^M$ is the probability that a particular diagram will step through all $A$ sites we then have

$$\Lambda_M = x^M K^M, \tag{6.2}$$

and we obtain

$$L(E\approx\epsilon_A)=xKV\,|\,g_A(E\approx\epsilon_A)|\,. \tag{6.3}$$

On the other hand, the general expression (3.4) for $L(E)$ gives $L(E\approx\epsilon_A)\to 0$ as $\delta\to\infty$ because all the $\tilde{G}$'s approach zero. Consider

$$\tilde{G}^{\vec{0}\cdots}_{\vec{n}_i}=\exp[x\ln\tilde{G}^{\vec{0}}_{\vec{n}_i,A}+(1-x)\ln\tilde{G}^{\vec{0}}_{\vec{n}_i,B}], \tag{6.4}$$

where $\ln\tilde{G}^{\vec{0}}_{\vec{n}_i,A}=\langle\ln|\tilde{G}^{\vec{0}\cdots}_{\vec{n}_i}|\rangle_{\mathrm{av},\vec{n}_i\equiv A}$ with a similar expression for $\tilde{G}^{\vec{0}\cdots}_{\vec{n}_i,B}$; but

$$\tilde{G}^{\vec{0}\cdots}_{\vec{n}_i,B}(E\approx\epsilon_A)\xrightarrow[\delta\to\infty]{}\frac{1}{\delta}$$

and by substituting this in (6.4) we obtain

$$\tilde{G}^{\vec{0}}_{\vec{n}_i}\xrightarrow[\delta\to\infty]{}\left(\frac{1}{\delta}\right)^{1-x}.$$

This shows the failure of the general $L(E)$ expression in this particular case.

Consider now the general expression for $L(E)$ but use the CPA to calculate the averages. Then we obtain

$$L(E\approx\epsilon_A)\approx L_{\mathrm{CPA}}(E\approx\epsilon_A)=KVg_{\mathrm{CPA}}(E\approx\epsilon_A). \tag{6.5}$$

But

$$g_{\mathrm{CPA}}(E\approx\epsilon_A)\equiv xg_{A,\mathrm{CPA}}(E\approx\epsilon_A) + (1-x)g_{B,\mathrm{CPA}}(E\approx\epsilon_A), \tag{6.6}$$

where

$$g_{B,\mathrm{CPA}}(E\approx\epsilon_A)\xrightarrow[\delta\to\infty]{}\frac{1}{\delta}.$$

Thus

$$L_{\mathrm{CPA}}(E\approx\epsilon_A)=xKV|\,g_{A,\mathrm{CPA}}(E\approx\epsilon_A)|\,, \tag{6.7}$$

which is roughly the same as the correct result (6.3).

This rather systematic cancellation of possible errors introduced by the assumption of strong correlation and the CPA demands that improvements in the procedures for calculating averages should be considered in conjunction with an effort to improve the assumption of strong correlation. Otherwise improvements in CPA may be proved counterproductive.

## VII. CONCLUSIONS

We have introduced in this paper a new refined criterion for localization, denoted as the $G^{\vec{0}}$ approach. The $G^{\vec{0}}$ approach employs the general localization function obtained by Economou and Cohen on the basis of the assumption of strong correlation among the diagrams contributing to the self-energy $\Delta_{\vec{0}}$. It also makes use of the coherent-potential approximation (or, more generally, any effective-medium theory) for the calculation of the averages entering the general expression for the localization function. By examining several particular examples, comparing with other approaches, testing against numerical results and against limiting cases where exact results are available, we have demonstrated that the $G^{\vec{0}}$ approach is far superior than the other approaches examined in this paper.

The success of the $G^{\vec{0}}$ approach was traced to a rather systematic cancellation of the possible errors introduced by the only two sources of possibly significant mistakes left in the theory, namely, the assumption of strong correlation and the use of CPA for calculating averages.

Any further progress in the subject should require an improved way to handle the correlations among the diagrams without omitting the self-energies in the propagators.

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[1]N. F. Mott and E. A. Davis, *Electronic Processes in Non-Crystalline Materials* (Oxford U. P., London, 1971).

[2]E. N. Economou, *New Developments in Semiconductors*, edited by P. R. Wallace, R. Harris, and M. J. Zuckermann (Noordhoff, Leyden, 1973); E. N. Economou, M. H. Cohen, K. Freed, and S. Kirkpatrick, in *Amorphous and Liquid Semiconductors*, edited by J. Tauc (Plenum, New York, 1974); E. N. Economou, in The Proceedings of the New Delhl Winter School 1972 (unpublished); D. J. Thouless, Phys. Rep. 13C, 94 (1974).

[3]P. W. Anderson, Comments Solid State Phys. 2, 193 (1970).

[4]P. W. Anderson, Phys. Rev. 109, 1492 (1958).

[5]J. M. Ziman, J. Phys. C 2, 1230 (1969).

[6]D. J. Thouless, J. Phys. C 3, 1559 (1970).

[7]M. Kikuchi, J. Phys. Soc. Jpn. 29, 296 (1970).

[8]E. N. Economou and Morrel H. Cohen, Phys. Rev. Lett. 25, 1445 (1970); Phys. Rev. B 5, 2931 (1972).

[9]D. J. Thouless, J. Non-Cryst. Solids 8–10, 461 (1972).

[10]D. C. Herbert and R. Jones, J. Phys. C 4, 1145 (1971).

[11]T. Lukes, J. Non-Cryst. Solids 8–10, 470 (1972).

[12]Although this basic picture is the underlying thesis used

throughout this work, different points of view have also been conjectured: See, e.g., M. A. Ball, J. Phys. C 4, 1747 (1971), who proposed a model in which the localized states are degenerate with nonlocalized ones. More recently, see N. Kumar and R. R. Subramanian, J. Phys. C 7, 1817 (1974).

[13]R. Haydock and A. Mookerjee, J. Phys. C 7, 3001 (1974).

[14]S. F. Edwards, in *New Developments in Semiconductors*, edited by P. R. Wallace, R. Harris, and M. J. Zuckermann (Noordhoff, Leyden, 1973), p. 249.

[15]K. F. Freed, Phys. Rev. B 5, 4802 (1972).

[16]R. Abou-Chacra, P. W. Anderson, and D. J. Thouless, J. Phys. C 6, 1734 (1973).

[17]A. R. Bishop, Philos. Mag. 27, 651 (1973); 27, 1489 (1973); J. Phys. C 6, 2089 (1973); report, 1974 (unpublished).

[18]D. C. Licciardello and E. N. Economou, Solid State Commun 15, 969 (1974).

[19]N. F. Mott, Phys. Rev. Lett. 31, 466 (1973)

[20]J. T. Edwards and D. J. Thouless, J. Phys. C 5, 807 (1972).

[21]K. Schönhammer and W. Brenig, Phys. Lett. A 42, 447 (1973), and private communication.

[22]E. N. Economou, S. Kirpatrick, M. H. Cohen, and T. P. Eggarter, Phys. Rev. Lett. 25, 250 (1970).

[23]S. R. Broadbent and J. M. Hammersley, Proc. Camb. Philos. Soc. 53, 629 (1957).

[24]V. K. S. Shante and S. Kirkpatrick, Adv. Phys. 30, 325 (1971), and references therein.

[25]In a recent paper, B. J. Last and D. J. Thouless, J. Phys. C 7, 699 (1974), examine the possibility of a power-law localization. They present some numerical evidence for such a hypothesis as well as some theoretical support.

[26]E. Feenberg, Phys. Rev. 74, 206 (1948).

[27]K. M. Watson, Phys. Rev. 105, 1388 (1957).

[28]R. Abou-Chacra and D. J. Thouless, J. Phys. C 7, 65 (1974).

[29]A. Mookerjee, J. Phys. C 7, 4069 (1974).

[30]E. N. Economou and Morrel H. Cohen, Phys. Rev. B 4, 396 (1971).

[31]P. W. Anderson, Proc. Natl. Acad. Sci. USA 69, 1097 (1972).

[32]R. A. Abram and S. F. Edwards, J. Phys. C 5, 1183 (1972); 5, 1196 (1972).

[33]B. Velicky, S. Kirkpatrick, and H. Ehrenreich, Phys. Rev. 175, 747 (1968).

[34]R. J. Elliott, J. A. Krumhansl, and P. L. Leath, Rev. Mod. Phys. 46, 437 (1974).

[35]P. Soven, Phys. Rev. 156, 809 (1967); D. W. Taylor, Phys, Rev. 156, 1017 (1967).

[36]Equation (4.19) includes for the square and simple-cubic lattices the additional approximation of treating each $m_i m_j$ pair as a next-nearest-neighbor spacial relationship, which is not exactly true. For example, the pairs which are separated by $2a$ are strictly speaking next next-nearest-neighbor pairs. We expect this simplification will have little or no effect on our results, and we do it only for convenience. For the diamond lattice this problem does not arise and the relation (4.19) is exact.

[37]D. C. Licciardello and E. N. Economou, Solid State Commun. 12, 1275 (1973).

[38]K. Schönhammer, Phys. Lett. A 36, 181 (1971).

[39]Actually the percentage of extended states in a given subband as $\delta \to \infty$ should be equal or *less than* the corresponding percolation probability since quantum states associated with a classically extended path may become localized due to surface scattering by the surrounding infinite walls.

[40]K. E. Khor and P. V. Smith, J. Phys. C 4, 2029 (1971); 4, 2041 (1971).

[41]A. Mookerjee, Ph. D. thesis (Cambridge University, 1972) (unpublished).

[42]E. N. Economou, Phys. Rev. Lett. 28, 1206 (1972).

[43]D. C. Licciardello, E. N. Economou, and C. Papatriantaphillou, *Amorphous Magnetism*, edited by H. O. Hooper and A. M. de Graaf (Plenum, New York, 1973), p. 387.

[44]See also F. Brouers, J. Phys. C 1, 1 (1971); 773 (1971).

[45]N. Kumar, J. Heinrichs, and A. A. Kumar (unpublished).

[46]A. R. Bishop, Phys. Lett. A 49, 5 (1974).