Science of Superconductivity, Stanford, 1969 (unpublished).
[9]W. D. Grobman, J. Appl. Phys. 42, 1456 (1971).
[10]A. M. Toxen and R. D. Parks (private communication).
[11]See Figs. 10 and 11.
[12]O. Lindberg, Proc. IRE 40, 1414 (1952).
[13]In addition, R. J. Gambino, W. D. Grobman, and A. M. Toxen (unpublished) will report on the Kondo behavior of $CeIn_3$.
[14]D. K. MacDonald, *Thermoelectricity: An Introduction to the Principles* (Wiley, New York, 1962), Sec. 4.1.1.
[15]L. B. Welsh, A. M. Toxen, and R. J. Gambino, Phys. Rev. (to be published).
[16]The use of γ rather than the bare density of states does not affect the validity of the argument since we are only making qualitative arguments about the curves in Fig. 2. Equation (2) assumes the rigid-band model.
[17]K. Levin, B. Velicky, and E. Ehrenreich, Phys. Rev. B 2, 1771 (1970).
[18]W. D. Grobman, J. Phys. Chem. Solids (to be published).
[19]J. M. Ziman, *Electrons and Phonons* (Oxford U. P., London, 1960).
[20]G. Gladstone, M. A. Jensen, and J. R. Schrieffer, *Superconductivity*, edited by R. D. Parks (Marcel Dekker, New York, 1969), Chap. 13.
[21]Reference 19, p. 487.
[22]A. C. Smith, J. F. Janak, and R. B. Adler, *Electronic Conduction in Solids* (McGraw-Hill, New York, 1966), Sec. 9.1.

PHYSICAL REVIEW B VOLUME 5, NUMBER 8 15 APRIL 1972

Existence of Mobility Edges in Anderson's Model for Random Lattices*

E. N. Economou† and Morrel H. Cohen
The James Franck Institute, The University of Chicago, Chicago, Illinois 60637
(Received 15 April 1971)

Anderson's theory of localization is critically reviewed and extended with particular emphasis on some controversial aspects. It is shown that when the randomness exceeds a certain critical value, all the eigenstates become localized in agreement with Anderson's original result. When the randomness is less than this critical value, the tails of a band consist of localized states. The character of the states changes sharply from localized to extended at mobility edges, in agreement with the Mott-CFO (Cohen-Fritzsche-Ovshinsky) model. As the randomness increases, the mobility edges move inwards into the band and they coincide at Anderson's critical value of the randomness. A criterion is developed which, under certain conditions, imposes upper limits on the extent of the portions of the energy spectrum consisting of extended states. These conditions are fulfilled exactly in the case of a Lorentzian distribution of single-site energies and approximately within the framework of any single-site approximation. Thus in the Lorentzian case upper bounds are obtained for the positions of the mobility edges and the critical value of the randomness for which Anderson's transition takes place. These results are in agreement with the Mott-CFO model.

I. INTRODUCTION

Considerable attention has been given recently to the problem of the electronic structure of disordered materials. Perhaps the most significant contribution to the field is Mott's notion[1] that there exist energies of sharp transition from localized states in the band tails to extended states in the interior of the band.[1-3] This notion is based on results obtained by Anderson in a remarkable paper entitled "The Absence of Diffusion in Certain Random Lattices"[4] as well as some other results suggesting the existence of localized states in the extreme tails of the bands in disordered materials.[5-12]

Anderson[4] considers what is essentially a tight-binding model, in which a single band is formed from s-like atomic orbitals with energies $\epsilon_{\vec{l}}$, corresponding to the site $\vec{l}$. The bandwidth is $B = 2VZ$, where V is an overlap energy integral and Z is the coordination number. Anderson introduces randomness into the system by assuming that the quantities $\epsilon_{\vec{l}}$ are random variables possessing a common distribution function with a width Γ around the mean value. He finds that there is a critical value $\Gamma_c \sim B \ln Z$ of Γ such that for $\Gamma \geq \Gamma_c$ the states at the middle of the band (and by inference all the states) are localized. On the other hand, for $\Gamma < \Gamma_c$ the states in the middle of the band are extended. Anderson has demonstrated that his results hold only if the off-diagonal matrix elements $V_{\vec{l}\,\vec{m}}$ are of range sufficiently short to give rise to bands of finite width. His main line of argument is as follows: The localizability of an eigenstate belonging to an eigenenergy $E = 0$ is related to the convergence of a renormalized perturbation expansion (RPE) for the self-energy $\Delta_{\vec{0}}(0)$. Since one is dealing with random quantities, the convergence is a matter of probability. We show here by comparison with a geometrical series that the series for $\Delta_{\vec{0}}(0)$ ($E = 0$ corresponds to the middle of the band) converges

with probability $p \to 1$ if $\Gamma \geq \Gamma_c$ and diverges with probability $p \to 1$ if $\Gamma < \Gamma_c$, thus proving the original statement. One expects on physical grounds that the last eigenstates which will become localized as the randomness increases are those with eigenenergies lying in the middle of the band, and consequently their localizability implies the absence of any extended states in the system. This disappearance of extended states from the system as the randomness exceeds a certain critical value is termed Anderson's transition by Mott. There is experimental evidence supporting Anderson's results, as has been pointed out by Mott.[13,14]

In Anderson's paper there were no suggestions for the energy distribution of those extended states which exist when the randomness is less than critical. The work on the eigenstates in the tails of the bands in disordered systems[5-12] is complementary to that of Anderson's, covering situations of small randomness. These two disjoint aspects of the problem were synthesized by Mott[1] into a single picture through the introduction of critical energies E_c separating regions in which all the states are localized from those in which all states are extended. The energies E_c depend, of course, on the characteristics of the system and, in particular, on the degree of randomness. In the framework of this picture, Anderson's transition can be understood as a disappearance of regions of extended states caused by coincidence of two adjacent E_c. This same picture was later arrived at independently by Cohen, Fritzsche, and Ovshinsky[2] (CFO) in their model for amorphous semiconducting alloys. In view of the experimental evidence and the reasonableness of the basic assumptions there seems little doubt about the basic correctness of the Mott-CFO model. In this paper we shall show how one can justify the Mott-CFO model by using an approach based on that of Anderson's.

Anderson's original paper is well known for being very complicated and difficult to read. Ziman[3] achieved considerable simplification and clarity of presentation at the expense of some rigor in the argument. Thouless[15] has achieved further clarification, has improved the mathematical analysis somewhat, and has given a critical discussion of some aspects of the paper. Nevertheless, some aspects of Anderson's paper are still unclear. We therefore present in this paper a critical review of Anderson's theory without restricting ourselves to a specific energy, the middle of the band, as Anderson did, but examining the problem as a function of energy.[3] This slight generalization, when coupled with a detailed analysis of the RPE for $\Delta_{\vec{0}}(E)$, permits a first-principles derivation of the Mott-CFO picture for the particular model that we examine through the introduction of a localization function[16] $L(E)$ such that the localized (extended) eigenstates correspond to $L(E) < 1$ (> 1) and the mobility edges E_c to $L(E_c) = 1$. Moreover, considerable progress has been achieved in estimating $L(E)$ under certain conditions.[16,17] which are exactly satisfied in the case where the single-site energies follow a Lorentzian distribution and approximately so within the framework of any single-site approximation.[18] Under these conditions a function $F(E)$ exists such that when $F(E) < 1$, $L(E) < 1$; the function $F(E)$ is no more difficult to calculate than is the average Green's function.

There have been claims that Anderson's proof of localization is so basically incorrect that localization does not exist.[3,19,20] These refutations of Anderson's results have been dealt with already by Anderson,[21] Mott,[22] and Thouless.[15] We hope that our analysis of Anderson's model together with the new exact results will end debate on the existence of localization.

In Sec. II the connection between the localizability of a state and the analytical properties of the self-energy is examined. The analytical properties are related to the convergence (or divergence) of a renormalized perturbation series expansion for this quantity. In Sec. III the problem of the convergence of this series is examined. Since the terms of the series are random variables, the convergence (or divergence) of the series for a given energy is a matter of probability. A function $L(E)$ is introduced and it is shown that when $L(E) < 1$ the series converges with probability unity and when $L(E) > 1$ the series diverges with probability unity. In Sec. IV estimates of the function $L(E)$ are presented and the results so obtained are compared to the similar ones of Anderson[4] and Thouless.[15] In Sec. V it is shown that under certain conditions a function $F(E)$ can be defined such that $L(E) < 1$ when $F(E) < 1$; moreover, the calculation of the function $F(E)$ is of the same difficulty as calculating the average Green's function. The particular case of the Lorentzian distribution of the single-site energies is considered and some exact results are derived. In Sec. VI we conclude this paper by discussing some interesting aspects of the present approach in relation to the status of the theory of disordered materials.

II. ROLE OF SELF-ENERGY, ITS ANALYTIC PROPERTIES, AND ITS PERTURBATION EXPANSIONS

Anderson has considered the motion of a particle in a three-dimensional array of potential wells such that in each well $\vec{n}$ the particle can occupy a Wannier state $|\vec{n}\rangle$ of energy $\epsilon_{\vec{n}}$. The Hamiltonian is assumed to be

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

where $V_{\vec{l}\vec{m}}$ is assumed to satisfy the periodicity condition

$$V_{\vec{l}\vec{m}} = V_{\vec{0},\vec{m}-\vec{l}} , \tag{2.2}$$

and $V_{\vec{l}\vec{l}} = 0$. The disorder is introduced into the system by allowing the quantities $\epsilon_{\vec{m}}$ to be random variables; any two quantities $\epsilon_{\vec{n}}$, $\epsilon_{\vec{l}}$ are taken as statistically independent whenever the distance $r_{\vec{n}\vec{l}}$ is larger than a finite correlation length. This eliminates long-range order from the system and is the basic requirement for the derivation of the Mott-CFO model. However, when explicit numerical results are sought, we shall make the unnecessary but simplifying assumption that the distribution function for the set $\{\epsilon_{\vec{n}}\}$ is given by

$$P(\{\epsilon_{\vec{n}}\}) = \prod_{\vec{n}} P(\epsilon_{\vec{n}}) . \tag{2.3}$$

If $V_{\vec{l}\vec{m}}$ in (2.1) were identically zero, then the eigenstates of H would be just the states $|\vec{n}\rangle$ which are by definition localized. On the other hand, if $V_{\vec{l}\vec{m}}$ were not identically zero and the quantities $\epsilon_{\vec{m}}$ were all identical, then we would have a periodic case for which according to Bloch's theorem all the eigenstates are extended. In the present problem it is not *a priori* clear what is the nature of the eigenstates. One way to decide about the localizability of the eigenstates is to consider what happens to a particle which initially was localized in a certain region of space. If there are localized eigenstates in the neighborhood of the region considered, the particle will have finite probability of being initially in each one of these eigenstates. Since these probabilities are time independent, there will be a finite probability of rediscovering the particle at the initial region as $t \to \infty$. On the other hand, if no localized states exist in the neighborhood of the region considered, the particle will diffuse away, and the probability of rediscovering it in the initial region will approach zero as $t \to \infty$. Thus, following Anderson, our criterion for the nature of the eigenstates is the behavior of the probability of rediscovering the particle in an initially ($t = 0$) localized state as $t \to \infty$.

More specifically, the particle is assumed to be initially at the site $\vec{0}$ with a wave function $|\vec{0}\rangle$. For $t > 0$, the wave function will be

$$\psi(t) = \sum_{\vec{n}} c_{\vec{n}}(t) |\vec{n}\rangle . \tag{2.4}$$

The quantity of interest is $p_{\vec{0}\vec{0}} = \lim |c_{\vec{0}}(t)|^2$, as $t \to \infty$, which gives the probability of finding the particle in the state $|\vec{0}\rangle$ at $t = \infty$, if initially ($t = 0$) it was in $|\vec{0}\rangle$. The probability $p_{\vec{0}\vec{0}}$ depends on the set of variables $\epsilon_{\vec{n}}$. According to what was said before, if for a set of values $\{\epsilon_{\vec{n}}\}$ of these variables, $p_{\vec{0}\vec{0}} = 0$, then there are no eigenfunctions of H localized near the site $\vec{0}$. On the other hand, if $p_{\vec{0}\vec{0}} \neq 0$, such localized eigenstates exist. Using the relation[19]

$$c_{\vec{0}}(t) = i \lim_{\eta \to 0^+} \int_{-\infty+i\eta}^{\infty+i\eta} G_{\vec{0}}(E) e^{-iEt} \frac{dE}{2\pi} , \tag{2.5}$$

where

$$G_{\vec{0}}(E) = \langle \vec{0} | \frac{1}{E - H} | \vec{0} \rangle \tag{2.6}$$

is the $\vec{0}$, $\vec{0}$ matrix element of the Green's function for the system, we can express $p_{\vec{0}\vec{0}}$ in terms of the Green's function as follows:

$$p_{\vec{0}\vec{0}} = \lim_{s \to 0^+} \frac{s}{\pi} \int_{-\infty}^{\infty} dE\, G_{\vec{0}}(E + is) G_{\vec{0}}(E - is) . \tag{2.7}$$

We define $p_{\vec{0}\vec{n}}$ as the probability of finding the particle for $t = \infty$ in the state $|\vec{n}\rangle$ if initially ($t = 0$) it was in $|\vec{0}\rangle$ Then (2.7) can be generalized to

$$p_{\vec{0}\vec{n}} = \lim_{s \to 0^+} \frac{s}{\pi} \int_{-\infty}^{\infty} dE\, G_{\vec{0}\vec{n}}(E + is) G_{\vec{n}\vec{0}}(E - is) , \tag{2.8}$$

where $G_{\vec{l},\vec{r}}$ is the $\vec{l}$, $\vec{r}$ matrix element of the Green's function for our system. Using the identity

$$\sum_{\vec{n}} G_{\vec{0}\vec{n}}(E + is) G_{\vec{n}\vec{0}}(E - is) = \frac{1}{2is} [G_{\vec{0}}(E - is) - G_{\vec{0}}(E + is)] \tag{2.9}$$

and the well-known relation

$$n_{\vec{0}}(E) = \frac{1}{\pi} \lim_{s \to 0^+} \operatorname{Im} G_{\vec{0}}(E - is) , \tag{2.10}$$

where $n_{\vec{0}}(E)$ is the contribution to the density of states from the site $\vec{0}$, we can prove the physically obvious relation

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

$$= \int_{-\infty}^{\infty} dE \lim_{s \to 0^+} \frac{1}{\pi} \operatorname{Im} G_{\vec{0}}(E - is) = \int_{-\infty}^{\infty} n_{\vec{0}}(E)\, dE = 1 . \tag{2.11}$$

The last step follows from the original assumption that there is just one state per site. Use has also been made of the relation

$$G_{\vec{0}\vec{n}}(E + is) = [G_{\vec{n}\vec{0}}(E - is)]^* , \tag{2.12}$$

which is a direct consequence of the hermiticity of the Hamiltonian.

Equation (2.7) can be rewritten as

$$p_{\vec{0}\vec{0}} = \int_{-\infty}^{\infty} f_{\vec{0}}(E)\, dE , \tag{2.13}$$

where

$$f_{\vec{0}}(E) = \lim_{s \to 0^+} \frac{s}{\pi} G_{\vec{0}}(E + is) G_{\vec{0}}(E - is) \tag{2.14}$$

is a nonnegative quantity. $G_{\vec{0}}(E)$ can be expressed in terms of the "self-energy" $\Delta_{\vec{0}}(E)$, defined by

$$G_{\vec{0}}(E) = \frac{1}{E - \epsilon_{\vec{0}} - \Delta_{\vec{0}}(E)} . \tag{2.15}$$

Using (2.10) and (2.15), $f_{\vec{0}}(E)$ can be written as

$$f_{\vec{0}}(E)=\frac{1}{\pi}\lim_{s\to 0^+}\frac{s}{2is-[\Delta_{\vec{0}}(E+is)-\Delta_{\vec{0}}(E-is)]}\times\left(\frac{1}{E-is-\epsilon_{\vec{0}}-\Delta_{\vec{0}}(E-is)}-\frac{1}{E+is-\epsilon_{\vec{0}}-\Delta_{\vec{0}}(E+is)}\right)$$

$$=n_{\vec{0}}(E)\lim_{s\to 0^+}\frac{1}{1-[\Delta_{\vec{0}}(E+is)-\Delta_{\vec{0}}(E-is)]/2is}\,. \tag{2.16}$$

From (2.16) we see that in order to have $f_{\vec{0}}(E)\neq 0$ for a certain E we should have (i) $n_{\vec{0}}(E)\neq 0$ (which means that eigenstates corresponding to energy E and overlapping with the state $|\vec{0}\rangle$ should exist) and

$$\text{(ii)}\quad Z_{\vec{0}}(E)\equiv\lim_{s\to 0^+}\frac{1}{1-[\Delta_{\vec{0}}(E+is)-\Delta_{\vec{0}}(E-is)]/2is}\neq 0\,. \tag{2.17}$$

We know, however, that extended states do not contribute to $p_{\vec{0}\vec{0}}$ and consequently for these states $f_{\vec{0}}(E)=0$, which, in turn, implies[23] that $Z_{\vec{0}}(E)=0$. Thus if $Z_{\vec{0}}(E)\neq 0$, the corresponding eigenstates cannot be extended and are necessarily localized.

From Eq. (2.17) it follows that a branch cut in $G_{\vec{0}}$ along the real axis corresponds to extended states. Conversely, it is not difficult to show that the extended states correspond to a branch cut. The localized states, on the other hand, correspond to $Z_{\vec{0}}(E)\neq 0$ and, of course, $n_{\vec{0}}(E)\neq 0$. The analytical behavior of $G_{\vec{0}}(E)$ for a typical configuration of a random system in the range of localized states is quite peculiar, as has already been discussed by Thouless.[15] There is a dense distribution at poles, but only a finite number of these have residues larger than any preset small value in a finite range of energy. Considerable simplification of the whole analysis results if one makes the physically justifiable assumption of considering a localized eigenfunction as completely confined within a finite volume, neglecting its extreme tails. In this case in the region of localized states, if any, $G_{\vec{0}}(E)$ has a finite number of isolated simple poles.

Consequently all singularities of $G_{\vec{0}}(E)$ and $\Delta_{\vec{0}}(E)$ lie on the real axis and are either simple poles (corresponding to localized states) or branch cuts (corresponding to extended states). The simple poles of $G_{\vec{0}}(E)$ and $\Delta_{\vec{0}}(E)$ never coincide, since the poles of $\Delta_{\vec{0}}(E)$ correspond to zeros of $G_{\vec{0}}(E)$. Thus, when $Z_{\vec{0}}(E)$ vanishes because of a pole in $\Delta_{\vec{0}}(E)$, it implies nothing about states of energy E because $G_{\vec{0}}(E)$ and therefore $n_{\vec{0}}(E)$ vanish. Using the general relation[19]

$$G_{\vec{n}\vec{m}}(E;\cdots\epsilon_{\vec{r}}'\cdots)=G_{\vec{n}\vec{m}}(E;\cdots\epsilon_{\vec{r}}\cdots)+G_{\vec{n}\vec{r}}(E;\cdots\epsilon_{\vec{r}}\cdots)G_{\vec{r}\vec{m}}(E;\cdots\epsilon_{\vec{r}}\cdots)\times\frac{\epsilon_{\vec{r}}'-\epsilon_{\vec{r}}}{1-(\epsilon_{\vec{r}}'-\epsilon_{\vec{r}})G_{\vec{r}}(E;\cdots\epsilon_{\vec{r}}\cdots)}\,, \tag{2.18}$$

and taking the limit $\epsilon_{\vec{r}}'\to\infty$, one can easily show from (2.15) that the poles of $\Delta_{\vec{0}}(E)$ correspond to poles of the diagonal elements $G_{\vec{n}}^{\vec{0}}$, where $\vec{n}$ is such that $G_{\vec{0}\vec{n}}$ is different from zero and a superscript $\vec{1}$ indicates that the corresponding quantity has been calculated for $\epsilon_{\vec{1}}\to\infty$. It is obvious from (2.15) that the branch cuts of $G_{\vec{0}}(E)$ and $\Delta_{\vec{0}}(E)$ always coincide. Thus $n_{\vec{0}}(E)$ is finite when $Z_{\vec{0}}(E)$ vanishes along a branch cut, corresponding to extended states. Having eliminated poles and branch cuts in $\Delta_{\vec{0}}(E)$ from consideration, we see that an eigenstate overlapping with the state $|\vec{0}\rangle$ and with eigenenergy E is localized if and only if the self-energy $\Delta_{\vec{0}}(E)$ is analytic at E.

In order to study the analytic properties of the self-energy $\Delta_{\vec{0}}(E)$, we first need to express it in terms of known quantities. One way to achieve this is the perturbation-series (PS) solution for $\Delta_{\vec{0}}(E)$, which has the form

$$\Delta_{\vec{0}}(E)=\sum_{\vec{n}}V_{\vec{0}\vec{n}}\frac{1}{E-\epsilon_{\vec{n}}}V_{\vec{n}\vec{0}}+\sum_{\vec{n}\vec{m}}V_{\vec{0}\vec{n}}\frac{1}{E-\epsilon_{\vec{n}}}V_{\vec{n}\vec{m}}\frac{1}{E-\epsilon_{\vec{m}}}V_{\vec{m}\vec{0}}+\cdots\,, \tag{2.19}$$

and can be represented by all paths starting from the site $\vec{0}$ and only returning to it at the end. To each step from one site $\vec{l}$ to another site $\vec{m}$ there corresponds a factor $V_{\vec{l}\vec{m}}$, and to each site $\vec{n}$ ($\vec{n}\neq\vec{0}$) there corresponds a factor $1/(E-\epsilon_{\vec{n}})$.

If the matrix elements $V_{\vec{l}\vec{m}}$ fall off at large distances $|\vec{r}_{\vec{l}}-\vec{r}_{\vec{m}}|$ slowly enough, even two-step processes (corresponding to lowest order in the PS) will delocalize the electron. Anderson[4] demonstrated that the matrix elements must be of sufficiently short range—falling off faster than $|r-r_m|^{-3}$—for there to be no transport in the lower orders of the PS. This is exactly the condition for having bands of finite width. We are interested only in those cases where the energy bands are of finite width so that the matrix elements $V_{\vec{l}\vec{m}}$ are automatically of sufficiently short range and thus localization persists to any finite order in the PS. To simplify the presentation we shall assume that

$$V_{\vec{l}\vec{m}}=V \text{ when } \vec{l},\ \vec{m} \text{ are nearest neighbors}$$
$$=0 \text{ otherwise}\,. \tag{2.20}$$

Equation (2.19) has a meaning only as long as the PS converges. If the quantities $\epsilon_{\vec{n}}$ are all finite, the PS for $\Delta_{\vec{0}}(E)$ converges for large E, and $\Delta_{\vec{0}}(E)$ is analytic in this region. As E approaches the origin the PS for $\Delta_{\vec{0}}(E)$ can diverge in two physically distinct ways: (a) because of the contribution of terms corresponding to paths of infinite extent, and (b) because of the contributions of portions of paths

going back and forth among a finite number of neighboring sites $\vec{l}$, $\vec{n}, \ldots, \vec{m}$ and possessing the property that

$$\left| \frac{1}{E-\epsilon_{\vec{l}}} V_{\vec{l}\vec{n}} \cdots \frac{1}{E-\epsilon_{\vec{m}}} V_{\vec{m}\vec{l}} \right| > 1 . \qquad (2.21)$$

It is only the divergence of the first kind which implies the delocalization of the eigenstates by introducing branch cuts along the real energy axis and by mixing sites of infinite separation. The divergence of the second kind exists even in systems of finite extent and corresponds to changes in the position of the isolated singular points (simple poles) of $G_{\vec{0}}(E)$, indicating that the localized eigenfunctions and their eigenenergies are not identical to those of the unperturbed situation. Thus the divergence of the second kind could be eliminated if in every stage of the perturbation expansion we changed the basis functions in such a way that they coincide with the eigenfunctions resulting from the perturbation approximation of the previous stage.

The PS for $\Delta_{\vec{0}}(E)$ in general diverges in a finite area of the complex E-plane symmetrical about the real axis with its extent along the real axis determined by the lower and upper bounds of the energy spectrum of the Hamiltonian (2.1) with $\epsilon_{\vec{0}} = \infty$. If the extremes of the spectrum correspond to localized [extended] states, the divergences there come through contributions of type (b) [(a)].

At this point it should be clear that Eq. (2.19) is not appropriate for our purpose of distinguishing between localized and extended states, since it has no meaning (diverges) in either case. On the other hand, an expression for $\Delta_{\vec{0}}(E)$ that will hold in one case only (localized or extended states) would be adequate for the purposes of the present investigation. This is exactly what is achieved by the renormalization method,[4] which eliminates the divergences of the second kind in such a way that the resulting renormalized perturbation expression for $\Delta_{\vec{0}}(E)$ holds everywhere on the complex E plane except along the branch cuts on the real axis.

To clarify the meaning of the renormalization approach we consider first what happens in a finite system. By allowing the dimensions of the system to grow larger and larger we shall eventually retrieve the results for an infinite system. We accomplish this program formally by introducing a set of Hamiltonians H_R differing from (2.1) in that

$$E_{\vec{m}} \to \infty \quad \text{for all } \vec{m} \text{ such that } r_{\vec{0}\vec{m}} > R , \qquad (2.22)$$

where R is a positive length. Obviously $H = \lim H_R$ as $R \to \infty$. We denote by G_R, Δ_R, etc., the Green's function, self-energy, etc., corresponding to the Hamiltonian H_R. For any finite R the quantity $\Delta_{\vec{0},R}(E)$ can be written in a renormalized form[4] using Watson's method,[24,25]

$$\Delta_{\vec{0},R}(E) = \sum_{\vec{n}\neq\vec{0}} V_{\vec{0}\vec{n}} \frac{1}{E-\epsilon_{\vec{n}}-\Delta^{\vec{0}}_{\vec{n},R}(E)} V_{\vec{n}\vec{0}} + \sum_{\substack{\vec{n}\neq\vec{0} \\ \vec{n}'\neq\vec{n},\vec{0}}} V_{\vec{0}\vec{n}'} \frac{1}{E-\epsilon_{\vec{n}'}-\Delta^{\vec{0},\vec{n}}_{\vec{n}',R}(E)} V_{\vec{n}'\vec{n}} \times \frac{1}{E-\epsilon_{\vec{n}}-\Delta^{\vec{0}}_{\vec{n},R}(E)} V_{\vec{n}\vec{0}} + \cdots , \qquad (2.23)$$

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 (2.23) can be represented by all paths starting from site $\vec{0}$ and returning to it. The restrictions on the summations mean that only paths which do not visit the same site twice must be considered. Thus for any finite system (finite R) the number of terms in (2.23) is finite, and consequently the renormalized perturbation series (RPS) for $\Delta_{\vec{0},R}$ ($R < \infty$) terminates. Note that the expression (2.23) is not an explicit solution for $\Delta_{\vec{0},R}$, since it contains the unknown quantities $\Delta^{\vec{0},\vec{1}}_{\vec{n},R}, \cdots$. These quantities, however, can be expressed through relations similar to (2.23). Substituting back into (2.23) and repeating the procedure, we obtain a continued-fraction-like expression for $\Delta_{\vec{0},R}(E)$ of the following form:

$$\Delta_{\vec{0},R} = \sum_{L} \sum\sum V_{\vec{0}\vec{n}_1} \cdots \frac{1}{E-\epsilon_{\vec{n}_L} - \sum_{N} \sum\sum V_{\vec{n}_L\vec{m}_1} \cdots \frac{1}{E-\epsilon_{\vec{m}_N} - \cdots} V_{\vec{m}_N\vec{n}_L}} V_{\vec{n}_L\vec{0}} . \qquad (2.24)$$

Since at each new step of the iteration procedure at least one additional site is absent, it follows that the continued-fraction-like expression (2.24) terminates after a finite number of steps large enough to exhaust all the sites within the sphere $(0, R)$. Thus formula (2.24) constitutes an explicit solution for $\Delta_{\vec{0},R}$ holding everywhere in energy.

Consider now what happens if $R = \infty$. Then both the RPS and the iteration procedure do not terminate. Hence possibilities of convergence or divergence of the renormalized perturbation expression (RPE) (2.24) arise. The convergence of the RPE for $\Delta_{\vec{0}}(E)$ is defined for each E as the existence of the limit

$$\lim_{R\to\infty} \Delta_{\vec{0},R}(E) = \Delta_{\vec{0}}(E) \quad \text{as } R \to \infty , \qquad (2.25)$$

which in turn implies the convergence of both the

RPS and the iteration procedure. Thus the RPE (2.24) diverges as $R \to \infty$ if either the RPS (2.23) or the iteration procedure implied in (2.23), or both, diverge.

It is not difficult to show that Eq. (2.25) is satisfied for every E except those lying along the branch cuts, as follows. Using the analytic properties of $\Delta_{\vec{0}}(E)$ and $\Delta_{\vec{0},R}(E)$, we can write

$$\Delta_{\vec{0},R}(E) = \sum_n \frac{f_{n,R}}{E - E_{n,R}} + \sum_i \frac{f_{i,R}}{E - E_{i,R}} , \qquad (2.26a)$$

$$\Delta_{\vec{0}}(E) = \int \frac{f(E')\,dE'}{E - E'} + \sum_i \frac{f_i}{E - E_i} , \qquad (2.26b)$$

where

$$f_{i,R} \to f_i \quad \text{as } R \to \infty , \qquad (2.27a)$$

$$E_{i,R} \to E_i \quad \text{as } R \to \infty , \qquad (2.27b)$$

$$\sum_{E<E_{n,R}<E+\Delta E} f_{n,R} \xrightarrow[R\to\infty]{} \int_E^{E+\Delta E} f(E')\,dE' . \qquad (2.27c)$$

In view of Eqs. (2.27) the convergence of $\Delta_{\vec{0},R}$ to $\Delta_{\vec{0}}$ as $R \to \infty$ depends on replacing the first sum in (2.26a) by the corresponding integral in (2.26b). If the difference $E - E_{n,R}$ remains finite as $R \to \infty$, this replacement is always permissible according to the definition of the integral. The difference $E - E_{n,R}$ remains finite as $R \to \infty$ if and only if E does not lie on the portions of the real axis where $f(E) \neq 0$, i.e., E does not lie on the branch cuts. If E lies on the branch cuts, Eq. (2.25) cannot be correct since $\Delta_{\vec{0}}(E)$ cannot be defined in this case. Thus the RPE for $\Delta_{\vec{0}}(E)$ [Eq. (2.24)] converges at a given energy E if and only if E does not lie on a branch cut. As has been already discussed, the RPE for $\Delta_{\vec{0}}(E)$ can diverge because either the series or the iteration procedure, or both, diverge. Detailed study of the one-dimensional case[26] strongly suggests that for the present three-dimensional case the convergence of the expression (2.24) is governed by the convergence of the series alone. In one dimension, any finite degree of randomness is enough to make the iteration procedure convergent[26] for every E.

It should be noted that the convergence of the RPS (2.23) should be examined as a self-consistency problem.[4] We assume in the beginning that E does not lie on the branch cuts since, otherwise, the terms of the RPS would not be defined. Then we know that the only singularities of the quantities $\Delta_{\vec{n}}^{\vec{0},\vec{r},\vec{1},\cdots}(E)$ are simple poles and the eigenstates, if any, are localized. Using this information, we can study the convergence of the series (2.23). If the series converges, then we have verified the initial assumption that E does not lie on the branch cuts. This last statement, however, assumes that the convergence of the series (2.23) is equivalent to the convergence of the RPE (2.24) as $R \to \infty$, since it is the latter that is equivalent to the assumed analytic structure of the quantities $\Delta_{\vec{n}}^{\vec{0},\vec{r},\vec{1},\cdots}(E)$. On the other hand, if the RPS (2.23) is found to diverge, it follows that the initial assumption that E does not lie on a branch cut is wrong and consequently the conclusion to be drawn is that the eigenenergies corresponding to E are extended and that even the individual terms of the series (2.23) are not defined for this E. This discussion can be summarized as follows: Assume that the series (2.23) is defined for every real E. Then the real E axis can be separated into portions in which the series either converges or diverges. In the regions of convergence the series is defined and the eigenstates, if any, are localized. The regions of divergence correspond to portions of the energy spectrum where all the eigenstates are extended and there the initial assumption that the series can be defined term by term is wrong.

We examine now a property of the terms of the RPS (2.23) which is essential for the study of its convergence. From (2.18) by taking the limit $\epsilon_{\vec{r}}' \to \infty$ we have

$$G_{\vec{n}\vec{m}}(E, \ldots, \epsilon_{\vec{r}} = \infty, \ldots) \equiv G_{\vec{n}\vec{m}}^{\vec{r}} = G_{\vec{n}\vec{m}}(E) - G_{\vec{n}\vec{r}}(E) G_{\vec{r}\vec{m}}(E)/G_{\vec{r}}(E) . \qquad (2.28)$$

From (2.28) it follows that the poles of $G_{\vec{n}\vec{m}}^{\vec{r}}(E)$ coincide with the zeros of $G_{\vec{r}}(E)$ if the indices $\vec{n}, \vec{m}$ are such that $G_{\vec{n}\vec{r}}$ and $G_{\vec{r}\vec{m}}$ are not negligible, i.e., if the distances $r_{\vec{r}\vec{n}}$ and $r_{\vec{r}\vec{m}}$ are finite; the poles in $G_{\vec{n}\vec{m}}(E)$ are canceled by those in the second term of (2.28). Let $T_i^{(N)}$ be one of the diagrams of Nth order of the RPS for $\Delta_{\vec{0}}(E)$. Then from (2.23) we have

$$T_i^{(N)} = V\, G_{\vec{n}_1}^{\vec{0}}\, V G_{\vec{n}_2}^{\vec{0},\vec{n}_1} \cdots G_{\vec{n}_N}^{\vec{0},\vec{n}_1,\ldots,\vec{n}_{N-1}}\, V . \qquad (2.29)$$

According to the property just established, the poles of $G_{\vec{n}_2}^{\vec{0}\vec{n}_1}$ coincide with the zeros of $G_{\vec{n}_1}^{\vec{0}}$, the poles of the next factor $G_{\vec{n}_3}^{\vec{0},\vec{n}_1,\vec{n}_2}$ with the zeros of $G_{\vec{n}_2}^{\vec{0},\vec{n}_1}$, and so on. This means that poles of each G in (2.29) are canceled by the zeros of the previous G. Thus the only poles of $T_i^{(N)}$ are the poles of the first factor and the only zeros are the zeros of the last one. If $\{E_p\}$ are the positions of poles of $G_{\vec{n}_1}^{\vec{0}}$ and $\{E_z\}$ the positions of the zeros of $G_{\vec{n}_N}^{\vec{0},\vec{n}_1,\cdots\vec{n}_{N-1}}$, then

$$G_{\vec{n}_1}^{\vec{0}} = \frac{G_{\vec{n}_1}^{\vec{0}'}}{\Pi_p (E - E_p)} \qquad (2.30)$$

and

$$G_{\vec{n}_N}^{\vec{0},\vec{n}_1,\ldots,\vec{n}_{N-1}} = \prod_z (E - E_z^i) G_{\vec{n}_N}^{\vec{0},\vec{n}_1,\ldots,\vec{n}_{N-1}'} . \qquad (2.31)$$

Using (2.30) and (2.31), Eq. (2.29) can be written as

$$T_i^{(N)} = V^{N+1} \prod_z (E - E_z^i) / \prod_p (E - E_p)$$

$$\times G^{\vec{0}'}_{\vec{n}_1} G^{\vec{0},\vec{n}_1}_{\vec{n}_2} \cdots G^{\vec{0},\vec{n}_1,\cdots,\vec{n}_{N-1}}_{\vec{n}_N}, \quad (2.32)$$

where the product $G^{\vec{0}'}_{\vec{n}_1} G^{\vec{0},\vec{n}_1}_{\vec{n}_2} \cdots G^{\vec{0},\cdots,\vec{n}_{N-1}}_{\vec{n}_N}$ is a smooth positive definite function of E. The latter follows from the fact that the product of G's in (2.32) has no zeroes and no poles and consequently it is either everywhere negative or everywhere positive. Examining the limiting case $E \to -\infty$ too, where we know that $T_i^{(N)}$ behaves like $|C|/E^N$, we can see that the product of G's is positive definite. It should be noted that the positions of the poles E_p are common for every diagram of any order, since, being the poles of the quantity $G^{\vec{0}}_{\vec{n}}(E)$, they are the eigenenergies of the Hamiltonian $H^{\vec{0}}$ corresponding to the eigenstates localized in the vicinity of the site $\vec{0}$. Consequently the factor $1/\Pi_p(E-E_p)$ is a common factor of every term in the RPS (2.23) and thus

$$\Delta^{\vec{0}}_{\vec{0}}(E) = \frac{1}{\Pi_p(E-E_p)} \sum_N \sum_j V^{N+1} \times \prod_z (E-E_z^j) G^{\vec{0}'}_{\vec{n}_1} G^{\vec{0},\vec{n}_1}_{\vec{n}_2} \cdots G^{\vec{0},\cdots,\vec{n}_{N-1}}_{\vec{n}_N}, \quad (2.33)$$

where the terms to be summed are now analytic everywhere. Note that Eq. (2.33) implies that the poles of $\Delta^{\vec{0}}_{\vec{0}}(E)$ coincide with the poles of $G^{\vec{0}}_{\vec{0}\vec{n}}$, or with the zeros of $G_{\vec{0}}(E)$ as it should be. It is worthwhile to remember that this description is valid as long as it is self-consistent, i.e., as long as the series (2.33) converges. Divergence of the series (2.33) implies lack of self-consistency and consequently the existence of extended states.

If we define the $\mathrm{Im}\Delta(E)$ as $\lim \mathrm{Im}\Delta(E-is)$ as $s \to 0^+$, then we can see from (2.33) that when the RPS converges, $\mathrm{Im}\Delta^{\vec{0}}_{\vec{0}}(E)$ is zero except at a finite number of points, coinciding with the zeros of $G_{\vec{0}}(E)$, where δ-function singularities appear. This point has been overlooked in the literature[3] and incorrect statements have been made suggesting that the localizability of states is equivalent to the reality of $\Delta_{\vec{0}}$ everywhere. In contrast, when the states are extended [i.e., when the series (2.33) diverges], $\mathrm{Im}\Delta_{\vec{0}}$ is a continuous nonzero function. This basic difference in the behavior of $\mathrm{Im}\Delta_{\vec{0}}$ for localized and extended states is wiped out if one tries to average the function $\Delta_{\vec{0}}$ over all possible values of $\{\epsilon_{\vec{m}}\}$, since then, even in the case of convergence, the δ functions in $\mathrm{Im}\Delta_{\vec{0}}$ will be broadened to continuous nonzero functions. In other words, quantities like $\langle G_{\vec{0}} \rangle$ or $\langle \Delta_{\vec{0}} \rangle$, where the symbol angular brackets denotes averaging over the values of $\{\epsilon_{\vec{m}}\}$, are not appropriate for finding the nature of the eigenstates, since the averaging procedure eliminates from the behavior of $G_{\vec{0}}$ and $\Delta_{\vec{0}}$ as a function E exactly those characteristics which would enable us to distinguish between the localized and the extended states. On the other hand, by averaging the quantity $f_{\vec{0}}(E)$ [Eq. (2.14)] we retain those properties which distinguish the extended states from the localized. Thus, if $\langle f_{\vec{0}}(E) \rangle$ is zero for a certain energy, the eigenstates corresponding to this energy are extended for all sets of values of the parameters $\{\epsilon_{\vec{m}}\}$ (except possibly for sets of zero total measure). If $\langle f_{\vec{0}}(E) \rangle \neq 0$, then for a nonnegligible proportion of the configurations ($\cong$ sets of values of the parameters $\{\epsilon_{\vec{m}}\}$), the eigenstates belonging to the energy E are localized. It should be pointed out that for a given configuration the eigenstates corresponding to a specific energy are all localized or all extended. The reason is that even an infinitesimally small perturbation can mix an extended and a localized state, if they belong to the same energy, and transform both of them into extended states. Thus their coexistence is a matter of accidental degeneracy and consequently the probability of its occurrence is negligible. It is not obvious *a priori*, however, if for *all* the configurations (except possibly for a set of measure zero) the eigenstates belonging to a given energy are either localized or extended. One can imagine intermediate situations such that for a nonnegligible proportion of the configurations the states for a given energy are localized while for the remaining nonnegligible proportion of the configurations the states for the same energy are extended. By finding $\langle f_{\vec{0}}(E) \rangle \neq 0$, one cannot know if the eigenstates are localized for all the configurations or simply for a nonnegligible part of them. This question will be naturally resolved in Sec. III, in which, following Anderson, we attempt a study of the convergence of the RPS (2.23) in a probabilistic way: i.e., we try to find for each energy E the probability that the RPS converges.

III. STATISTICAL CONVERGENCE CONSIDERATIONS

As has been explained in the previous section, the problem of localization can be solved by examining the convergence properties of the series

$$V \sum_{N=1}^{\infty} \Delta^{(N)}_{\vec{0}}, \quad (3.1)$$

where

$$\Delta^{(N)}_{\vec{0}} = \sum \frac{V}{e_1} \frac{V}{e_2} \cdots \frac{V}{e_N} \quad (3.2)$$

is the sum of the contributions from all N-step paths starting from and ending at the site $\vec{0}$ without visiting the same site twice. Since the quantities $e_{\vec{n}} \equiv E - \epsilon_{\vec{n}} - \Delta^{\vec{0},\vec{1},\vec{m},\cdots,\vec{n}-1}_{\vec{n}}$ are random functions, the convergence of the RPS (3.1) is a matter of probability. We define the notion of convergence (divergence) in probability[27] of a series of random terms as meaning that the series converges (diverges) for all sets of values of the random variables (except possibly for sets of zero total measure). More precisely, we say that the series

(3.1) converges (diverges) in probability if the absolute value of the Nth-order team $|\Delta_0^{(N)}|$ is bounded from above (below) by the Nth-order term of convergent (divergent) geometric series with probability approaching unity as $N \to \infty$, i.e.,

$$\text{probability}\,[\,|\Delta_0^{(N)}| \lesssim F^N\,] \to 1 \quad \text{as } N \to \infty\,, \tag{3.3}$$

where $F < 1$ (> 1) in the case of convergence (divergence).

It will be shown in this section that one can define a nonnegative function $L(E)$ of the real variable E such that the Nth-order term $|\Delta_0^{(N)}(E)|$ is sharply distributed around the quantity $L^N(E)$, i.e.,

$$\text{probability}\,[L^{N-Nq}(E) < |\Delta_0^{(N)}(E)| < L^{N+Nq}(E)\,] \to 1 \quad \text{as } N \to \infty\,, \tag{3.4}$$

where $\frac{1}{2} < q < 1$. Thus if $L(E) < 1$ (> 1), the RPS converges (diverges) in probability according to the definition given here and consequently the eigenstates are localized (extended) for almost all the sets of values of the random variables $\{\epsilon_n\}$.

Consider the particular contribution to $\Delta_0^{(N)}$

$$T_j^{(N)} = V^N \frac{1}{e_1 \cdots e_N}\,, \tag{3.5}$$

and define $X_j^{(N)}$ as

$$X_j^{(N)} \equiv \ln|T_j^{(N)}| = (N)\ln V - \sum_{i=1}^{N} \ln|e_j|\,. \tag{3.6}$$

The average value of $X_j^{(N)}$,

$$\langle X_j^{(N)}\rangle = N\ln V - \sum_{i=1}^{N} \langle \ln|e_i|\rangle\,, \tag{3.7}$$

is obviously proportional to N, and consequently one can write

$$\langle X_j^{(N)}\rangle = N\ln(V/\tilde{e}_j)\,, \tag{3.8}$$

where $\tilde{e}_j$ is defined by

$$N\ln\tilde{e}_j = \sum_{i=1}^{N} \langle \ln|e_i|\rangle\,. \tag{3.9}$$

The variance of the random variable $X_j^{(N)}$ is

$$\sigma^2_{X_j^{(N)}} = \sum_{k,l=1}^{N} \langle (\ln|e_k| - \langle \ln|e_k|\rangle)(\ln|e_l| - \langle \ln|e_l|\rangle)\rangle\,. \tag{3.10}$$

Any two random variables e_l, e_k are statistically independent if the distance r_{lk} exceeds a certain finite value. This is due to a similar assumption about the random variables $\{\epsilon_m\}$ and to the fact that for localized states—as we have assumed we have—the quantities e_l depend on a finite number of variables $\{\epsilon_m\}$ corresponding to sites within the regions where the localized states are different from zero. Thus for any given k in (3.10) and for most of the l's—except for a number remaining finite as $N \to \infty$—the average of the product is the product of the averages and consequently is zero. It follows that $\sigma^2_{X_j^N}$ is proportional to N and that

$$\sigma_{X_j^{(N)}} = \beta_j N^{1/2}\,, \tag{3.11}$$

where β_j tends to a finite value as $N \to \infty$. Because $N^{q-1/2}\,\sigma_{X_j^{(N)}} \to \infty$ more rapidly than $\sigma_{X_j^{(N)}}$ as $N \to \infty$ for $q > \frac{1}{2}$, the random variable $X_j^{(N)}$ satisfies the relation

$$\text{probability}\,[\,\langle X_j^{(N)}\rangle - N^{q-1/2}\sigma_{X_j^{(N)}} < X_j^{(N)} < \langle X_j^{(N)}\rangle + N^{q-1/2}\sigma_{X_j^{(N)}}\,] \to 1 \quad \text{as } N \to \infty\,. \tag{3.12}$$

Taking into account Eqs. (3.8) and (3.11), we can write (3.12) as

$$\text{probability}\,[\,N a_j - N^q \beta_j < X_j^{(N)} < N a_j + N^q \beta_j\,] \underset{N\to\infty}{\longrightarrow} 1\,, \tag{3.12'}$$

where $a_j \equiv \ln(V/\tilde{e}_j)$. Because q can be taken as < 1, i.e., $\frac{1}{2} < q < 1$, it follows that $X_j^{(N)}$ is sharply peaked around its average. From Eqs. (3.6) and (3.12) it follows that

$$\text{probability}\,[e^{Na_j - N^q\beta_j} < |T_j^{(N)}| < e^{Na_j + N^q\beta_j}] \to 1 \quad \text{as } N \to \infty\,, \ \tfrac{1}{2} < q < 1\,. \tag{3.13}$$

It is worthwhile to note that if all the random variables e_i were statistically independent, then Lindeberg's condition[27,28] for the applicability of the central limit theorem would be satisfied and the distribution of the quantity $X_j^{(N)}$ would be a normal one.[29] In this case the probability defined in Eqs. (3.12), (3.12'), and (3.13) approaches unity as $N \to \infty$ in the following way: $1 - e^{-N^{2q-1}}$. The fact, however, that the probability defined in (3.12) tends to unity as $N \to \infty$ is independent of the particular form of the distribution function as long as it possesses a standard deviation for finite N.

We examine now the distribution of the quantity $|\Delta_0^{(N)}|$. We want first to make plausible that

$$|\Delta_0^{(N)}| \equiv \Big|\sum_j T_j^{(N)}\Big| = \gamma(N)\sum_j |T_j^{(N)}|\,, \tag{3.14}$$

where $\gamma(N)$ is such that $[\gamma(N)]^{1/N} \to 1$ as $N \to \infty$. Equation (3.14) would be obviously correct if all the $T_j^{(N)}$ had the same sign. On the other hand, (3.14) would be violated if all the $T_j^{(N)}$ had random

signs. As we have seen in Sec. II, the sign of the quantities $T_j^{(N)}$ ($j=1, 2, \ldots$) for a given E is determined by the positions of the poles E_p and the zeros E_z of Eq. (2.32). We have already shown that the positions of the poles are common to all diagrams. Thus only the positions of the zeros E_z determine the relative sign of the quantities $T_j^{(N)}$. Any quantity E_z, being an eigenvalue of the Hamiltonian $H^{\vec{0}\cdots\vec{N}}$ (sites $\vec{0}, \ldots, \vec{N}$ define the diagram under consideration), depends only on the sites lying within the region where the corresponding localized eigenfunction is nonnegligible. We define the localization length as a measure of the linear dimensions of this region. It follows that the positions of the zeros E_z differ from one diagram to another owing to the noncommon sites within the localization region. One can consider two limiting classes of diagrams. The first class consists of those diagrams passing rapidly through the localization region. The other class of diagrams consists of those with a portion of them tightly packed within the localization region. Most of the diagrams belong to the first class. On the other hand, the diagrams belonging to the second class make the largest contributions. Localized states are generally associated with regions of the order of the localization length in extent in which the single-site energies happen to be interrelated, e.g., are all nearly the same, or all do not exceed some maximum value, etc. As a consequence, for states overlapping $\vec{0}$ at energy E, the values of the $e_{\vec{i}}$ for sites $\vec{i}$ within the localization length of $\vec{0}$ are much smaller on average than those for sites outside; whence it follows that the more tightly packed the diagram is inside the localization region, the larger it is.

For large localization lengths—as in the case where we approach a mobility edge—the diagrams of the first class differ among themselves only because they visit different excluded sites within the localization length, the number of which is negligible in comparison with the total number of sites in the localization region. Thus the relative shifts of the positions of the zeros for all these diagrams is very small and consequently they possess strongly correlated signs.[30] The diagrams of the second class also possess a common sign, because they have all the important sites in common. We conclude that the relative signs of the quantities $T_j^{(N)}$ ($j=1, \ldots, K^N$) cannot be random and that the class of the largest individual diagrams as well as the class of the most numerous each has a common sign. These arguments provide, in our opinion, adequate support for the supposition (3.14). Although the existence of localized states does not depend on whether Eq. (3.14) is true or wrong, the specific form of the function $L(E)$ that we derive depends on its correctness.

We have shown [Eq. (3.13)], that the individual $|T_j^{(N)}|$ are sharply distributed. We have just argued that [Eq. (3.14)] the magnitude of Δ_0^N, $|\sum_j T_j^{(N)}|$, is given, apart from a factor $\gamma(N)$ not of exponential order in N, by the sum of the individual $|T_j^{(N)}|$. We now intend to make plausible the supposition that the sum of the individual $|T_j^{(N)}|$, and therefore $|\Delta_0^N|$ itself, is sharply distributed, i.e., that

$$\text{probability}\left[\gamma^*(N)\sum_j e^{Na_j - N^\alpha\beta_j} < \left|\Delta_0^{(N)}\right| < \gamma^*(N)\sum_j e^{Na_j+N^\alpha\beta_j}\right] \underset{N\to\infty}{\longrightarrow} 1, \tag{3.15}$$

where $[\gamma^*(N)]^{1/N} \to 1$ as $N\to\infty$. If the quantities $T_j^{(N)}$ ($j=1, 2, 3$) were all equal, (3.15) would be a trivial consequence of (3.13) and (3.14) with $\gamma^*(N) = \gamma(N)$. Equation (3.15) would also be correct if the $T_j^{(N)}$ were so strongly correlated that most of them have large or small values simultaneously. We can, however, argue that the quantities $T_j^{(N)}$ are sufficiently well correlated for (3.15) to hold from the following three observations.

(1) The maximum number of sites available to an Nth-order diagram, and therefore the number of independent random variables, is of order N^3, whereas the number of distinct diagrams is of order K^N, as pointed out by Thouless[15] [look right after (3.19) for the definition of K].

(2) The e_i are correlated over the localization length. Thus two diagrams which are never further apart than the localization have about the same value.

(3) Important classes of diagrams have the same signs. This strong correlation of signs implies correlation of magnitudes as well.

We have not been able, however, to convert these physical arguments to a mathematically rigorous one. Nevertheless, it should be realized that the existence of localized states does not depend on the validity of (3.14) or (3.15). Anderson[4] has used just the opposite assumptions considering the signs of $T_j^{(N)}$ random and treating the quantities $T_j^{(N)}$ as statistically independent random variables, and has obtained results qualitatively similar to the ones to be presented here. However, as Thouless has shown, Anderson's assumption of statistical independence is incorrect. One therefore expects quantitatively more accurate results for localization from our proposal of strong correlation. In any event, since statistical independence and strong correlation are limiting situations, we ex-

pect that Anderson's results and our results bracket the correct localization criterion.

Equation (3.15) means that $|\Delta_{\vec{0}}^{(N)}|$ behaves like $\sum_i e^{Na_j}$ as $N \to \infty$. From Eqs. (3.7) and (3.8) and the definition of $a_j = \ln(V/\tilde{e}_j)$ we see that

$$\sum_j e^{Na_j} = \sum_j e^{\langle X_j^{(N)} \rangle} . \tag{3.16}$$

If we define $\ln \tilde{G}^{\vec{0},\vec{n}_i \cdots \vec{n}_{i-1}}_{\vec{n}_i}$ as $-\langle \ln |e_{\vec{n}_i}| \rangle$,

$$\ln \tilde{G}^{\vec{0},\vec{n}_1,\ldots,\vec{n}_{i-1}}_{\vec{n}_i} = \left\langle \ln \left| \frac{1}{E - \epsilon_{\vec{n}_i} - \Delta^{\vec{0},\vec{n}_1,\ldots,\vec{n}_{i-1}}_{\vec{n}_i}} \right| \right\rangle , \tag{3.17}$$

the quantity $V\sum_j e^{Na_j}$ can be written as

$$V\sum\nolimits_j e^{Na_j} = \sum\nolimits' V_{\vec{0}\vec{n}_1} \tilde{G}^{\vec{0}}_{\vec{n}_1} V_{\vec{n}_1\vec{n}_2} \tilde{G}^{\vec{0}\vec{n}_1}_{\vec{n}_2} \cdots V_{\vec{n}_N\vec{0}} , \tag{3.18}$$

where the $\sum'$ on the right-hand-side of (3.18) indicates summation over all indices $\vec{n}_1, \ldots, \vec{n}_N$ with the restrictions $\vec{n}_1 \neq \vec{0}$, $\vec{n}_2 \neq \vec{0}$, $\vec{n}_1, \ldots, \vec{n}_N \neq \vec{0}$, $\vec{n}_1, \ldots, \vec{n}_{N-1}$ corresponding to all self-avoiding paths of order N starting from and ending at the site $\vec{0}$. The number of these paths is given by $S(N)$ and

$$S(N) \sim K^N \quad \text{as } N \to \infty , \tag{3.19}$$

where K is the connective constant[3,31-33] of the lattice, which is generally[33] of the order $\frac{2}{3}Z$. A table of values of K for different lattices can be found in Domb's paper.[33] It is clear that the quantity $\sum_j e^{Na_j}$ depends exponentially on N so that one can define $L(E)$ by

$$L^N(E) = \sum\nolimits' V_{\vec{0}\vec{n}_1} \tilde{G}^{\vec{0}}_{\vec{n}_1} V_{\vec{n}_1\vec{n}_2} \tilde{G}^{\vec{0}\vec{n}_1}_{\vec{n}_2} \cdots V_{\vec{n}_N\vec{0}} , \tag{3.20}$$

where $L(E)$ is independent of N as $N \to \infty$.

From Eqs. (3.15), (3.18), and (3.20) it follows that the function $L(E)$ defined by (3.17) and (3.20) satisfies the basic relation (3.4), and can be used for discovering the nature of the eigenstates. If $L(E) > 1$, the eigenstates are extended for almost all configurations; if $L(E) < 1$, the eigenstates, if any, are localized; the equation $L(E_c) = 1$ determines the positions of the mobility edges E_c.

Having defined the localization function $L(E)$, it is possible to reach certain conclusions regarding its behavior. Suppose that Γ is a measure of the degree of randomness in the system; then $\Gamma = 0$ corresponds to the case of a perfect crystal and consequently the quantities $\tilde{G}^{\vec{0},\vec{n}_1,\ldots,\vec{n}_{i-1}}_{\vec{n}_i}(E)$ are equal to $|\mathcal{G}^{\vec{0},\vec{n}_1,\ldots,\vec{n}_{i-1}}_{\vec{n}_i}(E)|$, where the script $\mathcal{G}$ denotes the Green's function for the periodic case, $\Gamma = 0$. Since in the periodic case all the $T_j^{(N)}$ are positive or negative (there are no poles or zeros outside the branch cuts), we can conclude that for $\Gamma = 0$, $L^N(E)$ is just the absolute value of the Nth-order term of the RPS for $\Delta_{\vec{0}}(E)$, as it should be. Since all the eigenstates are extended, the RPS for $\Delta_{\vec{0}}(E)$ should diverge inside the band and converge outside. Thus for the periodic case, $\Gamma = 0$, $L(E)_{\Gamma=0} \geq 1$ for E inside the band with the equality obtained at the band edges, as was expected. On the other hand, when $\Gamma \to \infty$ the quantities $\tilde{G}^{\vec{0},\ldots,\vec{n}_{i-1}}_{\vec{n}_i}$ tend to zero everywhere so that $L(E) \to 0$ for every E as $\Gamma \to \infty$. Assuming that $L(E)$ is a continuous function of Γ for every E, we can conclude that for every E there is a critical value of Γ, $\Gamma_c(E)$ such that for $\Gamma \geq \Gamma_c(E)$, $L(E) \leq 1$. If we define

$$\Gamma_c = \max\{\Gamma_c(E)\} , \tag{3.21}$$

it follows that for $\Gamma \geq \Gamma_c$, $L(E)$ is smaller than unity for every E, which means, that for $\Gamma \geq \Gamma_c$ all the eigenstates of the system become localized. This disappearance of extended states has been termed Anderson's transition. For $0 < \Gamma < \Gamma_c$, the energy spectrum is separated by the mobility edges E_c, satisfying the equation $L(E_c) = 1$, into regions consisting alternately of localized $[L(E) < 1]$ and extended $[L(E) > 1]$ states in agreement with the Mott-CFO model. One can generalize the notion of Anderson's transition to denote the disappearance of a region of extended states through the merging of two adjacent mobility edges. In this case the total disappearance of extended states from the system takes the form of successive Anderson's transitions, each one eliminating one region of extended states.

In this section we have shown that each term of Nth order of the RPS for $\Delta_{\vec{0}}$ is sharply distributed [Eq. (3.11) or (3.13)]. This was a direct consequence of the assumed statistical independence of any two quantities $\epsilon_{\vec{m}}$, $\epsilon_{\vec{l}}$ when the distance $r_{\vec{m}\vec{l}}$ is larger than a given finite length—the mathematical condition expressing the absence of long-range order from the system. From Eq. (3.13) by using certain physical arguments, one demonstrates that the Nth-order term of $\Delta_{\vec{0}}$, $\Delta_{\vec{0}}^{(N)}$, is also sharply distributed in the sense of Eq. (3.15). Hence the RPS either converges or diverges in probability, which, in view of the analysis in Sec. II, means that there are regions of extended states, and regions of localized states with energies of sharp transition, the mobility edges, which are common for almost all the configurations (except some of total measure zero).

We conclude this section by pointing out that the results presented here for one band can be trivially generalized in the case of many (or even an infinite number of) bands as long as there is no band mixing in the original Hamiltonian, since in this case each band can be treated separately. If there are interband matrix elements or if there is nondiagonal disorder, the problem becomes exceedingly complicated. We feel, however, that these complications would change the present results only quan-

titatively, leaving the basic qualitative features untouched.

IV. EXPLICIT ESTIMATES AND RELATION TO EARLIER WORK

In this section we attempt first to make some rough estimates of the critical quantities E_c and Γ_c using the localization function $L(E)$ obtained in Sec. III. Then we review the earlier work on the same subject with particular emphasis on the similarities to and differences from our own. Our estimates are compared with those given by Anderson.

The simplest approximation one can do in trying to calculate $L(E)$ is to neglect the self-energies $\Delta^{\vec{0},\ldots,\vec{n}_i-1}_{\vec{n}_i}$ in Eq. (3.13). Then

$$\ln \tilde{G}^{\vec{0},\ldots,\vec{n}_i-1}_{\vec{n}_i} \simeq \langle \ln | 1/(E-\epsilon_{\vec{n}_i}) | \rangle = -\langle \ln | E-\epsilon_{\vec{n}_i} | \rangle , \tag{4.1a}$$

and

$$\tilde{G}^{\vec{0},\ldots,\vec{n}_i-1}_{\vec{n}_i} \simeq e^{-\langle \ln | E-\epsilon_{\vec{n}_i} | \rangle} . \tag{4.1b}$$

Substituting in (3.20) and performing the summation, we obtain

$$L^N(E) \simeq K^N V^{N+1} e^{-N\langle \ln | E-\epsilon_{\vec{n}_i} | \rangle} , \tag{4.2a}$$

or

$$L(E) \simeq KV e^{-\langle \ln | E-\epsilon_{\vec{n}_i} | \rangle} , \tag{4.2b}$$

where K is the connective constant defined earlier. Owing to the approximation (4.1a), $L(E)$ no longer reproduces the correct results in the periodic case where $\epsilon_{\vec{n}_i} = \epsilon_0 = \text{const}$ for every $\vec{n}_i$. In this case

$$L(E) \simeq KV/|E-\epsilon_0| , \tag{4.3}$$

which violates the basic property that $L(E) \geq 1$ for the periodic case and for E inside the band, with the equality achieved at the band edges. To remedy this deficiency we write

$$L(E) \simeq \alpha KV e^{-\langle \ln | E-\epsilon_{\vec{n}_i} | \rangle} , \tag{4.2'}$$

where α is a constant such that $L(E) \geq 1$ with $L(E_b) \simeq 1$ for the periodic case and for $|E-\epsilon_0| \leq E_b$, where $E_b = ZV$ is half the bandwidth. Equation (4.3) will then become

$$L(E) \simeq \alpha KV/|E-\epsilon_0| . \tag{4.3'}$$

It is obvious that the equation $L(E) \geq 1$ for $|E-\epsilon_0| \leq ZV$ is satisfied only if

$$\alpha KV = ZV \tag{4.4a}$$

or

$$\alpha = Z/K . \tag{4.4b}$$

Substituting (4.4b) in (4.2'), we obtain finally

$$L(E) \simeq ZV e^{-\langle \ln | E-\epsilon_{\vec{n}_i} | \rangle} . \tag{4.5}$$

It should be pointed out that the correction factor α is in general a function of E and depends on the distribution function for $\epsilon_{\vec{n}}$. All these dependences have been neglected in arriving at the oversimplified estimate (4.5).

It is worthwhile to note that Ziman[3] used Eq. (4.5) arbitrarily as an estimate of the convergence of the PS, which he associated with the localization properties of the eigenfunctions. Ziman,[3] using Eq. (4.5), has studied the particular cases of a rectangular distribution function for ϵ_i of total width W and of the random binary-alloy case, where ϵ_i can take two values ϵ_A or ϵ_B with probabilities p_A and $p_B = 1 - p_A$. In the rectangular distribution case the result, as calculated by Ziman, is

$$L(E) \simeq Z \exp\left\{1 - \frac{1}{2}\left[\left(1+\frac{2E}{W}\right)\ln\left|\frac{W}{2V}+\frac{E}{V}\right| + \left(1-\frac{2E}{W}\right)\ln\left|\frac{W}{2V}-\frac{E}{V}\right|\right]\right\} . \tag{4.6}$$

The critical value W_c of the total width W for which all the states become localized can be deduced[3] from (4.6) as

$$W_c \simeq 2.7B , \tag{4.7}$$

where $B = 2ZV$ is the bandwidth for the periodic case $W = 0$.

The binary-alloy case will not be discussed here.[17,34] We simply note that approximation (4.5) as used by Ziman reproduces in this case some of correct qualitative features and fails to reproduce others.[3,34]

We have next applied Eq. (4.5) to the case where the quantities $\epsilon_{\vec{n}}$ are distributed according to a Lorentzian of half-width Γ, i.e.,

$$P(\epsilon_{\vec{n}}) = \frac{1}{\pi}\frac{\Gamma}{\epsilon_n^2+\Gamma^2} . \tag{4.8}$$

In this case

$$L(E) \simeq \frac{ZV}{(E^2+\Gamma^2)^{1/2}} . \tag{4.9}$$

The mobility edges are then given by $L(E_c) = 1$, i.e.,

$$E_c = \pm (Z^2V^2 - \Gamma^2)^{1/2} , \tag{4.10}$$

and Anderson's transition occurs when $\Gamma = \Gamma_c$, where

$$\Gamma_c = ZV = \tfrac{1}{2}B . \tag{4.11}$$

We shall discuss the Lorentzian case in more detail in Sec. V in connection with some exact results.

If one uses the correspondence $\Gamma \leftrightarrow \frac{1}{4}W$ between the half-width Γ of the Lorentzian distribution and the total width W of the rectangular distribution stemming from the relation

$$\frac{1}{W}\int_{-W/4}^{W/4} dx = \tfrac{1}{2} = \frac{1}{\pi}\int_{-\Gamma}^{\Gamma}\frac{\Gamma}{x^2+\Gamma^2}\,dx , \tag{4.12}$$

one sees that we need degrees of randomness about 25% higher for the rectangular case than the Lorentzian case in order to obtain Anderson's transition. This can be attributed to the long tails of the Lorentzian distribution.

We shall discuss at some length Anderson's work in the light of the analysis which has been presented here. Anderson has used the simplifying approximations that the quantities e_i are statistically independent with identical distribution functions possessing a cutoff around the origin. He assumed, furthermore, that the distribution of e_i is the same as the distribution of ϵ_i except for the cutoff. This approximation is equivalent to our neglect of $\Delta^{\vec{0},\ldots,\vec{n}_{i-1}}_{\vec{n}_i}$ in Eq. (3.17). Anderson calculated directly the probability distribution $P(T_j^{(N)})$ of the quantity $T_j^{(N)}$. At this point use was made of a theorem that the tail of the probability distribution of a sum of random terms T_j each of which is distributed symmetrically around the origin with a long tail is the same as the tail of the distribution of the single largest term, $T_{\max} = \max\{T_1, T_2, \ldots\}$. In other words, this theorem states that

$$P_\Sigma(X) = P_M(X) \text{ for large } X , \tag{4.13}$$

where P_Σ and P_M are the probability distributions of the sum and the maximum term, respectively. As has been pointed out by Thouless,[15] Anderson implicitly assumes, in order to calculate the probability distribution for $T^{(N)}_{\max}$, that the random variables $T_j^{(N)}$ $(j=1, \ldots, K^N)$ are statistically independent. This assumption permits him to write

$$P_M(X) = K^N P(X) , \tag{4.14}$$

where P is the probability distribution of each term $T_j^{(N)}$. The criterion for convergence in probability stated without proof by Anderson is

$$W \geq W_c , \tag{4.15}$$

where W_c satisfies the equation

$$P_\Sigma(1)_{\substack{W=W_c \\ E=0}} = K^N P(1)_{\substack{W=W_c \\ E=0}} = 1 . \tag{4.16}$$

Anderson states that $\Delta_0^{(N)}$ is less than e^{-N} with probability $\sim 1 - e^{-N}$ when (4.15) is satisfied. This statement cannot be correct in general, since the the probability of $\Delta_0^{(N)}$ being smaller than a certain quantity is related to an integral of the distribution $K^N P(\Delta_0^{(N)})$ and not to the value of it at $\Delta_0^{(N)} = 1$. Thus Anderson's criterion (4.16) provides a reasonable order of magnitude estimate for the quantity W_c, but cannot be considered as justified within the framework of the theory of convergence in probability.

Thouless[15] in his critical and clarifying review of Anderson's work has justified Eq. (4.16) by deriving it from the correct criterion stating that the probability that $\Delta_0^{(N)} > (1-\epsilon)^N$ approaches zero for $W > W_c$.

For the rectangular distribution with total width W, and for a simple cubic lattice ($K \approx 4.5$), the best estimate of the critical randomness according to Eq. (4.16) is[4]

$$W_c \approx 5B . \tag{4.17}$$

The criterion according to our analysis corresponding to the approximations used to derive (4.16) is

$$\langle \ln(V/|E - \epsilon_{\vec{n}}|)\rangle + \ln K < 0 , \tag{4.18}$$

which gives for the critical randomness W_c in the case of a rectangular distribution and a simple cubic lattice,

$$W_c \approx 2B . \tag{4.19}$$

It can be seen by comparing our estimate (4.19) with the one given by Eq. (4.17) that Anderson's results overestimate the critical randomness in comparison with our results by about a factor of 2. It will be shown in Sec. V that our theory provided under certain conditions an upper limit for the critical randomness (and for the regions of extended states). In the case of a random binary alloy these upper limits are consistent with exact results from percolation theory.[16,17] This lends further support to our assertion that the quantities $T_i^{(N)}$ are strongly correlated. Be that as it may, one expects the true value of W_c to lie between $2B$ and $5B$ because statistical independence and strong correlation are limiting situations.

V. UPPER BOUNDS ON REGIONS OF EXTENDED STATES

A. General Theory

We show in this subsection that under certain conditions a function $F(E)$ can be found such that

$$F(E) < 1 \rightarrow L(E) < 1 . \tag{5.1}$$

From (5.1) and the discussion in Sec. III it would follow that all the eigenstates corresponding to eigenenergies E satisfying $F(E) < 1$ are localized. In addition, the mobility edges E_c satisfy the equation

$$F(E_c) > 1 , \tag{5.2}$$

except for the trivial case of zero randomness where $F(E_c) = 1$. The importance of Eq. (5.1) lies in the fact that the quantity $F(E)$ is no more difficult to calculate than the average Green's function. Consequently there is one case where $F(E)$ can be calculated exactly (Lorentzian distribution of the quantities $\{\epsilon_n\}$) and in every other case $F(E)$ can be calculated approximately using methods developed for the calculation of the average density of states, most notably the coherent potential approximation (CPA).[35,36]

Assume that

$$\tilde{G}^{\vec{0},\ldots,\vec{n}_{i-1}}_{\vec{n}_i}(E) \le \left| \mathcal{G}^{\vec{0},\ldots,\vec{n}_{i-1}}_{\vec{n}_i}(E-\Sigma(E)) \right| , \qquad (5.3)$$

where the script $\mathcal{G}^{0,\ldots,n_{i-1}}_{n_i}$ denotes the $\vec{n}_i$, $\vec{n}_i$ matrix element of the Green's function corresponding to a Hamiltonian of the form (2.1) with $\epsilon_{\vec{0}} = \cdots = \epsilon_{\vec{n}_{i-1}} = \infty$ and $\epsilon_{\vec{j}} = 0$ for every $\vec{j} \neq \vec{0}, \ldots, \vec{n}_{i-1}$. $\Sigma(E)$ can be in general a complex function of E. We shall show that, when the quantities $\tilde{G}$ defined in (3.17) satisfy Eq. (5.3), then a function $F(E)$ can be found such that (5.1) is true.

We shall first show that

$$\left| \mathcal{G}^{\vec{0},\ldots,\vec{n}_{i-1}}_{\vec{n}_i}(E-\Sigma(E)) \right| \le \mathcal{G}^{0,\ldots,n_{i-1}}_{n_i}(|E-\Sigma(E)|) \qquad (5.4)$$

holds if

$$|E-\Sigma(E)| > ZV. \qquad (5.5)$$

The function $\mathcal{G}^{\vec{0},\ldots,\vec{n}_{i-1}}_{\vec{n}_i}$ is a matrix element of a Green's function corresponding to a periodic Hamiltonian containing infinitely strong impurities at the sites $\vec{0}, \ldots, \vec{n}_{i-1}$. The quantity $\mathcal{G}_{\vec{n}_i}$, being a matrix element of the Green's function for a perfectly periodic Hamiltonian, possesses a branch cut from $-E_b$ to E_b, where $E_b = ZV$, and no other singularity. Using Eq. (2.28), one can see that the $\mathcal{G}^{\vec{0}}_{\vec{n}_i}$ possesses no other singularity than the branch cut along the interval $[-E_b, E_b]$. Repeated use of Eq. (2.28) shows that the same is true for $\mathcal{G}^{\vec{0},\ldots,\vec{n}_{i-1}}_{\vec{n}_i}$. The same result can be reached by repeated application of the Koster-Slater[37] method of treating one impurity. Because of this analytic structure the function $\mathcal{G}^{\vec{0},\ldots,\vec{n}_{i-1}}_{\vec{n}_i}$ can be written as

$$\mathcal{G}^{\vec{0},\ldots,\vec{n}_{i-1}}_{\vec{n}_i}(z) = \int_{-E_b}^{E_b} \frac{n(E')\,dE'}{z-E'} , \qquad (5.6)$$

where the indices have been suppressed from $n(E)$, which equals $(1/\pi)\lim \mathrm{Im}\mathcal{G}^{\vec{0},\ldots,\vec{n}_{i-1}}_{\vec{n}_i}(E-is)$ as $s \to 0^+$. It is not difficult to show that the function $n(E)$ is symmetrical around the origin $E=0$. Consider now a value z of the argument such that

$$|z| \ge E_b \equiv ZV . \qquad (5.7)$$

Then

$$\left| \mathcal{G}^{\vec{0},\ldots,\vec{n}_{i-1}}_{\vec{n}_i}(z) \right| \le \int_{-E_b}^{E_b} \frac{n(E')\,dE'}{|z-E'|} = \int_0^{E_b} n(E') \left(\frac{1}{|z-E'|} + \frac{1}{|z+E'|} \right) dE' . \qquad (5.8)$$

It is a matter of simple geometry to show that

$$\frac{1}{|z-E'|} + \frac{1}{|z+E'|} \le \frac{1}{|z|-E'} + \frac{1}{|z|+E'} \qquad (5.9)$$

if $|z| \ge E'$. Because of (5.7), Eq. (5.9) holds for every $E' \le E_b$. Hence, substituting inequality (5.9) in inequality (5.8), we obtain

$$\left| \mathcal{G}^{\vec{0},\ldots,\vec{n}_{i-1}}_{\vec{n}_i}(z) \right| \le \int_0^{E_b} n(E') \left(\frac{1}{|z|-E'} + \frac{1}{|z|+E'} \right) dE' = \int_{-E_b}^{E_b} \frac{n(E')dE'}{|z|-E'} = \mathcal{G}^{\vec{0},\ldots,\vec{n}_{i-1}}_{\vec{n}_i}(|z|) \qquad (5.10)$$

if (5.7) is satisfied. Substituting $z = E - \Sigma(E)$ in (5.10), we obtain (5.4). It is easy to see that the equality is obtained in (5.4) only if $\Sigma(E)$ is real.

From (5.3) and (5.4) it follows that

$$\tilde{G}^{\vec{0},\ldots,\vec{n}_{i-1}}_{\vec{n}_i}(E) \le \mathcal{G}^{0,\ldots,n_{i-1}}_{n_i}(|E-\Sigma(E)|) \qquad (5.11)$$

if (5.5) is satisfied. Hence the function $\mathfrak{L}(E)$, defined as

$$\mathfrak{L}^N(E) = \sum{}' V_{\vec{0}\vec{n}_1} \mathcal{G}^{\vec{0}}_{\vec{n}_1}(|E-\Sigma(E)|) \cdots V_{\vec{n}_N\vec{0}} , \qquad (5.12)$$

is larger than $L(E)$ as long as (5.5) is satisfied. However, $\mathfrak{L}^N(E)$ as defined in (5.12) is nothing else than the Nth-order term of the RPS for $\mathfrak{D}_{\vec{0}}(|E-\Sigma(E)|)$, where $\mathfrak{D}_{\vec{0}}$ is the self-energy corresponding to the periodic case $\epsilon_{\vec{n}} = 0$ for every $\vec{n}$. We have already seen that for a periodic system the RPS diverges if the argument is real and its magnitude is smaller than $E_b = ZV$ and converges in every other case. Hence, if

$$|E-\Sigma(E)| \ge E_b , \qquad (5.5')$$

then

$$\mathfrak{L}(E) \le 1 . \qquad (5.13)$$

Define now the function $F(E)$ as

$$F(E) = E_b / |E-\Sigma(E)| . \qquad (5.14)$$

If $F(E) \le 1$, then (5.5′) is satisfied and consequently $\mathfrak{L}(E) \le 1$. But if $F(E) \le 1$, then (5.5) is satisfied and thus $L(E) \le \mathfrak{L}(E)$. We can conclude that, when $F(E) \le 1$, then $L(E) < 1$. $F(E) = 1$ implies $L(E) = 1$ only in the case where $\Sigma(E)$ is real and the equality sign holds in (5.3). One can demonstrate, however, that $\Sigma(E_c)$ is real only in the trivial case of no randomness where $\Sigma(E) = 0$.

The energies E_c^*, where $F(E_c^*) = 1$, divide the energy spectrum into regions where $F(E) > 1$ and $F(E) < 1$. The latter consist of localized states. The mobility edges E_c lie in the regions where $F(E) > 1$, separating them into subregions of extended and localized states. As the degree of randomness Γ approaches zero the mobility edges E_c approach E_c^*. Thus for small randomness, $F(E)$ can be considered as a fair approximation to $L(E)$; this approximation overestimates the size of the regions of extended states. One can estimate the discrepancy between E_c and E_c^* by finding the difference $F(E_c^*) - L(E_c^*) = 1 - L(E_c^*)$. This difference for small randomness is proportional to the difference $\mathcal{G}(|z|) - |\mathcal{G}(z)|$, with $z \simeq E_b - \Sigma(E_b)$, if the equality sign holds in (5.3). $\mathcal{G}$ is a matrix element of the periodic Green's function. Because of the square-

root singularity in the density of states at the band edge one knows[38] that

$$\mathcal{G}(z)=\mathcal{G}(E_b)+\zeta\,\frac{(z-E_b)^{1/2}}{E_b^{1/2}}\ , \tag{5.15}$$

where ζ is a constant as $z\to E_b$. Assuming for convenience only that $|\mathrm{Re}\Sigma|\ll|\mathrm{Im}\Sigma|$ as $\Gamma\to 0$, it follows that

$$\mathcal{G}(|E_b-\Sigma(E_b)|)-\mathcal{G}(E_b-\Sigma(E_b))|\propto[\mathrm{Im}\Sigma(E_b)/E_b]^{1/2}$$

and consequently

$$\frac{|E_c-E_c^*|}{E_b}\propto\left(\frac{\mathrm{Im}\Sigma(E_b)}{E_b}\right)^{1/2}\quad\text{as }\Gamma\to 0\ . \tag{5.16}$$

In the framework of any single-site approximation for the evaluation of $G^{\vec{0},\cdots,\vec{n}_i-1}_{\vec{n}_i}$ the basic condition (5.3) is satisfied (with the equality sign holding) and the quantity $\Sigma(E)$ can be calculated with no more difficulty than the average Green's function. Hence $F(E)$ can be calculated. This method was used in the case of a random binary alloy[17,34] within the CPA. In this case $\Sigma(E)$ is the same as the quantity $\Sigma(E)$ appearing in the definition of $\langle G_{\vec{k}}(E)\rangle$, namely,

$$\langle G_{\vec{k}}(E)\rangle=\frac{1}{E-E(\vec{k})-\Sigma(E)}\ . \tag{5.17}$$

The results in the binary-alloy case were in striking agreement with the Mott-CFO model and with the available exact results. We shall examine next the case of Lorentzian distribution for the single-site energies where exact results can be obtained.

B. Exactly Solvable Model

We examine in this subsection the Lorentzian case for which $F(E)$ can be calculated exactly. Lloyd[19] and Brouers[20] have considered the same case and their conclusion that localized states do not exist constitutes an additional reason for examining it further. The Hamiltonian is of the form (2.1) and the distribution of each diagonal matrix element is a Lorentzian of the form

$$P(\epsilon_{\vec{m}})=\frac{1}{\pi}\,\frac{\Gamma}{\epsilon_{\vec{m}}^2+\Gamma^2}\ . \tag{5.18}$$

Lloyd was able to calculate exactly the average $\langle G_{\vec{m}\,\vec{n}}\rangle$, from which he proved that

$$\langle c_{\vec{0}}(t)\rangle\to 0\quad\text{as } t\to\infty\ , \tag{5.19}$$

where the quantities $c_{\vec{n}}(t)$ are given by Eq. (2.4). From (5.19) he concluded that there are no localized states. However, the vanishing of $\langle c_{\vec{0}}(t)\rangle$ does not imply that $\lim\langle|c_{\vec{0}}(t)|^2\rangle=P_{\vec{0}\vec{0}}$ as $t\to\infty$ vanishes, since $\langle c_{\vec{0}}(t)\rangle$ can vanish because of a random phase and not because of a vanishing amplitude. As Mott[22] pointed out for a single random level, $c_{\vec{0}}(t)=e^{iE_0t}$ but $\langle c_{\vec{0}}(t)\rangle=e^{-\Gamma t}$, if the distribution of E_0 is of the form (5.18). Brouers[20] has calculated $\langle\Delta_{\vec{0}}(E)\rangle$ exactly and has shown that $\mathrm{Im}\langle\Delta_{\vec{0}}(E)\rangle\neq 0$, from which he concluded that localized states do not exist. However, according to our discussion in Sec. II, one cannot reach any conclusion as to whether the eigenstates are localized or extended from the fact that $\mathrm{Im}\langle\Delta_{\vec{0}}(E)\rangle\neq 0$, since this quantity is different from zero for both localized and extended states.

Lloyd,[19] using an elegant trick, was able to prove that

$$\langle G_{\vec{m}\,\vec{n}}(E)\rangle=\mathcal{G}_{\vec{m}\,\vec{n}}(E+iS(E)\Gamma)\ , \tag{5.20}$$

where

$$S(E)=1\quad\text{if }\mathrm{Im}E>0$$
$$=-1\quad\text{if }\mathrm{Im}E<0\ , \tag{5.21}$$

and $\mathcal{G}$ is the Green's function for the periodic case $\{\epsilon_{\vec{m}}\}=\{0\}$.

This elegant result can be generalized to

$$\langle f(G^{\vec{r},\vec{k},\cdots}_{\vec{n}}(E))\rangle=f(\mathcal{G}^{\vec{r},\vec{k},\cdots}_{\vec{n}}(E+iS(E)\Gamma))\ , \tag{5.22}$$

for every function $f(z)$ whose every singularity lies on the real axis and/or at infinity. This is shown in the Appendix.

In the present case we want to calculate $\tilde{G}^{\vec{0},\cdots,\vec{n}_i-1}_{\vec{n}_i}(E)$. According to (3.17) we have

$$\begin{aligned}\ln\tilde{G}^{\vec{0},\cdots,\vec{n}_i-1}_{\vec{n}_i}(E)&=\langle\ln|G^{\vec{0},\cdots,\vec{n}_i-1}_{\vec{n}_i}|\rangle\\&=\tfrac{1}{2}\lim[\langle\ln G^{\vec{0},\cdots,\vec{n}_i-1}_{\vec{n}_i}(E+is)\rangle\\&\quad+\langle\ln G^{\vec{0},\cdots,\vec{n}_i-1}_{\vec{n}_i}(E-is)\rangle]\quad\text{as } s\to 0^+\ .\end{aligned} \tag{5.23}$$

As is shown in the Appendix, the $\ln G$ satisfies Eq. (5.22) and consequently

$$\begin{aligned}\ln\tilde{G}^{\vec{0},\cdots,\vec{n}_i-1}_{\vec{n}_i}(E)&=\tfrac{1}{2}\lim[\ln\mathcal{G}^{\vec{0},\cdots,\vec{n}_i-1}_{\vec{n}_i}(E+i\Gamma)\\&\quad+\ln\mathcal{G}^{\vec{0},\cdots,\vec{n}_i-1}_{\vec{n}_i}(E-i\Gamma)]\\&=\ln|\mathcal{G}^{\vec{0},\cdots,\vec{n}_i-1}_{\vec{n}_i}(E+iS(E)\Gamma)|\quad\text{as } s\to 0^+\ ,\end{aligned} \tag{5.24}$$

or

$$\tilde{G}^{\vec{0},\cdots,\vec{n}_i-1}_{\vec{n}_i}(E)=|\mathcal{G}^{\vec{0},\cdots,\vec{n}_i-1}_{\vec{n}_i}(E+iS(E)\Gamma)|\ . \tag{5.25}$$

Equation (5.25) is of the form (5.3) with the equality sign holding and

$$\Sigma(E)=-iS(E)\Gamma\ . \tag{5.26}$$

Hence the whole theory developed in Sec. V A is applicable. The function $F(E)$ is given by

$$F(E)=E_b/(E^2+\Gamma^2)^{1/2}\ . \tag{5.27}$$

The regions $F(E)<1$, i.e.,

$$|E|>E_c^*\equiv(E_b^2-\Gamma^2)^{1/2}\ , \tag{5.28}$$

consist of localized states. The mobility edges

$\pm E_c$ satisfy the relation $F(\pm E_c) > 1$, i.e.,

$$E_c < E_c^* \equiv (E_b^2 - \Gamma^2)^{1/2} . \tag{5.29}$$

According to the general discussion given in Sec. V A,

$$\frac{E_c^* - E_c}{E_b} \propto \frac{\Gamma^{1/2}}{E_b^{1/2}} \quad \text{as} \quad \Gamma \to 0 . \tag{5.30}$$

Anderson's transition occurs when the two mobility edges $\pm E_c$ merge together, i.e., when $E_c = -E_c$ or

$$E_c(\Gamma_c) = 0. \tag{5.31}$$

From (5.29) and (5.31) we have that

$$E_c^*(\Gamma_c) > 0 , \tag{5.32}$$

or, using (5.28)

$$\Gamma_c < E_b = \tfrac{1}{2} B . \tag{5.33}$$

Thus all eigenstates are localized for $\Gamma \geq \frac{1}{2}B$, although the disappearance of extended states happens at lower values of Γ.

Within the framework of the general theory developed in Secs. III and V, formulas (5.29) and (5.33) constitute exact inequalities that the mobility edges and the critical value of the randomness obey.

For $\Gamma = 0$, $E_c = E_c^* = E_b$, which means that for a periodic system the mobility edges coincide with the band edges as they should since there are no localized states in a perfectly periodic system. As Γ increases, the quantities $\pm E_c^*$ and, from (5.29), the mobility edges $\pm E_c$ move inwards into the band, broadening the intervals of localized states at the expense of the extended states. For a critical value of Γ, $\Gamma = \Gamma_c$, the two mobility edges $\pm E_c$ coincide. For a still higher value of Γ, $\Gamma = \frac{1}{2}B > \Gamma_c$, the quantities $\pm E_c^*$ merge together too.

This sequence of events is presented pictorially in Fig. 1 through a sketch of the average density of states per atom $\langle n(E) \rangle$ for three different values of the parameter Γ.

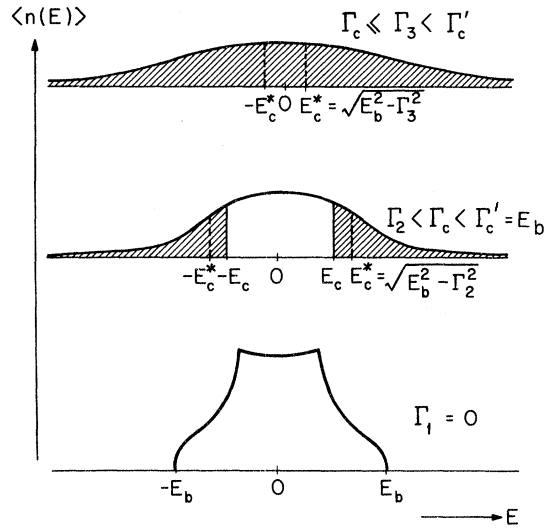

FIG. 1. Sketches of the average density of states per atom $\langle n(E) \rangle$ for three different values of the half-width Γ of the Lorentzian distribution of single-site energies. The mobility edges $\pm E_c$ separate regions of localized states (shaded) from those of extended states, and always lie within the interval $[-E_c^*, E_c^*]$. Γ_c is Anderson's critical value of the randomness (after Ref. 16).

VI. SUMMARY AND CONCLUSIONS

Because the derivations in the present paper were lengthy and complicated and many diverse aspects of them were discussed in a detailed way, we try here for the sake of clarity to present the skeleton of the logical structure of our work.

We started from a Hamiltonian of the form (2.1) satisfying conditions (2.2) and (2.3). Localized eigenstates overlapping with a given site $\vec{0}$ make a nonzero contribution to the quantity $p_{\vec{0}\vec{0}}$, where $p_{\vec{0}\vec{0}}$ is the probability of rediscovering a particle at $|\vec{0}\rangle$ as $t \to \infty$ if initially $t = 0$ was at $|\vec{0}\rangle$. It was shown that whether states of a given energy E contribute to $p_{\vec{0}\vec{0}}$ depends on the analytic structure of the $\vec{0}, \vec{0}$ matrix element $G_{\vec{0}}$ of the Green's function $G = (E - H)^{-1}$ and of the self-energy $\Delta_{\vec{0}} = E - \epsilon_0 - G_{\vec{0}}^{-1}$. $G_{\vec{0}}(E)$ and $\Delta_{\vec{0}}(E)$ have a branch cut for the regions of the spectrum corresponding to nonlocalized (i.e., extended) eigenstates. On the other hand, for the regions corresponding to localized eigenstates $G_{\vec{0}}(E)$ and $\Delta_{\vec{0}}(E)$ have a dense distribution of poles, but only a finite number of these have residues larger than any preset small value. This difference in the analytic structure of $G_{\vec{0}}$ or $\Delta_{\vec{0}}$ was used to reveal the nature of the eigenstates. The analytic behavior of $\Delta_{\vec{0}}$, and consequently the nature of the eigenstates, was then connected with the convergence properties of the renormalized perturbation series (RPS) for $\Delta_{\vec{0}}(E)$ as follows: Assume that the eigenenergy E belongs to a portion of the spectrum corresponding to localized eigenstates. One can then define the RPS for $\Delta_{\vec{0}}(E)$. If this series converges, the original assumption is true and the states there are really localized. If this series diverges, the initial assumption is wrong and consequently the states for that energy are extended. The Nth-order term of the RPS for $\Delta_{\vec{0}}$, $\Delta_{\vec{0}}^{(N)}$, was shown to be given by

$$\Delta_{\vec{0}}^{(N)} = \sum_{j=1}^{K^N} T_j , \tag{6.1}$$

for large N, where K is the percolation constant and T_j is the contribution from an Nth-order diagram. If

$$(|\Delta_{\vec{0}}^{(N)}|)^{1/N} \to L < 1 \quad \text{as} \quad N \to \infty , \tag{6.2}$$

then the RPS for $\Delta_{\vec{0}}$ converges. If $L > 1$, the series diverges. However, since the diagonal matrix ele-

ments of our Hamiltonian were assumed to be random variables, it is in general a matter of probability whether (6.2) is satisfied or not. In other words, one should find the probability distribution of $|\Delta_{\vec{0}}^{(N)}|$ in order to see if and under what conditions (6.2) holds. To this end the probability distribution for each $|T_j|$ was shown to be sharply peaked around a value of the form e^{Na_j}. Physical and mathematical arguments were developed to support the proposal that most of the quantities T_j have a common sign and that they are so strongly correlated that $\sum_j |T_j|$ and hence $|\Delta_{\vec{0}}^{(N)}|$ are sharply distributed around the value

$$\sum_{j=1}^{K^N} e^{Na_j} \equiv L^N(E).$$

Hence, if $L(E)<1$, the RPS converges with probability unity, and if $L(E)>1$, the RPS diverges with probability unity. It follows then that $L(E)$ is a localization function: The regions of the spectrum where $L(E)<1$ correspond to localized eigenstates, those where $L(E)>1$ correspond to extended states, and the critical energies E_c, where $L(E_c)=1$, are the mobility edges.

It should be emphasized that the existence of $L(E)$ does not depend on the validity of the assumption of strong correlations of the T_j. Anderson obtained qualitatively similar results assuming the other extreme of complete statistical independence of T_j's. The form of $L(E)$ does, of course, depend on which assumption is used. In any case, since statistical independence and strong correlation are limiting situations, we expect that our results and the ones deduced from Anderson's assumptions bracket the correct localization criterion. The binary-alloy case[17] and some preliminary numerical results reported by Thouless[39] provide some independent evidence that the correct answer lies closer to our result than those resulting from Anderson's assumption of statistical independence. The existence of $L(E)$ proves the correctness of the Mott-CFO model, which states there exist critical energies E_c, termed mobility edges, separating regions of the energy spectrum consisting entirely of localized states from those consisting entirely of extended states. As the randomness increases, $L(E)$ decreases and the regions of localized states expand while the regions of extended states shrink. Anderson's transition occurs locally within a band when a region of extended states disappears and globally when all regions of extended states have disappeared. Rough estimates of $L(E)$ were given and compared with related results in the literature.

The quantity $L(E)$ is difficult to calculate accurately, however. We consequently considered cases where

$$\exp\langle \ln|G_{\vec{n}_i}^{\vec{0},\cdots,\vec{n}_{i-1}}(E)|\rangle \leq |\mathcal{G}_{\vec{n}_i}^{\vec{0},\cdots,\vec{n}_{i-1}}(E-\Sigma(E))| \quad (6.3)$$

holds for all diagonal matrix elements $G_{\vec{n}_i}^{\vec{0},\cdots,\vec{n}_{i-1}}(E)$ of the Green's function with sites $\vec{0},\ldots,\vec{n}_{i-1}$ excluded, where $\mathcal{G}_{\vec{n}_i}^{\vec{0},\cdots,\vec{n}_{i-1}}$ is the corresponding matrix element for the periodic case and $\Sigma(E)$ is a self-energy. We then were able to define a function

$$F(E)=E_b/|E-\Sigma(E)|\ ,$$

where E_b is the half-width of a symmetrical band, which had the properties

$$F(E)\leq 1 \rightarrow L(E)<1\ .$$

Approximate positions of the mobility edges E_c^* were obtained from

$$F(E_c^*)=1\ ,$$

and the regions of extended states were shown to lie *within* the regions where $F(E)>1$ between adjacent E_c^*. Equation (6.3) does hold (with the equality sign) precisely for a Lorentzian distribution of single-site energies for which $\Sigma(E)=-iS(E)\Gamma$ and approximately for single-site approximations such as the CPA, where $\Sigma(E)$ is the CPA self-energy. It is expected that localization is described more accurately through $F(E)$ than through the approximate estimates thus far made of $L(E)$ directly.

The analysis just summarized was attempted as a contribution establishing the universal properties of disordered materials. In particular, we think that we have brought the subject to a stage such that the correctness of the Mott-CFO model should be considered as established, at least for Anderson's tight-binding Hamiltonian.

We conclude by pointing out the wide possibilities which open up for studying the positions of the mobility edges in different models using the function $F(E)$. In the case of a random binary alloy using $F(E)$ as calculated from the coherent potential approximation, results were already obtained[17] in striking agreement with the Mott-CFO model, with independent calculations, and with some exact results.[17,34]

ACKNOWLEDGMENTS

We have benefited from discussions with Karl Freed and Scott Kirkpatrick. This work was supported in part by ARO(D) and NASA and has benefited from general support of Materials Science at the University of Chicago by the Advanced Research Projects Agency. This work was partly supported by the Center for Advanced Studies at the University of Virginia.

APPENDIX

We want to calculate

$$\langle f(G_{\vec{n}}^{\vec{r},\vec{r},\cdots}(E))\rangle = \int d\{\epsilon_{\vec{i}}\} \prod_{\vec{i}} \frac{1}{\pi} \frac{\Gamma}{\epsilon_{\vec{i}}^2+\Gamma^2}$$

$$\times f\left(G_{\mathbf{n}}^{\mathbf{r},\mathbf{k},\cdots}(E;\{\epsilon_{\mathbf{i}}\})\right). \quad \text{(A1)}$$

We assume that all singularities of the function $f(z)$ lie on the real axis or/and at infinity. We consider first the case

$$\mathrm{Im}E>0, \quad \text{(A2)}$$

and try first to perform the integral over one of the variables $\{\epsilon_i\}$, e.g., ϵ_p. We define

$$\langle f\left(G_{\mathbf{n}}^{\mathbf{r},\mathbf{k},\cdots}(E)\right)\rangle_{\mathbf{p}}=\frac{1}{\pi}\int_{-\infty}^{\infty}d\epsilon_{\mathbf{p}}\,\frac{\Gamma}{\epsilon_{\mathbf{p}}^2+\Gamma^2}$$

$$\times f\left(G_{\mathbf{n}}^{\mathbf{r},\mathbf{k},\cdots}(E;\epsilon_{\mathbf{p}},\{\epsilon_{\mathbf{i}}\}')\right). \quad \text{(A3)}$$

We close the contour of integration by an infinite semicircle in the lower $\epsilon_{\mathbf{p}}$ half-plane. The contribution of this semicircle is zero. Thus

$$\langle f\left(G_{\mathbf{n}}^{\mathbf{r},\mathbf{k},\cdots}(E)\right)\rangle_{\mathbf{p}}=\frac{1}{\pi}\oint d\epsilon_{\mathbf{p}}\,\frac{\Gamma}{\epsilon_{\mathbf{p}}^2+\Gamma^2}$$

$$\times f\left(G_{\mathbf{n}}^{\mathbf{r},\mathbf{k},\cdots}(E;\epsilon_{\mathbf{p}},\{\epsilon_{\mathbf{i}}\}')\right). \quad \text{(A4)}$$

Since for every Hamiltonian

$$\mathrm{Im}(G_{\mathbf{n}})=-\sum_{\mathbf{r}}|G_{\mathbf{nr}}|^2\,\mathrm{Im}(E-\epsilon_{\mathbf{r}}), \quad \text{(A5)}$$

it follows that for $\mathrm{Im}\epsilon_i\leq 0$ and $\mathrm{Im}E>0$

$$\mathrm{Im}G_{\mathbf{n}}^{\mathbf{r},\mathbf{k},\cdots}(E;\epsilon_{\mathbf{p}}\{\epsilon_{\mathbf{i}}\})<0. \quad \text{(A6)}$$

Lloyd[19] has shown that when $\mathrm{Im}E>0$, $G_{\mathbf{n}}^{\mathbf{r},\mathbf{k},\cdots}$ cannot have a pole for $\mathrm{Im}\epsilon_i\leq 0$. Since the only singularities of $f(z)$ can occur when the argument is real or infinite, it follows that $f\left(G_{\mathbf{n}}^{\mathbf{r},\mathbf{k},\cdots}(E;\epsilon_{\mathbf{p}},\{\epsilon_{\mathbf{i}}\}')\right)$ has no singularities in the lower $\epsilon_{\mathbf{p}}$ half-plane. Hence the only pole inside the contour of integration is $\epsilon_{\mathbf{p}}=-i\Gamma$. Thus

$$\langle f\left(G_{\mathbf{n}}^{\mathbf{r},\mathbf{k},\cdots}(E;\epsilon_{\mathbf{p}},\{\epsilon_{\mathbf{i}}\}')\right)\rangle_{\mathbf{p}}$$

$$=f\left(G_{\mathbf{n}}^{\mathbf{r},\mathbf{k},\cdots}(E;-i\Gamma,\{\epsilon_{\mathbf{i}}\}')\right). \quad \text{(A7)}$$

Repeating the same analysis for the integration over every variable $\epsilon_{\mathbf{i}}$, we obtain finally

$$\langle f\left(G_{\mathbf{n}}^{\mathbf{r},\mathbf{k},\cdots}(E;\{\epsilon_i\})\right)\rangle=f\left(G_{\mathbf{n}}^{\mathbf{r},\mathbf{k},\cdots}(E;\{-i\Gamma\})\right), \quad \text{(A8)}$$

or

$$\langle f\left(G_{\mathbf{n}}^{\mathbf{r},\mathbf{k},\cdots}(E;\{\epsilon_i\})\right)\rangle=f\left(G_{\mathbf{n}}^{\mathbf{r},\mathbf{k},\cdots}(E+i\Gamma;\{0\})\right). \quad \text{(A9)}$$

The right-hand side of (A9) is nothing else than

$$f\left(\mathcal{G}_{\mathbf{n}}^{\mathbf{r},\mathbf{k},\cdots}(E+i\Gamma)\right), \quad \text{(A10)}$$

according to the definition of $\mathcal{G}_{\mathbf{n}}^{\mathbf{r},\mathbf{k},\cdots}(z)$. The same analysis can be repeated when $\mathrm{Im}E<0$. Then we should close the contours of integration in the upper $\epsilon_{\mathbf{i}}$ half-planes and consequently the quantity $i\Gamma$ in (A9) should be replaced by $-i\Gamma$. Introducing the function

$$S(E)=1 \quad \text{if } \mathrm{Im}E>0$$

$$=-1 \quad \text{if } \mathrm{Im}E<0, \quad \text{(A11)}$$

we can write the results for both cases as

$$\langle f\left(G_{\mathbf{n}}^{\mathbf{r},\mathbf{k},\cdots}(E;\{\epsilon_i\})\right)\rangle=f\left(\mathcal{G}_{\mathbf{n}}^{\mathbf{r},\mathbf{k},\cdots}(E+iS(E)\Gamma)\right). \quad \text{(A12)}$$

---

*This work was completed when one of the authors (E.N.E.) was at the University of Virginia.

†Present address: Department of Physics, University of Virginia, Charlottesville, Va. 22901.

[1]N. F. Mott, Advan. Phys. 16, 49 (1967).

[2]Morrel H. Cohen, H. Fritzsche, and S. R. Ovshinsky, Phys. Rev. Letters 22, 1065 (1969).

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

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

[5]H. Frölich, Proc. Roy. Soc. (London) A188, 521 (1947).

[6]A. I. Gubanov, *Quantum Electron Theory of Amorphous Conductors* (Consultants Bureau, New York, 1965).

[7]L. Banyai, *Physique des Semiconducteurs* (Dunod, Paris, 1964), p. 417.

[8]I. M. Lifshitz, Advan. Phys. 13, 483 (1964).

[9]V. L. Bonch-Bruevich, Fiz. Tverd. Tela 5, 1852 (1964) [Sov. Phys. Solid State 5, 1353 (1964)].

[10]B. I. Halperin and M. Lax, Phys. Rev. 148, 722 (1966).

[11]J. Zittarz and J. S. Longer, Phys. Rev. 148, 741 (1966).

[12]E. O. Kane, Phys. Rev. 131, 79 (1963).

[13]M. Cutler and N. F. Mott, Phys. Rev. 181, 1336 (1969).

[14]N. F. Mott, Rev. Mod. Phys. 40, 677 (1968).

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

[16]E. N. Economou and Morrel H. Cohen, Phys. Rev. Letters 25, 1445 (1970).

[17]E. N. Economou, S. Kirkpatrick, Morrel H. Cohen, and T. P. Eggarter, Phys. Rev. Letters 25, 520 (1970).

[18]See, e.g., B. Velický, S. Kirkpatrick, and H. Ehrenreich, Phys. Rev. 175, 747 (1968).

[19]P. Lloyd, J. Phys. C 2, 1717 (1969).

[20]F. Brouers, J. Non-Cryst. Solids 4, 428 (1970).

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

[22]N. F. Mott, Phil. Mag. 22, 7 (1970).

[23]We have supposed $Z_{\vec{0}}(E)$ must vanish for extended states because we expect that $n_{\vec{0}}(E)\neq 0$ for them, except precisely at the mobility edges. That this is so is obvious for ordinary extended states such as Bloch states in crystals, which extend everywhere. For energies near the mobility edges, the regions of the disordered material which are allowed in the semiclassical sense are of channel form, and follow the classical percolation probability (see Ref. 31 below). This vanishes at E_c, but inside E_c the channels cover a finite fraction of the volume and are never very far from any given sites. It seems highly probable, when quantum effects are included, that the amplitudes of the extended states are therefore everywhere finite.

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

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

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

[27]V. S. Pugachev, *Theory of Random Functions* (Pergamon, Oxford, 1965), pp. 136–140 and 273.

[28]R. VonMises, *Mathematical Theory of Probability and Statistics* (Academic, New York, 1964), pp. 289–305.

[29]The statement that the distribution of the quantity $X_i^{(N)}$ is a normal one means only that for arbitrary a and b

$$\lim\int_a^b P_i^{(N)}(x)\,dx = \int_a^b \Phi(x)\,dx \text{ as } N\to\infty,$$

where $P_i^{(N)}$ is the distribution function of $X_i^{(N)}$, and Φ is a normalized Gaussian with mean value and standard deviation equal to $\lim\langle X_i^{(N)}\rangle$ as $N\to\infty$ and $\lim\sigma_{X_i^{(N)}}$ as $N\to\infty$, respectively (see Refs. 27 and 28). It should be emphasized that the stronger condition $\lim P_i^{(N)}(X)=\Phi(X)$ as $N\to\infty$ is not in general true and as a consequence one *cannot* in general calculate the moments of $X_i^{(N)}$ using the normal distribution. This observation is particularly relevant to the present case, where, as Anderson pointed out (Ref. 4), the distributions of $T_i^{(N)}$ (and hence of $X_i^{(N)}$) are long tailed. This long tail in the distribution $P_i^{(N)}$ makes a zero contribution to any integral of the form $\int_a^b P_i^{(N)}(x)dx$ as $N\to\infty$, but a nonzero contribution to integrals of the form $\lim\int_\alpha^\infty x^n P_i^{(N)}(x)\,dx$ as $N\to\infty$ for $n>0$. Thus the central limit theorem should be used with extreme caution in the present case; e.g., it cannot be used to simplify Anderson's original analysis (Ref. 4), where an integral of the type $\lim K^N\int_{A_N}^\infty P_i^{(N)}(x)dx$ as $N\to\infty$ must be calculated with $\lim A_N\to\infty$ as $N\to\infty$, and $K>1$.

[30]This statement is correct only if the shift in the levels (due to the different sites omitted) is not much larger than the average level spacing. One can argue in favor of the latter statement assuming that the eigenstates are localized in a fashion similar to that suggested by classical percolation theory [i.e., that they tend to become extended as we approach the mobility edge in an essentially one-dimensional way (channels)]. In this case the shift of the levels is of the order $1/l$, where l is the length of the channel; the average spacing of the levels in a one-dimensional potential well of length l is of the order of $1/l$, i.e., of the same order of magnitude as the level shift. However, since the fluctuation of the potential along the channel is not uniform, one expects that the average level spacing in the channel would be larger than the corresponding uniform potential well. Thus the level shift is expected to be of the same order of magnitude or less than the average level spacing.

[31]S. R. Broadbent and J. M. Hammersley, Proc. Cambridge Phil. Soc. 53, 629 (1957).

[32]J. M. Hammersley, Trans. Cambridge Phil. Soc. 57, 516 (1961).

[33]J. M. Ziman, J. Phys. C 1, 1532 (1968); C. Domb, *ibid.* 3, 256 (1970).

[34]S. Kirkpatrick, E. N. Economou, Morrel H. Cohen, and Costas Papatriantafillou (unpublished).

[35]P. Soven, Phys. Rev. 156, 809 (1967); 178, 1136 (1969).

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

[37]G. F. Koster and J. C. Slater, Phys. Rev. 86, 1208 (1954).

[38]N. I. Muskhelishvili, *Singular Integral Equations* (Noordhoff, Groningen, The Netherlands, 1953), pp. 51–55.

[39]D. Thouless, in Proceedings of the Fourth International Conference on Amorphous and Liquid Semiconductors, Ann Arbor, Mich., 1971 (unpublished).

PHYSICAL REVIEW B VOLUME 5, NUMBER 8 15 APRIL 1972

Vacancy-Formation Entropy in Cubic Metals

J. J. Burton
Henry Krumb School of Mines, Columbia University, New York, New York 10027
(Received 25 October 1971)

Vacancy-formation entropies were computed for a number of face-centered-cubic solids from vibrational frequency distributions which were computed from pair potentials. The formation entropy is a monotonic function of the vacancy relaxation, computed from the same pair potential. It is shown that the relaxation of the nearest neighbors to the vacancy in fcc solids can be described by $\delta_1 = -5.8\times10^{15}(K/\alpha V)^2$, where δ_1 is in percent, K is the compressibility, α the linear thermal-expansion coefficient, and V is the molar volume. The computed vacancy-formation entropies are described by $\Delta S = 1.83 + 3.4\times10^{15}(K/\alpha V)^2$ in units of k/vacancy. Similar relations are obtained for bcc metals. The experimental relations found for model solids are used to predict vacancy relaxations and formation entropies from experimental values of K, α, and V. Vacancy relaxations are predicted to be less than 0.2% of the normal neighbor distance in most fcc metals and 2–5% in bcc metals. Vacancy-formation entropies are predicted to be $1.8k$–$2.0k$ in most fcc metals and $2.2k$–$2.6k$ in bcc metals. The predictions for the entropy are in satisfactory agreement with experimental data, where reliable data exist.

I. INTRODUCTION

There are questions as to the self-diffusion mechanism in rare-gas solids[1] and noble metals.[2] It is known that vacancies play an important role. This has motivated a number of workers to attempt to calculate the formation entropy,[3–12] motion entropy,[7,8] formation energy,[5,7,10,11,13–16] and motion