from the retarded interaction of surface plasmons. This result apparently is due to the fact that electromagnetic bulk excitations do not extend beyond surfaces[8] and thus do not contribute to an attractive force. Since the physical properties of surface plasmons are well understood, this new concept provides a much simpler intuitive understanding of van der Waals forces than the methods used before.[9,10–13] In particular, in the nonretarded limit, van der Waals forces are simply the attraction forces resulting from the interaction of the intrinsic surface-charge-density oscillations.

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Localization in One-Dimensional Disordered Systems*

E. N. Economou† and Morrel H. Cohen
The James Franck Institute, University of Chicago, Chicago, Illinois 60637
(Received 12 April 1971)

The basic idea that the convergence of the renormalized perturbation expression for the self-energy Δ_0 at a given energy is equivalent to the localizability of the eigenstates, if any, at this energy is applied to one-dimensional random systems, namely, electrons in the tight-binding approximation and phonons. For nearest-neighbor interactions all eigenstates are localized. If second-nearest-neighbor interactions are present, the possibility of the existence of extended states remains; we have shown that existing theories are unable to give a definite answer to the problem in this case.

I. INTRODUCTION

The study of disordered one-dimensional (1-D) systems has been focused on (a) numerical calculations of the average density of states, (b) theoretical efforts to show whether or not spectral gaps remain when disorder is introduced, and (c) theoretical and numerical studies to reveal the nature of the eigenstates, i.e., if they are localized or extended.

For the electronic case the early work was devoted to problems (b)[1–4] and (a)[3–8] above, although problem (c) was examined briefly in the work of Landauer and Helland.[4] Mott and Twose[9] were the first to suggest that all the electronic eigenfunctions in 1-D disordered systems are localized. Borland[10,11] was the first to present a rather general proof of this statement. A critical discussion of Borland's work is given in a review article by Halperin.[12] More recent work is discussed in review articles by Mott,[13] Hori,[14] Economou *et al.*,[15] and in books by Lieb and Mattis[16] and by Hori.[17]

For the problem of lattice vibrations in disordered 1-D systems the emphasis was on the calculation of the average spectral density. Since the pioneering work of Dyson,[18] many efforts have been made on analytical calculations of the spectrum. Dean,[19] in his remarkable numerical work, showed that the spectrum of an isotopically disordered linear chain has much fine structure with many well-defined peaks and valleys. Dean explained the existence of the peaks as due to states strongly localized around small islands of light masses surrounded by heavy masses. Hori *et al.*[20,21] gave a theoretical basis to Dean's finding by showing that such a fine structure should be expected for a wide variety of disordered systems. Dean[22] presented a proof, similar to that given by Borland for the electronic case, that all phonons in a 1-D disordered system are localized. It

seems, however, that his proof has not been widely accepted.[16,17]

Anderson[23] studied the problem of localization of the eigensolutions of a tight-binding Hamiltonian in a 3-D disordered system. He introduced the important idea that the nature of the eigenstates depends on whether or not a renormalized perturbation expression (RPE) for the self-energy Δ_0 converges. This idea was rigorously formulated recently by the present authors.[24] It has been established[24] that if the RPE for Δ_0 diverges at a certain real energy, the density of states is different from zero there and the corresponding eigenstates are all extended. On the other hand, if the RPE for Δ_0 converges for a given real energy, either the density of states is zero there or, if there are eigenstates corresponding to this energy, they are localized.

In the present work we use this idea to study some 1-D systems satisfying the criteria for its applicability, i.e., electronic systems in the tight-binding approximation and lattice vibrations within the harmonic approximation and for nearest-neighbor coupling. Some of these restrictions can probably be relaxed without affecting the final conclusions.

The basic result of the present completely different approach is in agreement with Borland's theorem: All eigenstates are localized. Our proof is direct and does not suffer from the presence of an ergodic assumption as Borland's does.[10,12,16] For the electronic case, Borland's method is more valuable since it covers a more realistic case than the present one. However, in the phonon case the present proof is especially needed in face of the skepticism which Dean's alternative proof has met.[16,17] It should be mentioned that our proof is based upon the convergence of a function $f_n(x)$ as $n \to \infty$, where

$$f_n(x) = \int_{-\pi/2}^{\pi/2} K(x', x) f_{n-1}(x')\, dx' \,. \tag{1.1}$$

We have shown here that the kernel $K(x', x)$ satisfies Frechet conditions[10] and consequently,[10] the function $f_n(x)$ converges uniformly as $n \to \infty$. Borland[10] was faced also with the convergence of a function $f_n(x)$ satisfying (1.1). In order to show that his kernel satisfies the Frechet conditions, he imposed certain restrictions that made his proof rigorously valid only for high energies. We have slightly extended Borland's method here so that no restriction on the values of the energy are needed. This slight generalization can be used in Borland's work also, making his proof valid for every energy.

Our proof is based upon the assumption of nearest-neighbor interaction only. If one permits the existence of, e.g., second-nearest neighbors, our proof breaks down, since new possibilities for the divergence of the RPE for Δ_0 appear which were absent previously. In this case the analysis of the convergence of the RPE can be carried on as in the 3-D case.[24] Thus a localization function $L(E)$ can be defined such that $L(E) > 1$ (< 1) if the eigenstates at E are extended (localized). However, we are neither able, in contrast to the 3-D case, to show that there are cases where $L(E) > 1$ (which would mean that there are extended states in 1-D disordered systems) nor able to show that $L(E) < 1$ always (which would mean that all the eigenstates in 1-D disordered systems remain localized even in the presence of second-nearest-neighbor interaction). We were able, however, to obtain under certain conditions an *inequality* restricting the regions where extended states, if any, can be found.

In Sec. II the tight-binding electronic case is considered in detail. It is shown that when the degree of randomness is different from zero all the eigenstates are localized.

In Sec. III the lattice vibration problem is examined and it is shown that it is equivalent to the electronic one, so that the proof given for the latter holds for the former, too.

In Sec. IV a model with second-nearest-neighbor interaction is examined. The analysis is similar to that used for the 3-D case and results in the definition of a localization function.

In Sec. V a brief discussion is given about the possibility of the existence of extended eigenfunctions in disordered 1-D systems.

II. ELECTRONS: TIGHT-BINDING APPROXIMATION

We consider here the motion of an electron in a one-dimensional array of potential wells (Fig. 1). We denote by $|i\rangle$ ($i = 0, \pm 1, \pm 2, \ldots$) a Wannier state localized around the ith potential well. The Hamiltonian describing the electron in this system is assumed to be

$$H_{ij} = \langle i | H | j \rangle = \epsilon_i \delta_{ij} + V_{ij}, \tag{2.1}$$

where

$$\begin{aligned} V_{ji} = V_{ij} &= V_j \delta_{i+1,j}, \quad j = 1, 2, 3, \ldots \\ &= V_i \delta_{i+1,j}, \quad j = 0, -1, -2, \ldots \,. \end{aligned} \tag{2.2}$$

Hamiltonian (2.1) describes the formation of a band from a single atomic orbital through nearest-neighbor interaction only. The theory based on (2.1) can be trivially generalized to more than one band as long as there are no matrix elements between different bands in the Hamiltonian. The disorder is introduced in the system by allowing the quantities ϵ_i and V_i to be random variables. More specifically, we assume that the pair ϵ_i, V_i is statistically independent from any other pair

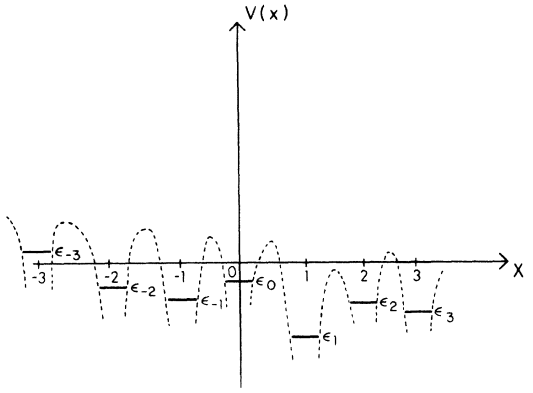

FIG. 1. Model 1-D random potential. Levels ϵ_i denote the energy eigenvalue of the ground state in each well if it was isolated.

ϵ_{i+k}, V_{i+k} ($k = \pm 1, \pm 2, \ldots$) with a common distribution function, i.e.,

$$\mathcal{P}\{\epsilon_i, V_i\} = \prod_i P(\epsilon_i, V_i). \tag{2.3}$$

The eigensolution $|\psi^{(r)}\rangle$ corresponding to the eigenvalue $E^{(r)}$ can be written as

$$|\psi^{(r)}\rangle = \sum_j c_j^{(r)} |j\rangle, \tag{2.4}$$

where the quantities $c_j^{(r)}$ satisfy the basic matrix equation

$$\sum_j H_{ij} c_j^{(r)} = E^{(r)} c_i^{(r)} \ . \tag{2.5}$$

The problem is to find whether the eigenfunctions $|\psi^{(r)}\rangle$ satisfying Eq. (2.5) are localized or not. An eigensolution is called localized when the coefficients $c_j^{(r)}$ are different from zero for values of j in the neighborhood, let us say, of j_0 and if

$$c_k^{(r)} \xrightarrow[|k-j_0|\to\infty]{} 0 \ .$$

It has been shown[24] that the localizability of an eigenfunction overlapping, e.g., with $|0\rangle$ and belonging to the eigenergy $E^{(r)}$ can be determined by the convergence properties of RPE for the self-energy Δ_0 ($E^{(r)}$). The proof has been given in Ref. 24 for the 3-D case, but it is easy to check that it is independent of the dimensionality of the system. The self-energy $\Delta_0(E)$ is defined by

$$G_0(E) \equiv \frac{1}{E - \epsilon_0 - \Delta_0(E)} \ , \tag{2.6}$$

where $G_0(E)$ is the 0, 0 matrix element of the Green's function of the system, i.e.,

$$G_0(E) \equiv \langle 0 | 1/(E - H) | 0 \rangle . \tag{2.7}$$

The RPE for Δ_0 corresponding to Hamiltonian (2.1) and (2.2) can be found[23,24] as the contributions from all self-avoiding paths starting from and ending at site 0 and linking only nearest neighbors. The last restriction stems from relation (2.2). To each step from site i to site j ($j = i \pm 1$) there corresponds a factor V_{ij}, and to each site j (except 0) there corresponds a factor $G_j^{0,\cdots}$, where $G_j^{0,\cdots}$ is the j-j matrix element of the Green's function corresponding to a Hamiltonian differing from (2.1) in that $\epsilon_k = \infty$, where k denotes every site which precedes site j in the particular path under consideration.

In the 1-D case there are only two self-avoiding paths starting from and ending at site 0 and linking nearest neighbors only, as shown in Fig. 2, and therefore only two terms in the RPE. On the other hand, for higher dimensionality there is an infinite number of such paths and therefore an infinite series of terms in the RPE. This basic difference between 1-D and higher dimensionality, stemming from the lack of alternative paths connecting two points in 1-D systems, accounts for the unique properties relating to localization of the eigensolutions in 1-D systems with nearest-neighbor interaction.

Thus, in our case, the RPE for Δ_0 is

$$\Delta_0(E) = V_{01} G_1^0 V_{10} + V_{0,-1} G_{-1}^0 V_{-10} \ . \tag{2.8}$$

The first term of the right-hand side of (2.8) can be written by taking into account (2.6) and (2.2),

$$V_{01} G_1^0 V_{10} = \frac{V_1^2}{E - \epsilon_1 - \Delta_1^0} \ . \tag{2.9}$$

The quantity Δ_1^0 is the self-energy corresponding to a Hamiltonian where $\epsilon_0 = \infty$. Writing the RPE for Δ_1^0 by the same rules as for Δ_0 we obtain

$$\Delta_1^0 = V_{12} G_2^{0,1} V_{21} \ , \tag{2.10}$$

where the other term $V_{10} G_0^{0,1} V_{01}$ is zero since $\epsilon_0 = \infty$. Equation (2.10) can be written

$$\Delta_1^0 = \frac{V_2^2}{(E - \epsilon_2 - \Delta_2^{0,1})} \ , \tag{2.11}$$

where $\Delta_2^{0,1}$ can be again expanded according to (2.11). Thus the final expression for $V_{01} G_1^0 V_{01}$ is

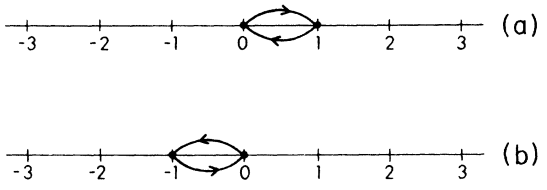

FIG. 2. The only two diagrams for RPE of the self-energy Δ_0 when only nearest-neighbor coupling is present.

$$V_{01}G_1^0V_{10}=\cfrac{V_1^2}{E-\epsilon_1-\cfrac{V_2^2}{E-\epsilon_2-\cfrac{V_3^2}{E-\epsilon_3-\cfrac{V_4^2}{E-\epsilon_4-\cdots}}}} \tag{2.12}$$

The RPE for $\Delta_0(E)$ is

$$\Delta_0(E)=\cfrac{V_1^2}{E-\epsilon_1-\cfrac{V_2^2}{E-\epsilon_2-\cfrac{V_3^2}{E-\epsilon_3-\cdots}}}+\cfrac{V_{-1}^2}{E-\epsilon_{-1}-\cfrac{V_{-2}^2}{E-\epsilon_{-2}-\cfrac{V_{-3}^2}{E-\epsilon_{-3}-\cdots}}}\,. \tag{2.13}$$

According to what was stated, if the RPE (2.13) converges for $E=E^{(r)}$, the eigensolution corresponding to $E^{(r)}$, if any, is localized. In contrast to the 3-D case where the RPE is an infinite series, the question of convergence arises only in relation to the two continued fractions in (2.13). On the other hand, if at least one of the two continued fractions diverge for a certain value of E, to this value of E there corresponds extended (i.e., nonlocalized) solutions. If only one of these continued fractions diverges, the eigensolution extends to infinity in the one direction only. Since both continued fractions have the same structure, it is enough to study the convergence of the first only. This can be achieved by reducing it to an infinite succession of Möbius transformations. If we denote the first continued fraction in (2.8) by t, we can write

$$t=w_1(w_2(\omega_3(\cdots))), \tag{2.14}$$

where

$$w_i(Z)=V_i^2/(E-\epsilon_i-Z)\,. \tag{2.15}$$

If we terminate at the nth step, we shall obtain

$$t_n=w_1(w_2(\cdots w_n(0)\cdots)). \tag{2.16}$$

The continued fraction (2.14) is defined as

$$t=\lim_{n\to\infty}t_n \tag{2.17}$$

if this limit exists.

We shall examine first the periodic case where $V_i^2=V^2$ and $\epsilon_i=\epsilon$ for every i. Denoting by Z_1, Z_2 the two solutions of the equation

$$Z=V^2/(E-\epsilon-Z)\,, \tag{2.18}$$

we can write (2.15) as

$$\frac{w(Z)-Z_1}{w(Z)-Z_2}=\frac{Z_1}{Z_2}\frac{Z-Z_1}{Z-Z_2}\,. \tag{2.19}$$

Combining (2.19) and (2.16) we obtain

$$\frac{t_n-Z_1}{t_n-Z_2}=\left(\frac{Z_1}{Z_2}\right)^{n+1}\,. \tag{2.20}$$

If $|Z_1/Z_2|\neq 1$, then one sees from (2.20) that $\lim t_n=Z_i$ as $n\to\infty$, where $|Z_i|<|Z_j|$, $i,j=1,2$. On the other hand, if $|Z_1/Z_2|=1$ and $\arg Z_1/Z_2=\phi\neq 0, 2\pi, \ldots$, then it follows from (2.20) that t_n does not converge as $n\to\infty$. From (2.18) we have that

$$Z_{1,2}=\tfrac{1}{2}\{E-\epsilon\pm[(E-\epsilon)^2-4V^2]^{1/2}\}. \tag{2.21}$$

Thus if E is real and $(E-\epsilon)^2>4V^2$ or if $\mathrm{Im}E\neq 0$, then $|Z_1/Z_2|\neq 1$ and the continued fraction converges; if E is real and $(E-\epsilon)^2<4V^2$, then $|Z_1/Z_2|=1$ with $\arg(Z_1/Z_2)\neq 0$ and the continued fraction diverges. The conclusion is that for the periodic case the RPE for $\Delta_0(E)$ diverges on the portion of the real axis $[\epsilon-2V, \epsilon+2V]$ and converges everywhere else. We have thus retrieved the standard result of a band of extended states with total bandwidth $B=4V$ as it should be for a 1-D case with nearest-neighbor interactions.

The motion of a point t_i lying on the real axis due to successive Möbius transformations (2.15) can be better visualized by considering the corresponding motion of the geometrically inverse point on a semicircle with center lying outside the real axis as shown in Fig. 3. The position of the inverse point is uniquely determined by an angle ϕ_i such that $-\frac{1}{2}\pi\leq\phi_i\leq\frac{1}{2}\pi$ and every transformation is characterized by an angle θ_i ($-\frac{1}{2}\pi\leq\theta_i\leq\frac{1}{2}\pi$) such that $\phi_{i+1}=\phi_i+\theta_i$, where θ_i is a function of the parameters of the Möbius transformation, the quantity ϕ_i, and the position of the center of the semicircle. The motion of the inverse point becomes particularly simple in the case where $|(E-\epsilon_i)/V_i|<2$ and the center of the semicircle has been chosen as $C_i=\frac{1}{2}\{E-\epsilon_i+i[4V_i^2-(E-\epsilon_i)^2]^{1/2}\}$.

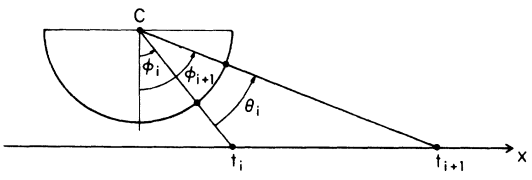

FIG. 3. Relation between the t and ϕ variables.

Then θ_i is independent of ϕ_i and is given by

$$\theta_i = \tan^{-1}\left[1-\left(\frac{E-\epsilon_i}{2V_i}\right)^2\right]^{1/2}\Big/\frac{E-\epsilon_i}{2V_i} \quad . \tag{2.22}$$

We return now to the disordered case where the quantities ϵ_i and V_i are independent random variables possessing a common distribution function $P(\epsilon_i, V_i)$. In this case, the quantites t_n are random variables themselves possessing a distribution function $f_n(t_n)$ which is a functional of $P(\epsilon_i, V_i)$. We shall show here that as $n \to \infty$ the function f_n converges uniformly for every x to a function $f(x)$ independent of n, as long as the distribution $P(\epsilon_i, V_i)$ is bounded in heights. This means that for every ensemble of random systems characterized by a bounded distribution $P(\epsilon_i, V_i)$, the distribution of the quantity t_n becomes independent of n as $n \to \infty$. The last statement is equivalent to asserting that for almost every member of the ensemble considered (except for some of total measure zero) the quantity t_n converges as $n \to \infty$ to a limiting value t which, of course, depends on the specific member of the ensemble. To prove this it is enough to show that t_{n+k} is independent of t_k as $n \to \infty$ for almost every value of t_k. But if t_{n+k} were depending on t_k as $n \to \infty$ for a non-negligible fraction of the members of the ensemble, then one could construct an ensemble with a bounded $P(\epsilon_i, V_i)$ such that $f_n(x)$ would not converge uniformly to $f(x)$ as $n \to \infty$, in contradiction to what will be proved here.

The distribution function $f_{n+1}(t_{n+1})$ is given in terms of the distribution function $f_n(t_n)$ by an integral equation of the form

$$f_{n+1}(t_{n+1}) = \int_{-\infty}^{\infty} K^*(t_n, t_{n+1}) f_n(t_n)\, dt_n , \tag{2.23}$$

where the kernel K^* is given by

$$K^*(t_n, t_{n+1}) = \frac{1}{t_{n+1}^2}\int dV_i\, V_i^2 P\left(E - t_n - \frac{V_i^2}{t_{n+1}},\ V_i\right) . \tag{2.24}$$

The $P(\epsilon_i, V_i)$ is the distribution function of the pair of random variables ϵ_i, V_i. In the case where V_i is not a random variable but just a constant V, Eq. (2.24) becomes

$$K^*(t_n, t_{n+1}) = \frac{V^2}{t_{n+1}^2} P_V\left(E - t_n - \frac{V^2}{t_{n+1}}\right) , \tag{2.25}$$

where $P_V(\epsilon_i)$ is the distribution of the random variable ϵ_i. On the other hand, if ϵ_i is constant ϵ_0 and if V_i is a random variable with a distribution function $P_\epsilon(V_i)$, then the kernel becomes

$$K^*(t_n, t_{n+1}) = \frac{1}{2}\left(\frac{E - t_n - \epsilon_0}{t_{n+1}}\right)^{1/2} P_\epsilon\left[(t_{n+1}(E - t_n - \epsilon_0))^{1/2}\right]$$

$$\text{if } t_{n+1}(E - t_n - \epsilon_0) > 0,$$

$$= 0 \quad \text{if } (E - t_n - \epsilon_0) t_{n+1} < 0 . \tag{2.26}$$

If the function $P(\epsilon_i, V_i)$ is bounded and $P(\epsilon_i, V_i) - g(V_i)/\epsilon_i^s$ as $\epsilon_i \to \infty$ with $s \geq 2$, where $g(V_i)$ is a bounded function of V_i, then the kernel (2.24) is always bounded. Similarly, if $P_V(\epsilon_i)$ is bounded and $P(\epsilon_i) \to \text{const}/\epsilon_i^s$ as $\epsilon_i \to \infty$ with $s \geq 2$, then the kernel (2.25) is bounded. Let us note that these restrictions on the asymptotic behavior of the distribution functions are of no physical importance, since any realistic distribution function would terminate. For the kernel (2.26) to be bounded one needs to assume that $P_\epsilon(V_i)$ is bounded by

$$P_\epsilon(V_i) \xrightarrow[V_i \to \infty]{} \text{const}/V_i^s \quad \text{with } s \geq 3$$

and

$$P_\epsilon(V_i) \xrightarrow[V_i \to 0+]{} \text{const} \times V_i^s \quad \text{with } s \geq 1.$$

Although we need to assume that the kernel in (2.23) is bounded to prove the localizability of the eigenfunctions, it is clear from the physical point of view that if we allow the functions $P_V(\epsilon_i)$ and $P_\epsilon(V_i)$ to violate the restrictions for the behavior around $\epsilon_i = \infty$ and $V_i = 0$, respectively, we actually help the localization of the eigensolutions.

Transforming from the variables $\{t_n\}$ to the variables $\{\phi_n\}$ introduced earlier we can write (2.23) as

$$P_{n+1}(\phi_{n+1}) = \int_{-\pi/2}^{\pi/2} K(\phi_n, \phi_{n+1}) P_n(\phi_n)\, d\phi_n , \tag{2.27}$$

where

$$P_i(\phi_i) = f_i(t(\phi_i))\frac{dt}{d\phi_i} , \quad i = 1, 2, \ldots \tag{2.28a}$$

$$K(\phi_i, \phi_{i+1}) = K^*(t(\phi_i), t(\phi_{i+1}))\frac{dt}{d\phi_{i+1}} , \quad i = 1, 2, 3, \ldots \tag{2.28b}$$

and $t(\phi)$ denotes the function relating ϕ with t. From (2.27) it follows that

$$P_n(\phi_n) = \int_{-\pi/2}^{\pi/2} K_n(\phi_0, \phi_n) P_0(\phi_0)\, d\phi_0 , \tag{2.29}$$

where K_n, the nth iterated kernel, is given by

$$K_n(\phi_0, \phi_n) = \int_{-\pi/2}^{\pi/2} K_{n-1}(\phi_0, \phi_{n-1}) K(\phi_{n-1}, \phi_n)\, d\phi_{n-1} \tag{2.30}$$

and

$$P_0(\phi_0) = \delta(\phi_0 - a) , \tag{2.31}$$

where a is the angle ϕ corresponding to $t = 0$ and $K_1 = K$.

Frechet has shown that $K_n(\phi_0, \phi)$ converges uniformly to a function $p(\phi)$ independent of ϕ_0 as $n \to \infty$, provided that $K(\phi_i, \phi_{i+1})$ satisfies certain conditions. Moreover, he has shown that $p(\phi)$ is a unique solution of the system defined by

$$p(\phi) = \int_{-\pi/2}^{\pi/2} K(\epsilon_0, \phi) p(\epsilon_0) d\epsilon_0 , \tag{2.32}$$

$$\int p(\phi) d\phi = 1 . \tag{2.33}$$

Thus, as can be seen by (2.29), $P_n(\phi)$ converges uniformly to $p(\phi)$ and consequently $f_n(t) \to f(t)$ as $n \to \infty$, where $f(t) = p(\phi(t)) d\phi/dt$. This proves that the distribution function $f_n(t_n)$ converges uniformly to a function $f(t_n)$ independent of n for any distribution $P(\epsilon_i, V_i)$, provided only that the Frechet conditions are satisfied. As has been already discussed, this convergence of $f_n(x)$ to $f(x)$ as $n \to \infty$ for any distribution $P(\epsilon_i, V_i)$ is equivalent to the convergence of the continued fraction (2.14) for almost every member of the statistical ensemble, which in turn means that all the eigensolutions are localized for almost every member of the ensemble (except, perhaps, of some of total measure zero). In the Appendix we prove that the Frechet conditions are satisfied, as long as the kernel K^* is bounded, which is true when $P(\epsilon_i, V_i)$ is bounded. The proof given in the Appendix holds for the case where the inequality $|(E - \epsilon_i)/2V_i| < 1$ is satisfied for a non-negligible portion of the configurations. A similar but not identical proof can be given for the case where this inequality is violated for almost all configurations. The case discussed in the Appendix is clearly the most unfavorable one for localization since it corresponds to small values of $|E - \epsilon_i|$ (limited degree of randomness) and large values of V_i (well within the band). The proof presented in the Appendix is a slight generalization of that given by Borland[10] for a mathematically similar problem. The generalization consists in that we do not impose, as Borland does, the condition that $K(\phi_{n-1}, \phi_n)$ is positive for all values of the arguments. It should be mentioned that the same generalization can be used in the case examined by Borland, and consequently, his result is valid rigorously for every electronic energy and not only for high enough energies as Borland stated.[10]

III. LATTICE VIBRATIONS

We shall consider in this section the longitudinal motion of the atoms of a linear chain. We assume that the mass of each atom is a random variable characterized by a bounded distribution function common for every atom. The spring constants are assumed to be the same k for every pair of nearest neighbors (isotopic disorder). No other coupling beyond that is present. The equation for the displacement x_i of the ith particle of mass m_i is given by

$$m_i \ddot{x}_i = -k(x_i - x_{i+1}) - k(x_i - x_{i-1}) . \tag{3.1}$$

Assuming a time dependence of the form $e^{i\omega t}$ we obtain

$$(2k - m_i \omega^2) x_i = k(x_{i-1} + x_{i+1}) . \tag{3.2}$$

Comparing (3.2) with (2.5) one sees that they are equivalent if one makes the substitutions

$$2k = E , \tag{3.3a}$$

$$m_i \omega^2 = \epsilon_i , \tag{3.3b}$$

$$k = V , \tag{3.3c}$$

$$x_i = c_i . \tag{3.3d}$$

Hence the whole theory of Sec. II can be repeated for the case of phonons in isotopically disordered 1-D systems. As a consequence, the basic theorem deduced in Sec. II is true in the present case: In a 1-D isotopically disordered system, where the masses are independent random variables possessing a common bounded distribution function, all the eigenmodes are localized.

From Eq. (3.3b) we can see that larger values of the eigenfrequency ω correspond to a larger spread of the random variable $m_i \omega^2$ and consequently to a larger degree of the randomness. Since, in general, larger values of the degree of randomness correspond to a higher degree of localization—although not always in a monotonic way—one expects that the localization length of the eigenmodes would be small for high frequencies and larger for smaller frequencies. This qualitative feature can be checked against the existing numerical results[11,12,17,22] on the average density of states in the following way: As has been stated already, the peaks in the density of states are due to strongly localized states.[17,19] On the other hand, localized states with long localization length or extended states lead to a rather smooth density of states. Thus one expects the fine structure to appear, if at all, at higher frequencies. This is actually the case in the available numerical calculations. One should, however, exclude from consideration those peaks which are the residual of singularities occurring in the periodic case before making the comparison.

IV. SECOND-NEAREST-NEIGHBOR INTERACTION

In this section we consider the electronic case—the phonon case would be identical—when in the Hamiltonian (2.1) V_{ij} is given by

$$\begin{aligned} V_{ij} &= V_1 \quad \text{if } i = j \pm 1 , \\ &= V_2 \quad \text{if } i = j \pm 2 , \\ &= 0 \quad \text{otherwise} . \end{aligned} \tag{4.1}$$

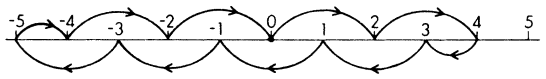

FIG. 4. Typical diagram contributing to the RPE of the self-energy Δ_0 in the presence of second-nearest-neighbor interaction.

The RPE for Δ_0 can be written as

$$\Delta_0 = \sum_{N=1}^{\infty} \Delta_0^{(N)}, \tag{4.2}$$

where the Nth order term $\Delta_0^{(N)}$ is given by

$$\Delta_0^{(N)} = \sum V_{0n_1} G^0_{n_1} V_{n_1 n_2} G^{0n_1}_{n_2} \cdots G^{0,\ldots,n_{N-1}}_{n_N} V_{n_N 0} . \tag{4.3}$$

The sum in (4.3) is over all self-avoiding paths starting from and terminating at zero. Every step links a site i with the nearest neighbors $i \pm 1$ or the second-nearest neighbors $i \pm 2$. A typical path is shown in Fig. 4. The number of terms in (4.3) is proportional to N for large N. In studying the convergence properties of the RPE (4.2) we assume, as in the 3-D case, [24] that the iteration procedure implicit in the RPE (4.2) converges for any nonzero degree of randomness, and consequently the convergence of (4.2) is equivalent to the convergence of the series (4.2). The problem of the convergence of a series of the form in (4.2) and (4.3) has been studied in detail in Ref. 24. The result is[24,25] that a function $L(E)$ exists, such that in the regions of the spectrum, where $L(E) > 1$, the series (4.2) diverges for almost all values of the random variables $\{\epsilon_i\}$ while in the regions where $L(E) < 1$ the series (4.2) converges for almost all values of the random variables $\{\epsilon_i\}$. The function $L(E)$ is given by

$$L^N(E) = \sum V_{0n_1} \tilde{G}^0_{n_1}(E) V_{n_1 n_2} \cdots \tilde{G}^{0,\ldots,n_{N-1}}_{n_N}(E) V_{n_N 0} \quad \text{as } N \to \infty , \tag{4.4}$$

where

$$\ln \tilde{G}^{0,\ldots,n_{i-1}}_{n_i}(E) = \langle \ln \left| G^{0,\ldots,n_{i-1}}_{n_i}(E) \right| \rangle \tag{4.5}$$

and the symbol $\langle\ \rangle$ denotes average over the variables $\{\epsilon_i\}$.

Thus the problem of finding if the eigenstates are localized or extended reduces to determining if $L(E)$ is smaller or larger than unity. In the 3-D case[24] with nearest-neighbor interaction there is a single V which enters in the definition of $L(E)$ and which determines the bandwidth. In the present case, however, $L(E)$ depends mainly on the quantity V_2 whereas the bandwidth depends on both V_1 and V_2. As a result of this, one can no longer show, along the same lines used in the 3-D case, that $L(E) > 1$ within the band as the randomness tends to zero. Consequently, one cannot decide if extended states exist. On the other hand, we were unable to show that $L(E) < 1$ always, so that the possibility of extended states remains open.

We conclude this section with some comments regarding the specific case where the distribution of ϵ_i is Lorentzian. Its importance lies in the fact that, in this case, [24,25]

$$\tilde{G}^{0,\ldots,n_{i-1}}_{n_i}(E) = \left| G^{0,\ldots,n_{i-1}}_{n_i}(E + is(E)\Gamma) \right| , \tag{4.6}$$

where $G^{0,\ldots,n_{i-1}}_{n_i}$ is the n_i, n_i matrix element of the Green's function corresponding to Hamiltonian (2.1) with $\epsilon_j = 0$, $j \neq 0$, $n_1, \ldots, n_{i-1}$ and $\epsilon_j = \infty$, $j = 0, n_1, \ldots, n_{i-1}$; Γ is the half-width of the Lorentzian distribution and $S(E) = 1$ if $\mathrm{Im}E > 0$ and $S(E) = -1$ if $\mathrm{Im}E < 0$.

Using Eq. (4.6) one can show, in a similar way[24] as in the 3-D case, that

$$L(E) < 1 \quad \text{if } F(E) \leq 1, \tag{4.7}$$

where

$$F(E) = E_b / \left| E + i\Gamma \right| . \tag{4.8}$$

The E_b is half the bandwidth for a symmetrical band. Equation (4.7) can be used to provide outer bounds for the region of extended states, if any, but it does not imply the existence or nonexistence of a region of extended states.

V. DISCUSSION

The proof of the localizability of all eigenstates in 1-D disordered systems with nearest-neighbor coupling presented in this paper attributes this peculiar feature, which is absent in higher dimensionality, to the unique property of 1-D lattices, i.e., that there is only one self-avoiding path linking nearest neighbors between two points in the lattice. Indeed, as a consequence of the latter property, the series in the RPE for Δ_0 terminates and the convergence properties of the RPE are determined by the behavior of the resulting continued fraction.

This connection between the unique localization properties and the unique topological behavior of 1-D systems is an extremely desirable feature of the present analysis because it expresses in rigorous mathematical language the vague but reasonable physical idea that all the eigenstates are localized in 1-D because of the existence of a unique path of propagation from one point to another. What we have shown here is that the existence of a unique path connecting two points implies the localization of all the eigenmodes. If one could

show that second-nearest-neighbor interaction allows extended states, then the condition of a unique path connecting two points would be not only sufficient for localization of all the eigenmodes but also necessary.

In this case one could make the following general statement which we present here as a conjecture: The localizability of all eigensolutions is a universal property of only those random systems which are characterized by a unique path along which the disturbance can propagate from one point to another.

This conjecture contains as special cases the 1-D lattice vibration problem with nearest-neighbor coupling, and the 1-D Schrödinger problem (which possesses the property of the uniqueness of the propagation path due to the local nature of Schrödinger equation). On the other hand, in the second-nearest-neighbor-coupling problem described by the Hamiltonian (4.1), extended states should be present according to this conjecture. This particular case can probably be checked numerically by calculating quantities depending on the localization length.[10,26,27]

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APPENDIX

Let

$$K_n(\phi_0, \phi_n) = \int_{-\pi/2}^{\pi/2} K_{n-1}(\phi_0, \phi_{n-1}) K(\phi_{n-1}, \phi_n) d\phi_{n-1} \tag{A1}$$

with

$$K_1(\phi, \phi') = K(\phi, \phi') \ . \tag{A2}$$

The quantity K_n is related to the probability distribution $P_n(\phi_n)$ by

$$P_n(\phi_n) = \int_{-\pi/2}^{\pi/2} K_n(\phi_0, \phi_n) P_0(\phi_0) d\phi_0 \ , \tag{A3}$$

where $P_0(\phi_0) = \delta(\phi_0 - \alpha)$. Thus

$$P_n(\phi_n) = K_n(\alpha, \phi_n). \tag{A4}$$

Let $d_n(\alpha)$ be the total width over which the function $K_n(\alpha, \phi_n)$ is different from zero, i.e.,

$$d_n(\alpha) = \int_{-\pi/2}^{\pi/2} T(K_n(\alpha, \phi_n)) d\phi_n , \tag{A5}$$

where

$$T(K_n(\alpha, \phi_n)) = 1 \quad \text{if } K_n(\alpha, \phi_n) \neq 0$$
$$= 0 \quad \text{if } K_n(\alpha, \phi_n) = 0 \ .$$

By a proper choice of the center of the semicircle on which the angles ϕ_n are measured and using the fact that there are ϵ_i V_i satisfying $|E - \epsilon_i| < 2V_i$, it is always possible to find a constant $\theta_0 \neq 0$ such that the probability distribution $f_n(\theta_n)$ of the quantity

$$\theta_n \equiv \phi_{n+1} - \phi_n \tag{A6}$$

satisfies the relation

$$f_n(\theta_0) \neq 0, \quad n = 1, 2, 3, \ldots \ . \tag{A7}$$

As was explained in the text, θ_0 is related to the choice of the center of the semicircle [see Eq. (2.22)]. Since, in general, $f_n(\theta_n)$ has a nonvanishing width around the value θ_0, it follows that the width d_n of the distribution function K_n is an increasing function of n and that for large enough n, $K_n(\alpha, \phi_n)$ will be different from zero everywhere in $-\frac{1}{2}\pi \leq \phi_n < \frac{1}{2}\pi$.

Frechet[10] has shown that the iterated kernel $K_n(\alpha, \phi_n)$ converges uniformly to a function independent of α as $n \to \infty$ if the following four conditions are satisfied[10]:

$$\text{(i)} \ \int_{-\pi/2}^{\pi/2} K(\alpha, t) dt = 1 \ . \tag{A8}$$

(ii) There is no eigenvalue of K of modulus 1 other than unity.

(iii) There is a unique solution of the system of equations

$$P(\phi) = \int_{-\pi/2}^{\pi/2} K(t, \phi) P(t) dt \ , \tag{A9}$$

$$\int_{-\pi/2}^{\pi/2} P(\phi) d\phi = 1 \ . \tag{A10}$$

(iv) The kernel is bounded.

Condition (iv) is satisfied if the distribution function $P(\epsilon_i, V_i)$ is bounded and approaches zero fast enough as $\epsilon_i \to \infty$ [see discussion after Eq. (2.26)]. Condition (i) is automatically satisfied since $K(\alpha, t)$ is a probability distribution for the quantity t. To show that conditions (ii) and (iii) are satisfied, we use a slight generalization of Borland's method.[10] Consider the associated homogeneous equations

$$\int_{-\pi/2}^{\pi/2} K(t, \phi) P(t) dt = \lambda P(\phi) \ , \tag{A11}$$

$$\int_{-\pi/2}^{\pi/2} K(\phi, t) y(t) dt = \gamma y(\phi) \ . \tag{A12}$$

It is well known that for bounded kernels these equations have the same eigenvalues and the same number of linearly independent solutions corresponding to each eigenvalue. The function $y(t)$

= const is a solution of Eq. (A12) corresponding to the eigenvalue $\gamma = 1$. We shall now show that there are no other solutions corresponding to eigenvalues of modulus unity. Let $y(t)$ be a solution of Eq. (A12) and ϕ_m be such that $|y(\phi_m)|$ is maximum. Then one can easily prove using Eq. (A12) that

$$|\gamma|\,|y(\phi_m)| \leq |y|_{\max'}, \qquad \text{(A13)}$$

where $|y|_{\max'}$ is the maximum value of $|y(\phi)|$ in the region of ϕ where $K(\phi_m, \phi)$ is different from zero. This region has been denoted by $d_1(\phi_m)$ previously [Eqs. (A2) and (A5)]. The equality in (A13) holds only if $y(\phi)$ is constant in $d_1(\phi_m)$. Thus, $|\gamma| < 1$ except if $y(\phi)$ is constant in $d_1(\phi_m)$ and such that $|y(\phi)| = |y(\phi_m)|$, $\phi \in d_1(\phi_m)$. In this last case one can repeat the argument taking as ϕ_m any point in $d_1(\phi_m)$. Then, it follows, using in addition the continuity of $d_1(\phi_m)$ that $|\gamma| < 1$ unless $y(\phi)$ is constant in $d_2(\phi_m)$ and such that $|y(\phi)| = |y(\phi_m)|$, $\phi \in d_2(\phi_m)$. Repeating the argument again and again we conclude that $|\gamma| < 1$, unless $y(\phi)$ is constant in every $d_j(\phi_m)$ ($j = 1, 2, 3, \ldots$). But we have shown that for large enough j, $d_j(\phi_m)$ coincides with the whole region $[-\frac{1}{2}\pi, \frac{1}{2}\pi]$. Thus $|\gamma| < 1$ unless $y(\phi)$ is constant everywhere.

*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.

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Optical Absorption of Sodium*

A. S. Karakashian† and A. Bardasis
Department of Physics and Astronomy, University of Maryland, College Park, Maryland 20742
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The imaginary part of the transverse dielectric tensor has been calculated for sodium using a two-band model and including both phonons and the interactions between conduction electrons in the random-phase approximation. It is found that the resulting expression reduces to the Hopfield dielectric constant for the case of an electron gas in a perturbing crystal potential. Reasonable agreement with N. V. Smith's data has been found in the range of photon energies 0.5–3.0 eV. However, at higher energies the agreement is not as good, since many-body effects become more important in this region.

I. INTRODUCTION

In recent years it has become possible to measure the optical absorption of the alkali metals over a fairly large range of photon energies. Mayer and co-workers[1-3] performed a series of careful ab-