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Localization Lengths of Electronic States in One-Dimensional Disordered Potential Chains*†

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We present a simple approach to the calculation of localization lengths of electronic states in a one-dimensional tight-binding model with nearest-neighbor interactions only. Monte Carlo calculations for a binary alloy with diagonal randomness only show longer-ranged states at energies which are allowed for both constituents and shorter-ranged states in the tails. The length of the longest-ranged states decreases continuously with increasing randomness, without any sharp transition. These results are compared with transmission calculations, and a simple physical interpretation is obtained thereby.

I. INTRODUCTION

It is well known that electronic states, which are infinitely extended in pure crystals, are not always so extended in disordered materials. In two or three dimensions there are ranges of energy in which the states are extended, and other ranges in which the states are localized. The energies at which the transition takes place are called mobility edges.[1-5] The positions of these mobility edges have been estimated to be $E_c \lesssim (E_b^2 - \Gamma^2)^{1/2}$ by Economou and Cohen[5] for an Anderson model with Lorentzian distribution of diagonal energies, where Γ is the half-width of the Lorentzian distribution and E_b is the half-bandwidth of the unperturbed potential $E_b = ZV$. Economou, Kirkpatrick, Cohen, and Eggarter have also done some calculations for binary alloys.[6] Their results show that the mobility edges lie close to the edges of the coherent-potential-approximation (CPA) density of states, especially in the majority subband. They do not give, however, any estimate of the energy dependence of the localization length outside the band. Some estimates of the localization length $L(E)$ have been made by Mott[2] $[L(E) \propto |E_c - E|^{-1/2}]$, by Freed[7] $[L(E) \propto |E_c - E|^{-2/3}]$, and by Lukes[8] $[L(E) \propto |E_c - E|^{-3/5}]$.

Because of its importance in characterizing localized states, we need more information about $L(E)$ than this, so we shall turn to the simplest case, that of a one-dimensional binary alloy, first. The one-dimensional problem has been investigated by several authors. They generally agree that all states in the infinite chain are localized,[9-15] but a completely general and rigorous proof has not been given.[16] It is a simple enough matter to calculate numerically the detailed dependence of the localization length on energy and randomness, although general analytic expressions have not yet been devised. Yet we should not assume that these results are completely irrelevant to the real world. Borland has shown[11] that the localization length and phase coherence length are the same in one dimension, whereas in three dimensions the phase coherence length is the mean free path for the infinitely extended states. Thus, the localization length in one dimension may give information about the phase coherence length in the extended region of the band, and may give information directly about the localization lengths of the states in the band tails of localized states. In addition, most approximations to the solution of the three-dimensional problem can also be calculated in one dimension, so these results provide a test for those approximations. Finally, Bloch, Weisman, and Varma[17] have identified a large number of materials which act like one-dimensional disordered conductors. For these reasons we have calculated the localization lengths for a particularly simple model.

II. MODEL AND NUMERICAL METHOD

Consider the tight-binding Hamiltonian in one dimension:

$$H = \sum_n \epsilon_n \, | n \rangle \langle n | + \sum_n \sum_m V_{mn} \, | m \rangle \langle n | \ , \qquad (1)$$

where the states $|n\rangle$ are (orthonormal) Wannier functions. In our calculations the diagonal elements ϵ_n of the Hamiltonian are random variables. For most of our calculations we chose a binary alloy $\epsilon_n = \delta$ with probability x, and $\epsilon_n = 0$ with probability $1 - x$, where x is the concentration of impurity potentials. The method can be generalized trivially to almost any form of diagonal randomness. We shall only consider nearest-neighbor interactions, i.e., $V_{mn} = 0$ unless $m = n \pm 1$. We have used $V_{n,n+1} = V_{n,n-1} = V = \text{const}$, although generalization to off-diagonal randomness would not be difficult.

The wave functions are also linear combinations of Wannier functions:

$$\psi = \sum_n a_n \, |n\rangle \ . \qquad (2)$$

We are interested in computing the coefficients a_n as functions of the energy E, impurity concentration

x, and impurity diagonal energy δ, in order to obtain a measure of the localization length. We define the "localization length" to be that distance over which the wave function increases, on the average, by a factor of e. That is, we are looking for a quantity L such that a_n fluctuates minimally about

$$b_n = b_0 e^{n/L + i\phi_n} , \tag{3}$$

where ϕ_n is a phase factor which we have not calculated. This definition agrees (apart from factors of the order of 2) with that of Borland,[11] Rubin,[12] Tong,[13] Minami and Hori,[14] Matsuda and Ishii,[16] and Reading and Sigel.[18]

For our simple Hamiltonian, Schrödinger's equation reduces to

$$a_{n+1} = [(E - \epsilon_n)/V] a_n - a_{n-1} . \tag{4}$$

A wave function localized around the site n_0 is one which for $n \ll n_0$ is of the form

$$a_n \approx A \exp\left(\frac{n - n_0}{L} + i\phi(n)\right) . \tag{5}$$

For $n \gg n_0$, it is

$$a_n \approx A \exp\left(\frac{-(n - n_0)}{L} + i\phi(n)\right) . \tag{6}$$

For $n \approx n_0$, it is

$$a_n \approx A e^{i\phi(n)}; \tag{7}$$

i.e., we are allowing the possibility that there is a region around the center of localization in which the wave function does not decay exponentially in either direction. Our method of calculating the localization length does not determine whether such a region exists or how long it is, but is simply concerned with the growth and decay of the tails. The wave function described by Eqs. (5)–(7) is a normalized (by proper choice of A) eigenfunction of the Hamiltonian (1). If we are considering only a finite chain, such a wave function must satisfy particular boundary conditions at the ends; an arbitrary choice of boundary conditions will not lead, as a rule, to a normalized eigenfunction. In addition, the chain of length N (i.e., with N sites) has exactly N eigenfunctions, and at most N distinct eigenvalues of energy. Any arbitrary energy, not an eigenvalue, is not likely to lead to a normalizable solution.

It has, in fact been shown,[11,13,16,18] that a wave function ψ, which satisfies Schrödinger's equation for an arbitrary energy E with arbitrary boundary conditions (i.e., arbitrary phase) at a point z_0, will increase exponentially in either direction from z_0 with probability 1. That this should occur is not particularly surprising, for if

$$\phi(x) = Ce^{\gamma x} + De^{-\gamma x}, \tag{8}$$

there is always an $x_1 > 0$ large enough that $\phi(x > x_1) \sim Ce^{\gamma x}$, unless $C = 0$ exactly, and similarly, there is always an $x_2 < 0$ for which $\phi(x < x_2) \sim De^{-\gamma x} = De^{\gamma |x|}$ unless $D = 0$; i.e., with probability 1, ϕ grows in either direction. Similarly, by analogy, in this case, the wave-function amplitude changes at the impurities, and it would be a rare event indeed if the average effect of the impurities were to cause a decrease in the amplitude (for a more careful statement of this property, see Ref. 13).

A normalizable eigenfunction could be constructed for a chain of length N by starting simultaneously at $n = 0$ and at $n = N$ with exponentially growing solutions and making them match at some point in between. This matching of amplitude and phase can only be done at eigenvalues of the energy, and the details of the procedure are described elsewhere.[11,14,19] The extreme difficulty in finding an eigenfunction is pointed out by Roberts and Makinson,[20] who calculated wave functions for various values of E near eigenvalues for a short chain. All their wave functions are growing exponentially at the right end of the chain, even those which had grown to a peak and decreased earlier in the chain. Roberts and Makinson estimate that the energy would have to be accurate to one part in 10^{10} to give a good approximation to the eigenfunction for 500 sites. Their graphs shown distinctly that the rate of growth of the wave function is the same when approaching the point of localization as it is in the exponential runaway at the right end of the chain. This lends credence to our method of calculating localization lengths, as will be seen below.

Our method of calculation of the localization length is quite straightforward. We chose values for the energy E, the impurity diagonal energy δ, and the impurity concentration x. We programmed a computer to produce a sample chain of randomly placed host and impurity potentials and to compute a wave function of the from (2) by using Schrödinger's equation (4) and two arbitrary constants, here taken to be a_0 and a_1. Then, in order to be certain that ϕ_n [defined in (3) above] satisfied $|e^{i\phi_n}| \approx \pm 1$, we selected only certain sites n_i and coefficients a_{n_i}. We chose various "critical amplitudes" A_i, and selected n_i and a_{n_i} if n_i was the smallest n for which $|a_n| \geq A_i$. By doing this we are assured that we have eliminated the effect of the oscillations of the wave function. Having found m values of n and a_n in this way, we approximated the graph of n_i vs $\ln |a_{n_i}|$ to a straight line, by at least-squares fit (see Fig. 1). The slope of this graph is the average of L, the localization length for that particular sample. We repeated the process many times, and, in so doing, averaged L over different samples. This ensemble average of L is our computed value of the localization length.

This localization length as so defined is remark-

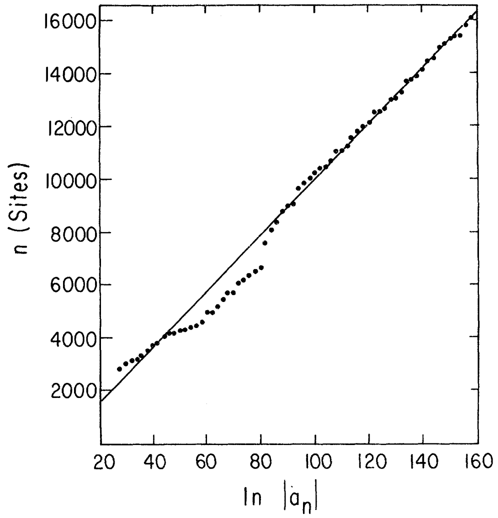

FIG. 1. Distance n vs $\ln|a_n|$, for $\delta = V$, $x = 0.10$, $E = 0.10\ V$. The slope of the line is the localization length, computed by least-squares fit to the data.

ably constant, for a given E, δ, x. We checked this by varying the other parameters we have available, the initial conditions a_0 and a_1, the critical amplitudes A_i, and the chains in the ensemble. As a rule, we chose for our critical amplitudes the even powers of e from 4 to 42 (i.e., 20 points) but in the initial testing we occasionally chose e^{20} for A_1 and e^{160} for A_m without causing any significant change in the localization length. Thus L appears to be well defined. We also varied the initial conditions (e.g., choosing $a_1 = 0$, $a_0 = 1$ instead of vice versa, or choosing $a_1 = a_0 = 1$, etc.) without producing any effect on L. We found that the average over 20 points per chain only justified the use of 15 chains. Averaging over more chains did not improve the statistics.

III. NUMERICAL RESULTS

As we expected, all the states are localized, although the range of localization found was about three orders of magnitude (see Figs. 2–5). For small impurity concentrations ($x \leqslant 0.1$) those states whose energy is in the range $+2V < E < 2V + \delta$ are very short ($L \lesssim 2$ sites). Those states in the host band ($-2V < E < 2V$) are considerably longer. There is no single characteristic length for the longer states, which have a localization length as long as 200 sites for the center of the $x = 0.05$, $\delta = V$ case or as short as 16 sites for $x = 0.1$, $\delta = 3V$. There is a simple empirical relation among all these lengths. If we plot the maximum localization length from each spectrum against the product $[x(1-x)\delta^2]^{-1}$ we get a straight line (Fig. 6). The equation for this is

$$L_{\max}(x, \delta) = 9.36 \text{ sites} \times [x(1-x)(\delta/V)^2]^{-1}. \quad (9)$$

This equation is certainly reasonable since it predicts $L_{\max} \to \infty$ as $x \to 0$, $x \to 1$, or $\delta \to 0$, all of which correspond to a perfect lattice; the sign of the impurity diagonal energy does not affect the value of $L_{\max}$, and x and $1 - x$ appear symmetrically—it does not matter which constituent is labeled "impurity." Thus we see that there is no "phase transition" as there is in two or three dimensions, at least not in the range we have investigated; that

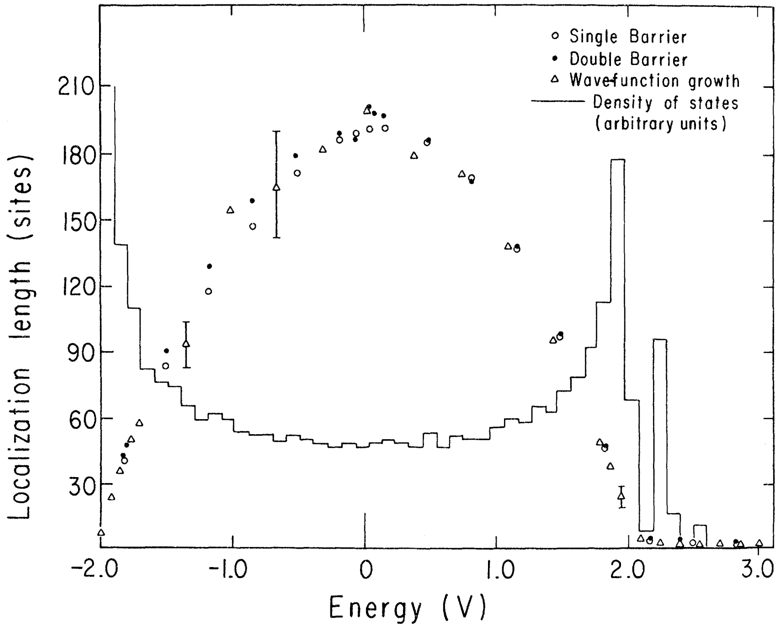

FIG. 2. Localization length and approximate density of states vs energy, for $\delta = V$, $x = 0.05$. The localization length was calculated by three methods, described in Secs. II and IV. The error bars indicate one standard deviation from the mean of 15 samples. Other points with similar localization lengths have similar standard deviations.

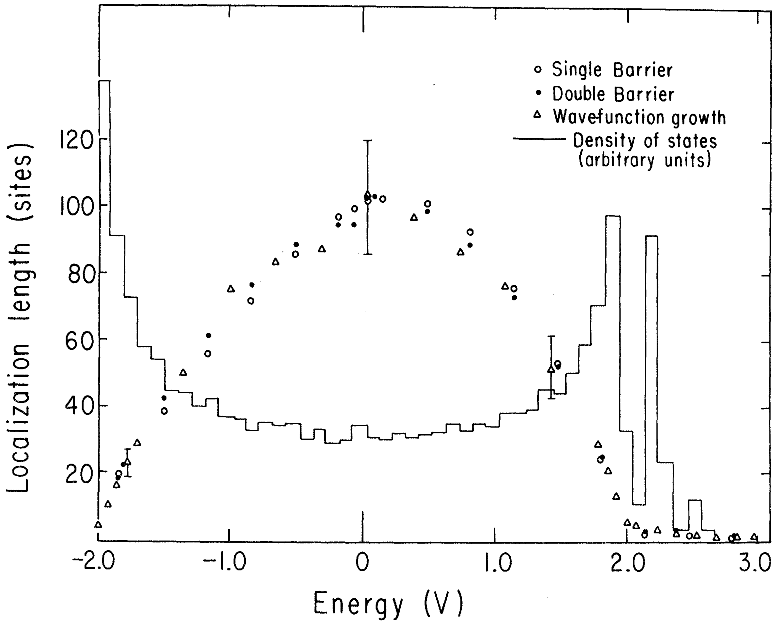

FIG. 3. Localization length and approximate density of states vs energy, for $\delta=V$, $x=0.10$.

is, the maximum localization length goes smoothly from infinity to zero as a function of x and δ. Economou and Cohen[21] predicted a rapid change in the localization length as a function of energy, near the band edges, based on numerical results of Williams and Matthews.[22] This is clearly borne out by these results. Although there can be no true mobility edges in this model (all the states are localized), if we view the inflection points of the graph of L vs E as a transition between the shorter and longer states, i.e., as a pseudomobility edge, we observe that these points move closer together as the randomness is increased. (Note especially the $x=0.5$, $\delta=V$ case, Fig. 4.)

There is also an interesting anomaly near $E=0$ on Figs. 2 and 3. $L(E)$ appears to jump by a finite amount in crossing this energy. A likely reason for this will be proposed in Sec. IV.[23] Economou and Papatriantafillou[24] have also calculated localization lengths by a completely independent method. At all points where we both have data, the results are in very good agreement.

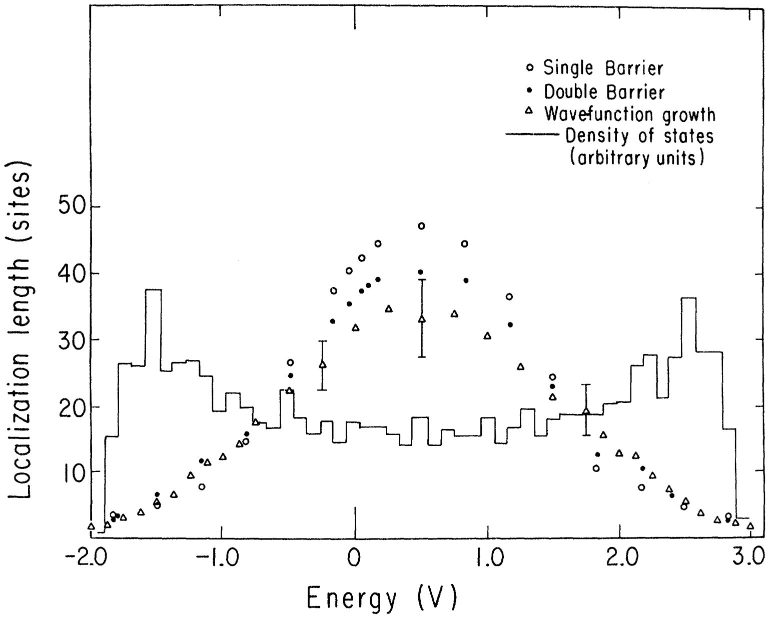

FIG. 4. Localization length and approximate density of states vs energy, for $\delta=V$, $x=0.50$.

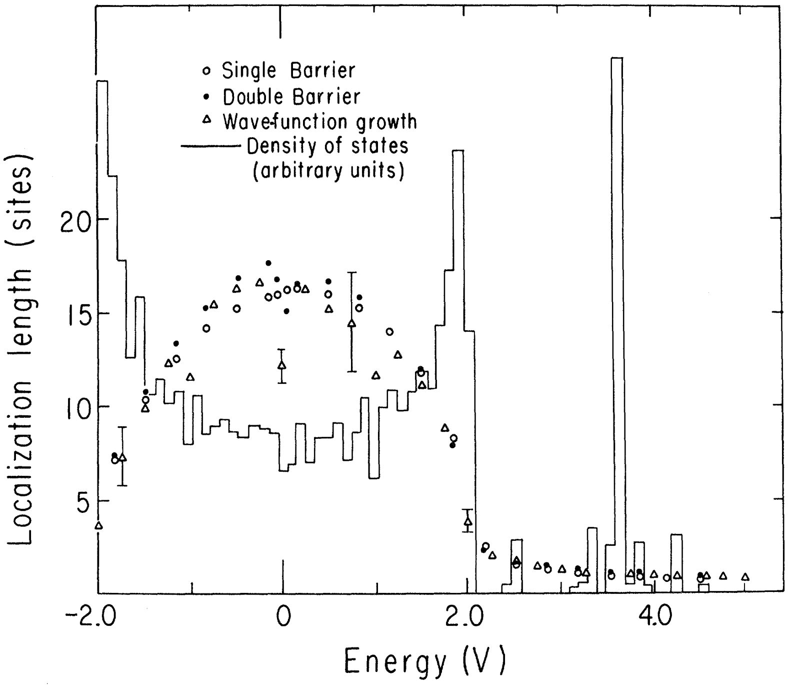

FIG. 5. Localization length and approximate density of states vs energy, for $\delta = 3V$, $x = 0.10$.

IV. TRANSMISSION AND REFLECTION COEFFICIENTS

As a check on our method and to interpret our results physically, we considered this problem to be a barrier-transmission problem, similar to those treated in any elementary text on quantum mechanics. We shall only discuss binary alloys in this section for reasons of algebraic complexity, which will shortly become obvious. Consider first a single boundary between host atoms (H) and impurity atoms (I):

(a) $\cdots HHHIII \cdots$, (b) $\cdots IIIHH \cdots$.

We can consider our chain of potentials as a series of boundaries, with forms (a) and (b) occurring alternately. As a zero-order approximation to the transmission coefficient of the chain, we could compute the transmission coefficient of each boundary and multiply them together. This is, of course, only a poor approximation, because it ignores all multiple reflections and interference effects, but is justified in view of the randomness. If we make this approximation, then we write

$$|\psi_N| = (T_a)^{n(N)/2}(T_b)^{n(N)/2}|\psi_0| \ , \qquad (10)$$

where ψ_N is the wave function at site N corresponding to a "plane wave" incident on site 0 with amplitude $|\psi_0|$, T_a and T_b are the transmission coefficients of type (a) and (b) boundaries, respectively, and $n(N)$ is the number of type (a) or type (b) boundaries occurring in N sites. The $\frac{1}{2}$ in the exponent occurs because the transmission coefficient relates probabilities, rather than wave-function amplitudes. In a completely random binary alloy, in which each site is independent of all others, the number of boundaries is given by

$$n(N) = x(1-x)N \ , \qquad (11)$$

since the number of boundaries in a length N is the product of the number of sites (N) and the probability of a boundary occurring at a site. This probability for a type (a) boundary is the probability

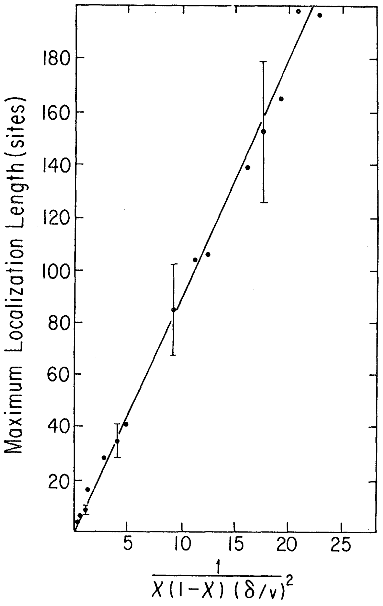

FIG. 6. Maximum localization length vs $[x(1-x)(\delta/V)^2]^{-1}$.

of a H atom at site $j-1$ multiplied by the probability of an I atom at site j, i.e., $x(1-x)$. As we want to compare this to a localization length, we rewrite it in the form of an exponential:

$$|\psi_N| = |\psi_0| \exp[\tfrac{1}{2}x(1-x)N(\ln T_a + \ln T_b)]. \tag{12}$$

If the reflection coefficient, $R \equiv 1-T$, is small, we may expand the logarithm to first order in R:

$$\ln T_a = \ln(1-R_a) \approx -R_a \, . \tag{13}$$

The reflection coefficients R_a and R_b are both given by

$$R_a = R_b = R = \frac{1-\cos(k-q)}{1-\cos(k+q)} \, , \tag{14}$$

where

$$\cos k = E/2V, \quad \cos q = (E-\delta)/2V \, ; \tag{15}$$

$k(q)$ is the Bloch wave vector of a wave of energy E traveling to the right in a pure $H(I)$ lattice. In the limit in which k and q are both small, we may expand the $\sin q \sin k$ to first nonvanishing order, giving

$$R = \delta^2[16V^2 - (2E-\delta)^2]^{-1} \, . \tag{16}$$

R clearly has a minimum value of $\delta^2/16V^2$ at $E=\frac{1}{2}\delta$. This corresponds to a maximum localization length [we have combined Eqs. (12), (13), and (16), and noticed that $1/L$ is the coefficient of $-N$ in the exponent] of

$$L = 16 \text{ sites} \times [x(1-x)(\delta/V)^2]^{-1} \, , \tag{17}$$

which compares reasonably well, considering the crudeness of this approximation, with our previous result (9).

To improve the approximation, and consider some double reflections, let us consider configurations of the form

$$\text{(c)} \quad \cdots H\underbrace{I\cdots H}_{n}I\cdots \, .$$

This is a barrier-penetration problem, and the methods for treating it are similar to those just described. This method, however, does not require that the states be wavelike in the impurity region, but only in the host region. We may therefore expect reasonable results for all energies in the host band, $-2V < E < 2V$. Also by considering barriers of the form

$$\text{(d)} \quad \cdots I\underbrace{H\cdots H}_{n}I\cdots$$

we may obtain results for $2V < E < 2V+\delta$. As before,

$$|\psi(N)| = (T_{(j)} \cdots T_{(1)})^{1/2} |\psi(0)| \, , \tag{18}$$

where $T_{(i)}$ is the transmission coefficient of the ith barrier. Since the $T_{(i)}$ are numbers, we may commute them, and order them from the shortest to the longest:

$$|\psi(N)| = (T_1^{p_1(N)} T_2^{p_2(N)})^{1/2} |\psi(0)| \, , \tag{19}$$

where T_n is the transmission coefficient for a barrier of the type (c) or (d) and $p_n(N)$ is the number of such barriers in N consecutive sites. Again, $p_n(N)$ is the probability of the next $n+2$ sites forming such a barrier after a particular site, multiplied by the number of such sites available. The number of barriers of type (c) is then

$$p_n(N) = (1-x)^2 x^n N \, . \tag{20}$$

We then write (19) in the form of an exponential:

$$|\psi(N) = |\psi(0)| \exp[\tfrac{1}{2}N(1-x)^2 \textstyle\sum_n x^n \ln T_n]. \tag{20$'$}$$

From this we identify

$$1/L = -\tfrac{1}{2}(1-x)^2 \textstyle\sum_n x^n \ln T_n \tag{21}$$

(recall that $T_n < 1$, so L is positive).

The calculation of the $T_n(E, \delta)$ is straightforward, and the result is

$$T_n = \frac{\sin^2 q \sin^2 k}{\sin^2 q \sin^2 k + (\delta^2/4V^2)\sin^2 qn} \tag{22}$$

for $-2V + \delta < E < 2V$, where q and k are defined by (15). Similar expressions can be calculated for $-2V < E < -2V + \delta$, $2V < E < 2V + \delta$. When these transmission coefficients are computed and inserted into (21), the localization lengths computed agree very well with those of the previous method for low concentrations (Figs. 2–5), but the agreement is not as good for high impurity concentrations (Fig. 4). For these concentrations, multiple reflections between barriers, which are of course closer together, become more important, and simply do not average to zero.

We then considered the possibility of reflections between consecutive barriers, by treating configurations of the form

$$\text{(e)} \quad \cdots H\underbrace{I\cdots I}_{l}\underbrace{H\cdots H}_{m}\underbrace{I\cdots I}_{n}H\cdots \quad ,$$

for which equation (19) reduces to

$$1/L = -\tfrac{1}{4}(1-x)^2 \textstyle\sum_l \sum_m \sum_n x^{l+n}(1-x)^m \ln T_{lmn} \, , \tag{23}$$

where T_{lmn} is the transmission coefficient of the configuration (e). The algebra of calculating T_{lmn} is much more tedious, but no more difficult, than that which led to Eq. (22). This procedure leads to values of L which are also shown in Figs. 2–5. We see a significant improvement in the case of 50% concentration, and little change in the others.

Higher-order approximations can be made in similar fashion, and the results should be more accurate. Rubin[12] has done some calculations for the phonon problem and reports similar results—

in the limit of low concentrations the effect of n barriers is just n times the effect of one.

The jump at $E=0$ in Figs. 2 and 3 can be explained in terms of these double-barrier-transmission coefficients. The effect is not observed at all in the results of the single-barrier calculation, but is quite pronounced in the results of the double-barrier program. We discover that configurations of the form

$$\text{(f)}\quad \cdots HI\underbrace{HH\cdots HH}_{\text{even number}}IIH\cdots$$

are perfectly transmitting for $E=0$, $\delta = V$. Thus they do not contribute to the localization length. The other configurations transmit more on the positive side than on the negative side, giving the asymmetric form to this energy region.[23]

V. CONCLUSIONS

A quantity called localization length is well defined for electron states in one-dimensional random systems, and the various methods of calculating these lengths agree. There are many areas for further work in this field. Off-diagonal randomness may be introduced, the existence of a region near the center of localization where the wave function is neither decaying nor growing should be investigated, and the question of localization of the second-neighbor interaction Hamiltonian[15] should be investigated.

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