Transmission resonances and the localization length in one-dimensional disordered systems

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Numerically obtained results concerning the transmittance and localization length of a one-dimensional disordered system are presented. We show that as a function of the energy of the incoming particle the transmittance is characterized by randomly positioned exponentially narrow resonances. Depending upon the relationship between the length of the system and the localization length, the transmittance may appear to be either a perfectly smooth function of energy (the resonances being invisible on any practical energy scale) or a highly structured function varying in a random way.

It has long been known[1] that the solutions to the Schrödinger equation for a one-dimensional random system exhibit exponential growth in the sense that with probability unity a solution finite at the beginning of a semi-infinite system will diverge exponentially with increasing distance along the chain. A well-known consequence of this property is that the transmittance $T_L(k)$ of a one-dimensional disordered system of length L decreases exponentially with the length of the system in the sense that an appropriate average of $\ln T_L(k) \to -2L/L_0$ as $L \to \infty$. In this expression L_0 is the localization length and is a function of the energy k^2 of the states as well as the nature of the disorder. A second consequence is that the eigenfunctions in the disordered system are localized in the sense that they decay exponentially on both sides of their maximum. Our purpose in this paper is to present some numerically obtained results concerning the specific nature of the function $T_L(k)$ and some characteristics of the eigenfunctions, and to discuss the way in which the same localization length affects both aspects of the quantum mechanics of the disordered system.

We make the following points:

(1) The transmittance $T_L(k)$ is an exceedingly complex function of k whose detailed nature depends critically upon the interplay of the length L of the system and the localization length L_0.

(2) For a specified random system $T_L(k)$, and indeed, its logarithm $\ln T_L(k)$, exhibits extreme maxima (corresponding to transmission resonances) at energies with an average separation in k (the square root of the energy) of the order of π/L. The energies at which the resonances occur are themselves random in that they are specific to each particular random sequence of scatterers. These transmission resonances correspond, in a sense to be discussed below, to the eigenfunction of the random system.

(3) The width of the resonances, as a function of the variable k, becomes exponentially small as the length of the system increases; the width is of order $\exp(-aL/L_0)$, where a is a number of order unity. Within the resonance region the transmittance increases dramatically, in the sense that the change in its logarithm obeys $\Delta \ln T_L(k) \approx \ln T_L(k)$. Thus $T_L(k)$, which for a system long compared to the localization length is of order $\exp(-2L/L_0)$, at the resonance positions becomes exponentially larger than its typical value and in particular instances can be of order unity.

(4) According to Landauer,[2] the conductance of a one-dimensional system, in units of $e^2/\pi\hbar$, is equal to $T_L(k)/[1-T_L(k)]$ or effectively to $T_L(k)$ since the transmittance is exponentially small. Azbel[3] has generalized Landauer's result and finds that at finite temperatures the conductance is related to the thermal average

$$\bar{T}_L = -\int T_L(k) \frac{\partial n_F(k)}{\partial k} dk \ ,$$

where $n_F(k)$ is the Fermi distribution function. At any practical temperature, therefore, one should regard the effective localization length as referring to a thermal average over an interval large compared to the spacing between transmission resonances. Even though the width of the resonances is "exponentially small" the transmittance at the resonance position is

"exponentially large" compared to the background, and the resonances contribute an amount comparable to the background to an average of $T_L(k)$ over an interval large compared to the spacing between them. It is probable, therefore, that the effective localization length is significantly different from that characterizing an arbitrarily chosen energy.

The specific numerical calculations were done for a lattice of δ-function potentials (with unit lattice spacing)

$$V(x)=\sum V_n\delta(x-x_n)\,, \tag{1}$$

where the coefficients V_n may have either of two values $V^{(1)}$ and $V^{(2)}$. For $x_{n-1}<x<x_n$ the wave function may be written

$$\psi(x)=A\exp\left[\frac{G_n}{2}\right]\cos\left[k(x-x_{n-1})-\frac{\varphi_n}{2}\right]\,, \tag{2}$$

where A is arbitrary and the overall amplitude and phase may be obtained in terms of their values at one end of the system by straightforward application of the transfer matrices appropriate to the δ-function potentials. However, in a disordered system in which the amplitude of the solutions grow exponentially it is convenient to work with the exponent G_n directly. We show in the Appendix that

$$G_{L+1}=\sum_{n=1}^{L}\ln\left[\frac{1+X_n^2}{\omega_{n-1}+\omega_{n-1}^{-1}X_n^2}\right]\,, \tag{3}$$

where $G_1=0$ and $X_n=\tan\{\frac{1}{2}[\varphi_n+(\pi/2)+h_{n-1}]\}$, $\omega_n=\tan^2[(h_n/2)+(\pi/4)]$, and $\tan(h_n)=V_n/2k$. The quantities X_n satisfy the recursion relation

$$X_n=\omega_{n-1}\frac{X_{n-1}-r_{n-1}}{1+X_{n-1}r_{n-1}}\,, \tag{4}$$

where $r_n=\tan[k-(h_n+h_{n-1})/2]$ with $h_0=0$. Two independent solutions are obtained by choosing $\varphi_1=0$ and $\varphi_1=\pi$. We show in the Appendix that these may be combined to form an eigenfunction having only an outgoing wave at one end of the chain, from which we derive the expression for the transmittance

$$T=4/[\exp(G)+\exp(G')+2]\,, \tag{5}$$

where the G and G' are the values of G_{L+1} for the two particular solutions just mentioned.

The results presented in this paper were obtained using the preceding expressions. We frequently refer to the localization length of a particular system, which we calculate by evaluating $-\ln T_L(k)/2L$ for a single system (or at most, a few systems) of the same nominal concentration of scatterers as the one of interest but very long compared to L_0 itself. The point is that according to (3), the G and G' entering into Eq. (5) are the sums of independent quantities, provided that the length L exceeds all characteristic lengths of the system. Thus it is to be expected, and indeed we find, that for large L the random variables G and G' have the same mean and are normally distributed about their average value. Therefore, for all practical purposes, we may calculate the localization length using $L_0=2L/G$. Alternatively, we may use the prescription of Azbel and Soven[4] to determine L_0 through an analytical procedure.

In Fig. 1 we show $\ln T_L(k)$ for a system containing 100 sites with equal concentrations of zero and unit strength δ-function potentials. The system was chosen to reflect a regime in which $L\gg L_0$. Numerical and analytical calculations show that L_0 is approximately four lattice constants for this system. The curve should be viewed as composed of a smooth background interrupted by maxima at the approximate spacing mentioned previously. For a few of the maxima we show a blowup of the graph on a much expanded wave-vector scale. Note that both the main plot of $\ln T_L(k)$ and the insets refer to the same vertical scale. Our numerical results for many chains show that the width of the fine structure may vary widely from resonance to resonance but is always of the order of $\exp(-aL/L_0)$ (where a is of order unity) for whatever system we studied. In the immediate vicinity of the transmission maxima (except for a very small rounding region reflecting the finite length of the sample) the function $\ln T_L(k)$ varies as $|k-k_m|^{1/2}$, where k_m is the resonance position. For a chain twice as long as the one used to generate Fig. 1 the analogous plot is simply a smooth curve with no apparent structure; only after very detailed probing on a wave-vector scale of order 10^{-14} do we discover a pattern of exceedingly sharp transmission maxima.

The intervals between transmission resonances decrease only as $1/L$ whereas the width of the resonances decreases exponentially. In the limit $L\gg L_0$ the function $\ln T_L(k)$ has the "appearance" of a smooth function, since the probability is overwhelmingly great that a randomly chosen energy will not lie close to a resonance. It is in this regime that for all practical purposes $\ln T_L(k)$ is characterized by the single parameter L_0.

Figures 2(a)–2(d) illustrate $\ln T_L(k)$ for a chain 2000 lattice sites long for which the localization length is approximately 200 lattice sites. Figure 2(a) is plotted on a wave-vector scale chosen to illustrate the extreme fluctuations exhibited by $\ln T_L(k)$ in a regime in which $\pi/L\approx\exp(-L/L_0)$. The dotted curve is the function $-2L/L_0(k)$, where $L_0(k)$ was

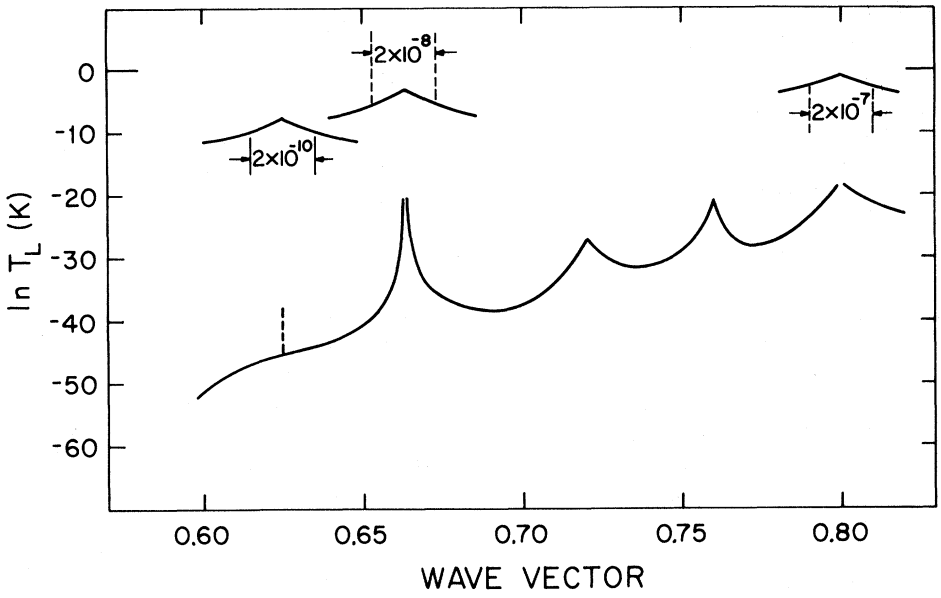

FIG. 1. Logarithm of the transmittance for a system 100 lattice sites in length. The insets show the transmittance on a much expanded wave-vector scale, as indicted, to illustrate the details of the transmission maxima.

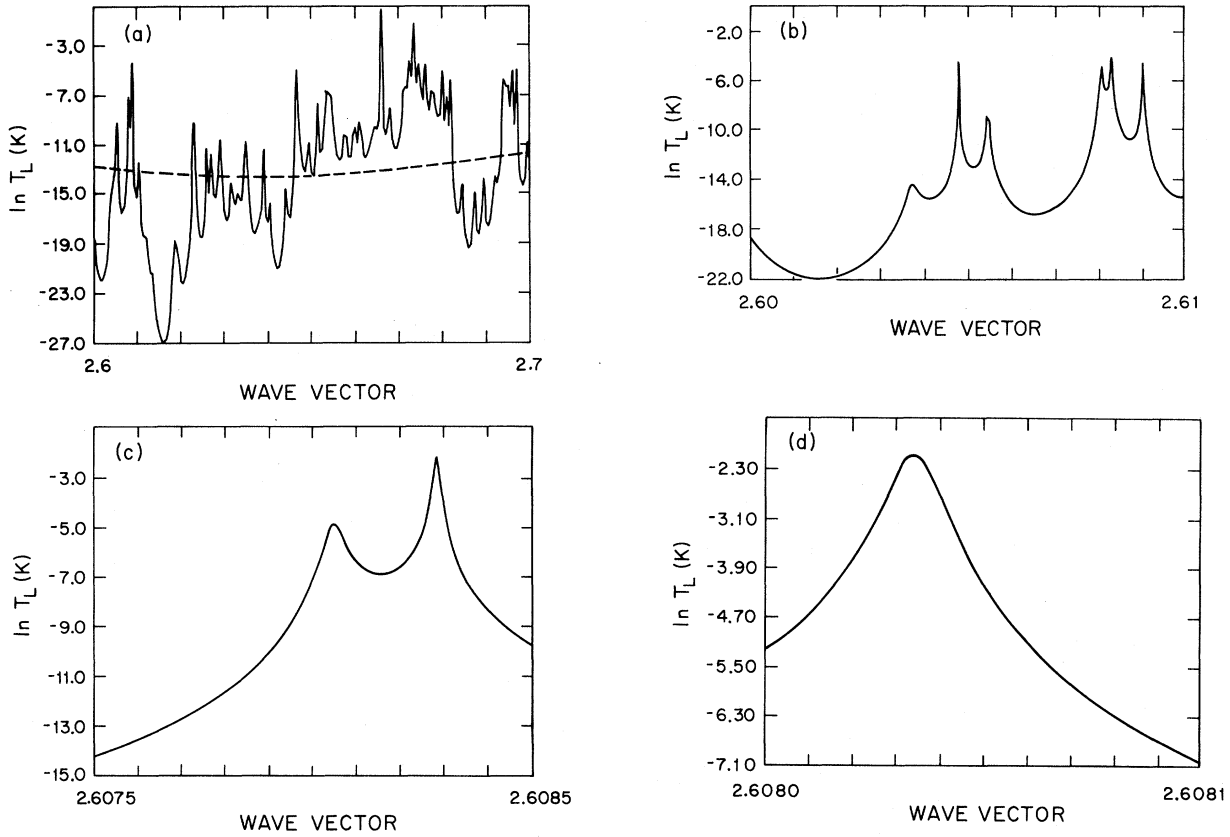

FIG. 2. (a) Logarithm of the transmittance for a system whose length is approximately ten times the localization length. (b) Same as (a) but for a wave-vector scale ten times smaller. (c) Same as (b) but for a wave-vector scale ten times smaller. (d) Same as (c) but for a wave-vector scale ten times smaller.

calculated using the procedure of Azbel and Soven[4] and verified by explicit calculations of the transmittance for much longer chains but the same nominal concentrations of potentials. Our point that in a short sample $\ln T_L(k)$ simply oscillates about its nominal value is well illustrated by this plot. Figures 2(b)—(2d) show $\ln T_L(k)$ for the same system on successively smaller energy intervals. In accordance with our earlier comment, the structure persists down to a scale of order $\exp(-aL/L_0)$.

The transmission resonances correspond to the eigenfunctions of the disordered system in the sense that, as is true for any resonance phenomena, the phase φ_{L+1} at the end of the chain of the two independent solutions referred to above (and therefore of any solution) varies by nearly π over the resonance region. Therefore it is possible to satisfy arbitrary boundary conditions at the ends of the chain for an energy within the resonance region. While there is no doubt that the eigenfunctions resulting from imposition of boundary conditions at the ends of the system are exponentially localized, it is of interest to study them in more detail in order to determine their decay length and the spatial distribution of the maxima within the chain.

We investigated the special case corresponding to standing wave boundary conditions at the ends of system. In summary, we found, as might be expected, that the maxima of the eigenfunctions are randomly positioned along the chain and decay away from their maxima with an exponential falloff corresponding to the localization length L_0. In Fig. 3

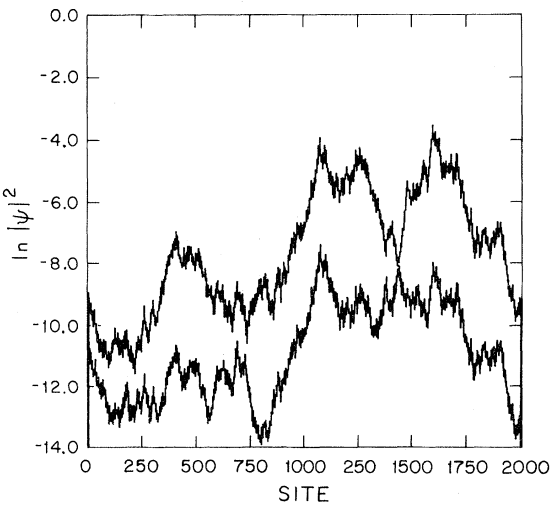

FIG. 3. Two successive eigenfunctions satisfying standing wave-boundary conditions at the end of a system 2000 lattice sites in length for which the localization length is approximately 200 lattice sites. Note that what is plotted is the logarithm of the square magnitude and not the eigenfunctions themselves.

we show the logarithm of the square amplitude [i.e., the quantities G_n of Eq. (2)] of typical normalized eigenfunctions. The eigenfunctions illustrated are adjacent in regard to the energy eigenvalue, but are otherwise arbitrarily chosen. The positions of the absolute and relative maxima are, of course, specific to the particular eigenfunctions and random system, but the general nature is typical of our results. Note that the absolute maxima of the eigenfunctions occurs at some random position along the chain. It is interesting that even the magnitude of the eigenfunctions are exceeding complex of position; the actual eigenfunctions, including the phases, oscillate with periods of the order of a few lattice constants.

In summary, we have shown that the transmittance of a one-dimensional disordered system is characterized by randomly positioned and exponentially narrow resonances. In addition, we have illustrated how the localization length L_0 is the characteristic length of a random one-dimensional system, in the sense that it determines the transmittance (and hence, conductance) of the system, the width in energy of the transmission resonances, and the scale of exponential falloff of the eigenfunctions satisfying arbitrary boundary conditions at the ends of the system.

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APPENDIX

The numerical calculations presented here refer to a one-dimensional system of δ-function potentials. Although this model has been studied for half a century, the specific algebraic expressions we use to describe it are somewhat unusual; accordingly, we present a brief derivation at this point.

We study a system of L δ-function potentials with a uniform lattice spacing of unity; the nth potential is located at x_n and has a strength V_n. In this paper we only consider a system in which V_n can have either of two values, although the expressions we derive are more general. In the region $x_{n-1} < x < x_n$ an arbitrary solution to the Schrödinger equation for energy k^2 may be expressed in the form

$$\psi = A_n e^{ik(x-x_{n-1})} + B_n e^{-ik(x-x_{n-1})} . \tag{A1}$$

Imposing the continuity in value and discontinuity in slope[5] appropriate to a δ-function potential of strength V_n we find the relations

$$A_{n+1} = [1 - i\tan(h_n)]e^{ik}A_n - i\tan(h_n)e^{-ik}B_n ,$$
$$B_{n+1} = i\tan(h_n)e^{ik}A_n + [1 + i\tan(h_n)]e^{-ik}B_n , \tag{A2}$$

where $\tan(h_n)=V_n/2k$.

It is convenient to use real solutions to the Schrödinger equation. Defining G_n and φ_n through the relations

$$A_n=\exp[(G_n-i\varphi_n)/2]\,,$$
$$B_n=\exp[(G_n+i\varphi_n)/2]\,, \tag{A3}$$

and substituting into (A2) we obtain

$$\sin\left[\frac{\varphi_{n+1}-\varphi_n}{2}+k-h_n\right] =\sin(h_n)\cos\left[\frac{\varphi_{n+1}+\varphi_n}{2}-k\right] \tag{A4}$$

and

$$\exp\left[\frac{G_{n+1}-G_n}{2}\right] =\sec(h_n)\cos\left[\frac{\varphi_{n+1}-\varphi_n}{2}+k-h_n\right] +\tan(h_n)\sin\left[\frac{\varphi_{n+1}+\varphi_n}{2}-k\right].$$

Defining the auxiliary quantity

$$a_n=\frac{1}{2}\left[\varphi_n+\frac{\pi}{2}-h_{n-1}\right],$$

we derive, after considerable manipulation

$$\tan(a_{n+1})=\omega_n\tan(a_n-\tan^{-1}r_n) \tag{A5}$$

and

$$\exp(G_{n+1}-G_n)=\frac{1+\tan^2 a_{n+1}}{\omega_n+\omega_n^{-1}\tan^2(a_{n+1})}\,,$$

where

$$\omega_n=\tan^2\left[\frac{h_n}{2}+\frac{\pi}{4}\right].$$

Expansion of the tangent in the first of these and taking logarithms in the second leads directly to Eqs. (4) and (3).

The transmittance is found by direct application of the preceding expressions. Choose a solution which, for $x_0<x<x_1$, has the form

$$\psi=e^{ikx}+re^{-kx} =(1+r)\cos(kx)+i(1-r)\sin(kx)\,. \tag{A6}$$

The cosine and sine functions have the form (2) with $\varphi_1=0$ and π, respectively. Letting G and φ denote G_{L+1} and φ_{L+1} for the case $\varphi_1=0$, and G' and φ' the same quantities for the case $\varphi_1=\pi$, the wave function for $x>x_l$ takes the form

$$\psi=\tfrac{1}{2}e^{ik(x-x_L)}[(1+r)e^{(G-i\varphi)/2}+i(1-r)e^{(G'-i\varphi')/2}]+\tfrac{1}{2}e^{-ik(x-x_L)}[(1+r)e^{(G+i\varphi)/2}+i(1-r)e^{(G'+i\varphi')/2}]\,. \tag{A7}$$

Imposing the condition that there be no leftward moving wave for $x>x_L$ leads immediately to

$$r=\frac{e^{(i\varphi'-G)/2}-ie^{(i\varphi-G')/2}}{e^{(i\varphi'-G)/2}+ie^{(i\varphi-G')/2}}\,. \tag{A8}$$

The transmission coefficient t is the amplitude of the rightward moving wave in (A7). Substituting (A8) into the original formula leads to

$$t=\frac{2i\sin[(\varphi'-\varphi)/2]}{e^{(i\varphi'-G)/2}+ie^{(i\varphi-G')/2}}\,. \tag{A9}$$

The unitarity condition that $|r|^2+|t|^2=1$ provides the constraint

$$\sin\left[\frac{\varphi'-\varphi}{2}\right]=e^{-(G+G')/2} \tag{A10}$$

which leads immediately to

$$T=|t|^2=\frac{4}{e^G+e^{G'}+2}$$

as was given in the text.

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[1]See, e.g., D. J. Thouless, Phys. Rep. 13, 93 (1974).
[2]R. Landauer, Philos. Mag. 21, 863 (1970).
[3]M. Ya. Azbel, Phys. Lett. 78A, 410 (1980).
[4]M. Ya. Azbel and Paul Soven, Phys. Rev. Lett. 49, 751 (1982).
[5]See, e.g., Eugen Merzbacher, *Quantum Mechanics* (Wiley, New York, 1961).