New method for calculation of quantum-mechanical transmittance applied to disordered wires

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We introduce a stable, accurate method for calculating the quantum-mechanical transmittance of random media. A Hamiltonian is constructed for a system consisting of a sample with a few simple, semi-infinite leads. This Hamiltonian is transformed into a block-tridiagonal matrix. Three-term matrix recurrences are then used to find the scattering matrix for electron waves impinging on the sample from the leads. In calculations for narrow wires described by the Anderson model we observe nearly transparent resonances in the transmittance as a function of energy in nearly all cases examined; the mean of the logarithm of the transmittance scales linearly with system length even for very short length scales, where resonances dominate the distribution. We also find agreement with previous results, including the statistics of the transmittances of an ensemble of wires and analytically predicted localization lengths. These methods are easily applicable to two- and three-dimensional systems, as well as four-lead devices.

I. INTRODUCTION

The purpose of this paper is to introduce a stable, accurate technique[1] for calculating the transmission properties of waves propagating in an arbitrary medium, such as electrons in a disordered solid or electromagnetic waves in a disordered dielectric. The usefulness of this method is then demonstrated by application to the statistics of electron transport in small, narrow wires.

Despite many years of study this problem remains interesting, primarily as a means of investigating Anderson localization in disordered systems.[2] Even the simplest, best understood case of disorder, that of a one-dimensional (1D) system, has received renewed interest since improvements in etching techniques have made fabrication of very narrow wires,[3] and hence measurements of their electrical conductance, possible. Related experiments have also been performed by sending microwaves down a waveguide filled with randomly positioned dielectric slabs.[4]

The theory of wave propagation in disordered systems is far from complete. Analytic work is so difficult that most descriptions of the properties of a particular disordered medium rely on averages over a statistical ensemble of systems,[5] obscuring exceptional behavior that can dominate the characteristics of typical samples. Only the most general results are universally agreed upon; for example, all states in one dimension have probability 1 of being exponentially localized no matter how weak the disorder.[6] Although it is generally accepted that some similar statement is true in 2D systems, the type of localization for states near the center of the band in weak disorder remains controversial.[7-10]

Because of the difficulty in obtaining analytic results, much of the work in this area has relied on numerical calculations.[11-20] However, many techniques used to date have numerical instabilities, particularly from divergent recursions or matrix inversions. Most of those of that are highly stable are not applicable to samples of dimension higher than 1. Our technique is highly stable and easily generalized to two or three dimensions.

After introducing our technique and describing its relation to previous work, we apply it to the case of the statistics of wave propagation in one-dimensional disordered chains. We find the following results: As expected, such chains, even those much longer than the average localization length, typically display certain energies which are nearly transparent to wave propagation. It is shown that these resonances are not consistent with fluctuations of the well-known log-normal distribution of the transmittance. The resonant states carry little probabilistic weight in the weakly transmittive regime, but dominate the statistics for strongly transmittive chains. In this latter regime the distribution of the transmittance is significantly skewed from log-normality, yet the mean of the distribution still scales linearly with chain length. In addition, we find agreement with other previously reported results, with the exception that we do not observe size-dependent localization lengths in the strongly transmittive regime.

II. THE CALCULATION

We demonstrate our technique by calculating the transmittance of a narrow wire described by an Anderson model,[2] a tight-binding Hamiltonian with a basis set of orbitals which are localized around a set of $2N$ atoms. $\{\phi_n\}$, $1 \le n \le 2N$ is the set of annihilation operators for these basis orbitals. Each atom has a site energy ε_n. If only nearest neighbors interact, the Hamiltonian is

$$H_{\text{sample}} = \sum_{n=1}^{2N} \varepsilon_n \phi_n^\dagger \phi_n + \sum_{n=1}^{2N-1} v\left[(\phi_{n+1}^\dagger \phi_n + \phi_n^\dagger \phi_{n+1})\right] . \tag{1}$$

The ε_n are randomly distributed between $-w/2$ and $w/2$ so that w/v is a parameter which describes the strength of the disorder. This model is thought to display all the

important features of 1D localization [with the possible exception of isolated extended states [see Sec. IV)].

We then attach the ends (sites $n=1$, $n=2N$) to semi-infinite leads with periodic potentials and single bands of states. The Hamiltonians of the leads are

$$H_{\text{lead 1}}=\sum_{n=0}^{-\infty} v(\phi_{n+1}^{\dagger}\phi_n+\phi_n^{\dagger}\phi_{n+1})$$

and

$$H_{\text{lead 2}}=\sum_{n=2N}^{\infty} v(\phi_{n+1}^{\dagger}\phi_n+\phi_n^{\dagger}\phi_{n+1})\ . \tag{2}$$

These, the simplest possible leads in this model, will be referred to as elemental leads. Their basis orbitals are again described by annihilation operators $\{\phi_n\}$, but with $-\infty<n\leq 0$ for lead 1 and $2N<n<\infty$ for lead 2, so that the $\{\phi_n\}$ with $-\infty<n<\infty$ describe the basis of the whole system of sample and leads. The Hamiltonian H for this infinite system can be expressed in matrix form in the ϕ_n basis as

$$H=\begin{pmatrix}
\ddots & & & & & & & & & & & & \\
 & 0 & v & & & & & & & & & & \\
 & v & 0 & v & & & & & & & & & \\
 & & v & \varepsilon_1 & v & & & & & & & & \\
 & & & v & \varepsilon_2 & v & & & & & & & \\
 & & & & v & & \ddots & & & & & & \\
 & & & & & & & v & & & & & \\
 & & & & & & v & \varepsilon_{2n} & v & & & & \\
 & & & & & & & v & 0 & v & & & \\
 & & & & & & & & v & 0 & & & \\
 & & & & & & & & & & \ddots & &
\end{pmatrix}, \tag{3}$$

where all elements of H are zero except for the diagonal elements $\{\varepsilon_n\}$ and the nearest-neighbor hopping integral v, which is a constant.

We now wish to find solutions of the time-independent Schrödinger equation,

$$H\psi=E\psi\ , \tag{4}$$

and from them the scattering matrix for the disordered region. This is depicted in Fig. 1. The solutions to (4) in the leads are Bloch waves of the form $\sum_n e^{\pm in\theta}\phi_n^{\dagger}$, where $\cos\theta=E/2v$. This can be easily seen by substituting (2) into (4) and trying $e^{in\theta}$ as a solution. Now in lead 1 there will be an incoming wave of the form $\sum_n e^{in\theta}\phi_n^{\dagger}$ and a reflected wave $\sum_n re^{-in\theta}\phi_n^{\dagger}$. In the other lead there will be a transmitted wave $\sum_n te^{in\theta}\phi_n^{\dagger}$. The problem, then, is to solve (4) in the disordered region (the region of sites numbered $1-2N$) with these boundary conditions.

In order to do this we perform a simple transformation on H by rearranging its rows and columns. This is equivalent to rearranging the basis as follows. The Hamiltonian (3) has a basis of orbitals created by $\{\ldots,\phi_{-2}^{\dagger},\phi_{-1}^{\dagger},\phi_0^{\dagger},\phi_1^{\dagger},\phi_2^{\dagger},\ldots\}$ of Fig. 1, and the condition of nearest-neighbor interactions gives H the special tridiagonal form of (3). When H operates on $\phi_n^{\dagger}$, the nth state in this infinite sequence, the result can be expressed in terms of $\phi_n^{\dagger}$, $\phi_{n-1}^{\dagger}$, and $\phi_{n+1}^{\dagger}$ only, the states adjoining $\phi_n^{\dagger}$. If the order of the sequence is changed the structure of H will be different; H operating on one of the orbitals $\phi_n^{\dagger}$ will give a state with projections along basis orbitals not adjoining $\phi_n^{\dagger}$ in the new sequence.

Now let us choose the particular rearrangement

$$\{\ldots,\phi_{-1}^{\dagger},\phi_{2N+2}^{\dagger},\phi_0^{\dagger},\phi_{2N+1}^{\dagger},\phi_1^{\dagger},\phi_{2N}^{\dagger},\phi_2^{\dagger},\phi_{2N-1}^{\dagger},\ldots,\phi_N^{\dagger},\phi_{N+1}^{\dagger}\}\ .$$

In this semi-infinite sequence, the last $2N$ states describe the wire, and all other states describe the leads. It is clear from the ordering that in this "new" basis there are second-nearest-neighbor interactions, but no nearest-neighbor interactions (except between the last two states). When the appropriate rows and columns of (3) are rearranged, H becomes

$$\begin{pmatrix}
\ddots & 0 & 0 & v & 0 & & & & & & & & & \\
 & 0 & 0 & 0 & v & & & & & & & & & \\
 & v & 0 & \varepsilon_1 & 0 & v & 0 & & & & & & & \\
 & 0 & v & 0 & \varepsilon_{2N} & 0 & v & & & & & & & \\
 & & & v & 0 & \varepsilon_2 & 0 & v & 0 & & & & & \\
 & & & 0 & v & 0 & \varepsilon_{2N-1} & 0 & v & & & & & \\
 & & & & & v & 0 & & & & & & & \\
 & & & & & 0 & v & & & \ddots & & & & \\
 & & & & & & & & & & v & 0 & & \\
 & & & & & & & & & & 0 & v & & \\
 & & & & & & & & & v & 0 & \varepsilon_N & v & \\
 & & & & & & & & & 0 & v & v & \varepsilon_{N+1} &
\end{pmatrix}, \tag{5}$$

which divides itself naturally into 2×2 blocks:

$$\begin{bmatrix}
\ddots & & \underline{vI}_{2\times2} & & & & & & \\
 & \underline{vI}_{2\times2} & \underline{0}_{2\times2} & \underline{vI}_{2\times2} & & & & & \\
 & & \underline{vI}_{2\times2} & \underline{A}_1 & \underline{vI}_{2\times2} & & & & \\
 & & & \underline{vI}_{2\times2} & \underline{A}_2 & \underline{vI}_{2\times2} & & & \\
 & & & & \underline{vI}_{2\times2} & & & & \\
 & & & & & & \ddots & & \\
 & & & & & & & \underline{vI}_{2\times2} & \\
 & & & & & & \underline{vI}_{2\times2} & \underline{A}_N &
\end{bmatrix} . \tag{6}$$

where $\underline{0}_{2\times2}$ is the 2×2 zero matrix, $\underline{I}_{2\times2}$ is the 2×2 identity matrix, and

$$\underline{A}_n = \begin{bmatrix} \varepsilon_n & 0 \\ 0 & \varepsilon_{2N-n+1} \end{bmatrix} . \tag{6a}$$

The Hamiltonian matrix is now semi-infinite. In this "block-tridiagonal" form one can define a recursion relation for ψ, a solution of (4), which terminates at block A_N. This solution can be specified by $\{\psi_n\}$, the projections of ψ on the basis orbitals:

$$\psi = \sum_n \psi_n \phi_n^\dagger .$$

Since we already know the solution in the leads, it is sufficient to find the solution of the truncated $(N+2)\times(N+2)$ Hamiltonian

$$\begin{bmatrix}
\underline{0}_{2\times2} & \underline{vI}_{2\times2} & & & & & \\
\underline{vI}_{2\times2} & \underline{A}_1 & \underline{vI}_{2\times2} & & & & \\
 & \underline{vI}_{2\times2} & \underline{A}_2 & \underline{vI}_{2\times2} & & & \\
 & & \underline{vI}_{2\times2} & & & & \\
 & & & & \ddots & & \\
 & & & & & \underline{vI}_{2\times2} & \\
 & & & & \underline{vI}_{2\times2} & \underline{A}_N &
\end{bmatrix} \tag{7}$$

whose basis is $\{\phi_0^\dagger, \phi_{2N+1}^\dagger, \phi_1^\dagger, \phi_{2N}^\dagger, \ldots, \phi_N^\dagger, \phi_{N+1}^\dagger\}$. Such solutions must obey the boundary conditions

$$\begin{aligned}
\psi_0 &= (1+r) , \\
\psi_{2N+1} &= t , \\
\psi_1 &= (e^{i\theta} + re^{-i\theta}) , \\
\psi_{2N} &= te^{-i\theta} .
\end{aligned} \tag{7a}$$

The numbering of the states here corresponds to that of Fig. 1, i.e., the states in the basis before being rearranged. This boundary condition on (7) means that at the ends of the isolated Hamiltonian (1) the solution to (4) must match the Bloch waves in the leads.

We now define a set of 2×1 matrices $\{\underline{z}_n\}$ such that the first row of $\underline{z}_n$ is ψ_n and the second is ψ_{2N-n+1}. We denote this matrix by

$$\underline{z} = \begin{bmatrix} \psi_n \\ \psi_{2N-n+1} \end{bmatrix} . \tag{8}$$

The subscript n of $\underline{z}$ now corresponds to that of the 2×2 blocks in (6), while the ψ subscripts have the same meaning as before. Thus, $\underline{z}_0$ gives the projection of ψ on the basis states at the ends of the leads, and when $N \geq n > 0$ the $\underline{z}_n$ give the projection of ψ on the basis of the sample.

In this notation the boundary condition (7a) can be represented in terms of the $\underline{z}_n$ as

$$\underline{z}_0 = \begin{bmatrix} 1+r \\ t \end{bmatrix}$$

and

$$\underline{z}_1 = \begin{bmatrix} e^{i\theta} + re^{-i\theta} \\ te^{-i\theta} \end{bmatrix} . \tag{9}$$

Each $\underline{z}_n$ can be written as

$$\underline{z}_n = \underline{X}_n \underline{z}_0 + \underline{Y}_n \underline{z}_1 , \tag{10}$$

where the $\underline{X}_n$ and $\underline{Y}_n$ are 2×2 matrices. By operating with the Hamiltonian (7) on the $\underline{z}_n$ with the Schrödinger equation (4), we find a three-term recurrence relation for the $\underline{X}_n$ and $\underline{Y}_n$. If the energy E and the site energies ε_i are expressed in units of v, the nearest-neighbor hopping, these relations are

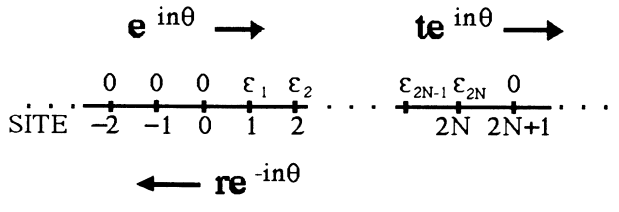

FIG. 1. A wave of the form $\sum_{n=0}^{-\infty} \phi_n^\dagger e^{in\theta}$ incident on the sample from the right-hand side gives rise to a transmitted wave $\sum_{n=2N+1}^{\infty} t\phi_n^\dagger e^{in\theta}$ on the left-hand side and a reflected wave $\sum_{n=0}^{-\infty} r\phi_n^\dagger e^{in\theta}$ on the right..

$$\underline{X}_{n+1}=(E\underline{I}_{2\times2}-\underline{A}_n)\underline{X}_n-\underline{X}_{n-1}\,,$$

$$\underline{X}_0=\underline{I}_{2\times2},\quad \underline{X}_1=\underline{0}_{2\times2}\,, \tag{11}$$

$$Y_{n+1}=(E\underline{I}_{2\times2}-\underline{A}_n)\underline{Y}_n-\underline{Y}_{n-1}\,,$$

$$\underline{Y}_0=\underline{0}_{2\times2},\quad \underline{Y}_1=\underline{I}_{2\times2}\,.$$

Since $\underline{H}$ extends only to $\underline{A}_N$, $\underline{z}_{n+1}$ must be zero. Mathematically, this amounts to another boundary condition on ψ, although its origin is not physically profound. It reflects the fact that a wave at site $N+1$, the last state in the basis of (7), must propagate to either site N or $N+2$. There are no states further along in the basis of (7) for it to propagate into. In terms of $\underline{X}_{n+1}$ and $\underline{Y}_{n+1}$ this boundary condition can be expressed as

$$\underline{X}_{N+1}\underline{z}_0+\underline{Y}_{N+1}\underline{z}_1=\underline{0}_{2\times2}\,. \tag{12}$$

Since $\underline{z}_0$ and $\underline{z}_1$ are simply expressed in terms of the transmission and reflection coefficients t and r, (12) gives two linear equations which can be solved for t and r in terms of $\underline{X}_{N+1}$, $\underline{Y}_{N+1}$, and $e^{\pm i\theta}$. By starting with boundary conditions for an incident wave in lead 2 instead of lead 1,

$$\underline{z}_0=\begin{pmatrix} t \\ 1+r' \end{pmatrix} \tag{9'}$$

and

$$\underline{z}_1=\begin{pmatrix} te^{-i\theta} \\ e^{-i\theta}+r'e^{i\theta} \end{pmatrix},$$

we get a similar pair of equations for t and r', where r' is the reflection coefficient for waves incident from lead 2. It can be shown through time-reversal symmetry that t must be the same for waves of the same energy incident from either lead, so it is unnecessary to define a separate t'. If we solve these equations we find that

$$\underline{S}=-(\underline{X}_{N+1}+\underline{Y}_{N+1}e^{-i\theta})^{-1}(\underline{X}_{N+1}+\underline{Y}_{N+1}e^{i\theta})$$
$$=\begin{pmatrix} r' & t \\ t & r \end{pmatrix}. \tag{13}$$

This is the scattering (S) matrix for the disordered region. For a given sample at energy E, $\underline{X}_{N+1}$ and $\underline{Y}_{N+1}$ may be calculated using (11). Such a calculation is extremely stable since at each step in the recursion the three numbers being added are of roughly the same order of magnitude, minimizing the effects of rounding error.

Although we only present results for one dimension here, the real power of this technique becomes evident when one wishes to generalize to higher dimensions. It can be shown[1] that a sample described by *any* finite discrete Hamiltonian which is attached to elemental leads of the form (2) can be transformed into a form very similar to (6). Specifically, the general form of this transformed matrix is

$$\begin{pmatrix}
\underline{0}_{2\times2} & \underline{I}_{2\times2} & & & & \\
\underline{I}_{2\times2} & \underline{A}_1 & \underline{B}_2 & & & \\
 & \underline{B}_2^{\dagger} & \underline{A}_2 & & & \\
 & & \underline{B}_3^{\dagger} & & & \\
 & & & \ddots & & \\
 & & & & \underline{B}_N & \\
 & & & \underline{B}_N & \underline{A}_N^{\dagger} &
\end{pmatrix}, \tag{14}$$

where the $\underline{A}_n$ and $\underline{B}_n$ are 2×2 blocks and all energies are again in units of the nearest-neighbor hopping v so that $v=1$. This transformation is done by using a generalization of the recursion method.[20] Applying the same boundary conditions and finding solutions to (4) leads to a recurrence relation analogous to (11):

$$\underline{B}_{n+1}^{\dagger}\underline{X}_{n+1}=(E\underline{I}_{2\times2}-\underline{A}_n)\underline{X}_n-\underline{B}_n\underline{X}_{n-1}\,,$$
$$\underline{B}_{n+1}^{\dagger}\underline{X}_{n+1}=(E\underline{I}_{2\times2}-\underline{A}_n)\underline{X}_n-\underline{B}_n\underline{X}_{n-1}\,, \tag{15}$$

where $\underline{X}_n$ and $\underline{Y}_n$ have the same meaning as before. Note that (15) reduces to (11) when all the $\underline{B}_n=\underline{I}_{2\times2}$ and all the $\underline{A}_n$ are diagonal. A system with more than two leads can be similarly transformed into a form tridiagonal in $n\times n$ blocks where n is the number of leads. This allows calculation of an S matrix by solution of a set of linear equations analogous to (12).

In practice, this transformation introduces large rounding errors into the $\underline{A}_n$ and $\underline{B}_n$. It can be shown that these errors do not affect calculation of the transmittance. Such justification will be presented in a later publication on 2D calculations.

In the context of electron transport in solids the calculation of transmittance describes an electric current in a disordered solid in the low-temperature, low-current limit. If the temperature is low enough there will be a few inelastic-scattering events while the electron is within the sample; in the low-current limit the density of excitations is sufficiently low for their interactions to be negligible. Therefore, the system is well defined by an elastic, random, independent-particle Hamiltonian. From this standpoint, the transformed matrix (14) can be thought of as an "equivalent quantum circuit."

In the remainder of this paper we consider calculations involving 1D samples of the form (1).

III. RELATION TO OTHER METHODS

A large amount of numerical work has been done on Anderson models, particularly in one dimension. It is therefore reasonable to ask how this technique differs from others and what advantages it has to offer. Most techniques use recursion relations in one form or another because they are easily and stably computable, although it should be noted that some compelling work has been done with other techniques.[21] In the remainder of this section the block-recursion technique will be compared to some other recursive technique in one and higher dimensions. Comparison of results to other types of techniques or disorders will be presented in a later section.

Previous recursive techniques generally fall into two categories: those that use more stable three-term recurrences to calculate $t(E)$ or an equivalent quantity but are limited to one dimension, and many-term or "slice" recursions that are applicable to higher dimensions but are not as stable.

A. 1D calculations

Perhaps the most extensive calculations of the statistics of 1D systems were performed by Czycholl, MacKinnon, and Kramer.[13] They used the Kubo formula[22] to find the conductance of isolated 1D Anderson models (i.e., without leads) by three methods: integrating the time-dependent Schrödinger equation, recursively computing matrix elements of the resolvent $G=(E-H)^{-1}$ between ends of the sample, and computing matrix elements of G by use of continued fractions. Since a finite system was used it was necessary to add a small imaginary component to the energy; otherwise the discrete eigenvalue spectrum of a finite Hamiltonian would make quantities such as $t(E)$ very sensitive to whether or not E is an eigenvalue. However, states with complex energies do not describe elastic scattering because they decay in time.

The problem of discrete energy spectra in calculation of elastic scattering can be solved by adding leads that make the system infinite and the spectrum continuous. This is a more physical calculation as electrons in a circuit whose elements have length comparable to the electronic localization length cannot be expected to have eigenfunctions that are confined to the sample. A calculation which included semi-infinite leads and very closely resembled our method was performed by Economou and Soukoulis.[23] $t(E)$ was recursively calculated for the Hamiltonian (3) without transforming it to (5) as we have done; instead a scalar recurrence relation analogous to (11) was used to find the $\psi_n(E)$, from which $t(E)$ was found. A related technique is that of transfer matrices.[11,12,14,18] In this method the sample is divided into individual site scatterers, each of which is represented by a matrix that describes its effect on a wave propagating through the lattice. The product of all the matrices is another matrix whose eigenvalues are related to the scattering matrix.

Both of these methods have the advantage of including the leads in the calculation; however, both require a matrix in the tridiagonal form of (3) to give stable three-term recurrences for the wave functions. These techniques are therefore not so useful in higher dimensions, or for long-range hopping. For a sample with a Hamiltonian more complicated than (1) that is attached to simple leads, the transformation we have applied to make the leads block tridiagonal allows the rest of the Hamiltonian (that describing the sample) to be transformed into a similar block-tridiagonal form without affecting the leads, so that the efficient recursive calculation (15) for the wave functions can be performed and the boundary conditions can still be matched.

B. "Slice" recursions in higher dimensions

Recursive calculations on samples of higher dimension have usually involved dividing the sample into "slices," arrays of sites of dimension $d-1$, where d is the dimension of the sample. Some recursion relation is then defined which calculates the properties of the system from those of the slices. Lee and Fisher[24] connected their 2D samples to 2D leads and recursively calculated matrix elements of $G=(E-H)^{-1}$ between states in the two leads. At each step of the recursion the resolvent of an isolated slice was calculated and a matrix of order comparable to that of the resolvent was inverted. Performing such an inversion at each step is time consuming.[25] Instead, MacKinnon and Kramer[25] used a different slice recursion to find the operator $G^{-1}=E-H$ from the G^{-1} for each of the slices, so that it was unnecessary to invert a large matrix until the end of the calculation. Matrix elements of G^{-1} between ends of an isolated sample were found. However, since the object of the calculation was to observe gross spatial features of the wave functions (such as localization lengths), only the exponent of the most rapidly diverging component of G was measured.

By defining a recursion in terms of slices, both methods have introduced an instability that was not present in the 1D calculations described earlier. For systems described by a Hamiltonian with a discrete basis, quantities such as G or $t(E)$ contain polynomials or ratios of polynomials in E whose orders are comparable to the number of basis states. In the case of $t(E)$ this is evident from Eqs. (10)–(13). We have noted the desirability of using three-term recurrences to calculate polynomials since in a relation such as (11) all additions involve a few numbers of roughly the same order of magnitude. However, in a slice recursion G for an isolated but large slice is a sensitive function of E with zeros and singularities close to the real axis. Many numbers of greatly differing magnitudes are added together, creating errors that accumulate much more rapidly than for the recurrence (11).

The use of elemental (one-band) leads does not limit the application of our method. In the low-temperature limit we are considering, electron transport in the leads takes place only in those bands which intersect the Fermi surface. It can be shown[20] that any nondegenerate Hamiltonian can be transformed into tridiagonal form, so that if the Fermi surface intersects n bands, then the Hamiltonian for electrons near the Fermi surface can be transformed into n decoupled tridiagonal Hamiltonians. Each of these Hamiltonians, although in general somewhat more complicated than those in (2), can still be thought of as an elemental lead in the sense that it describes wave propagation into and out of the sample by a single band of states. A lead with more than one band involved in transport can therefore be adequately described by transforming it into a number of elemental leads equal to the number of bands crossing the Fermi surface. As we indicated in Sec. II, this merely means tridiagonalizing in $n\times n$ blocks, where n is the number of elemental leads. If an excessive number of such leads (comparable to the number of basis states of a slice) were required, the calculation would have an instability similar to that of the slice recursions. However, almost all cases of interest can be described in terms of leads with at most two bands, so this is not a problem. It is therefore unnecessary to perform a slice recursion to describe 2D or 3D

systems.

The ability to attach leads to different parts of the device also has obvious applications to the description of four-lead devices, a problem of great experimental interest.[26]

IV. RESULTS FOR ONE-DIMENSIONAL CHAINS

We have studied one-dimensional Anderson models ranging in size from 1 to 400 sites and in disorder from $w/v=0.5$ to $w/v=5$. Figure 2 shows typical plots of $|t(E)|^2$ for two systems with $w/v=2$. The first is the entire band for a chain 20 sites long; the second is a narrow resonance in a chain 180 sites long. The Lorentzian appearance of the peaks is due to the previously noted fact that $|t(E)|^2$ is a ratio of polynomials in E. Although the sample is almost transparent at one energy in Fig. 2(b), the peak is *not* an unusual feature; at $w/v=2$ we examined large portions of the band for 28 chains of different lengths from 10 to 250 sites and in each case found at least one peak whose height was greater than 0.7 and in all but one case greater than 0.9, with average widths decreasing as the length increases. At this disorder average localization lengths (see below) are about ten sites.

Several authors have suggested the presence of resonances and their possible origins. For a model of one dimensional disorder very different from the Anderson model, Denbigh and Rivier[27] and Condat and Kirkpatrick[28] noted that at each of an infinite, discrete set of energies their lattice had an extended state and was therefore completely transparent to wave propagation. (This set of energies was of measure zero, i.e., was a set which was infinite but discretely spaced in E and so carried no probability weight when compared to the full continuous spectrum of eigenstates.) It is not clear whether the Anderson model supports such solutions in general. Azbel has suggested[29] that localized states with a single maximum very near the middle of the sample would couple equally with both leads and would produce strong transmittance at that energy. Previous numerical studies of resonances and phase-correlation lengths[16,18] indicate this phenomenon is an important cause of resonances. In a picture somewhere between these two, Pendry has argued[30] that "necklace" states, probabilistically exceptional states with more than one maximum located in a broad area near the sample center would dominate the transmittance and provide very transparent resonances. Which of these effects causes a particular resonance is interesting experimentally since this will determine the characteristic time for an electron to traverse the sample (longest time for resonant tunneling, shortest for extended states). We

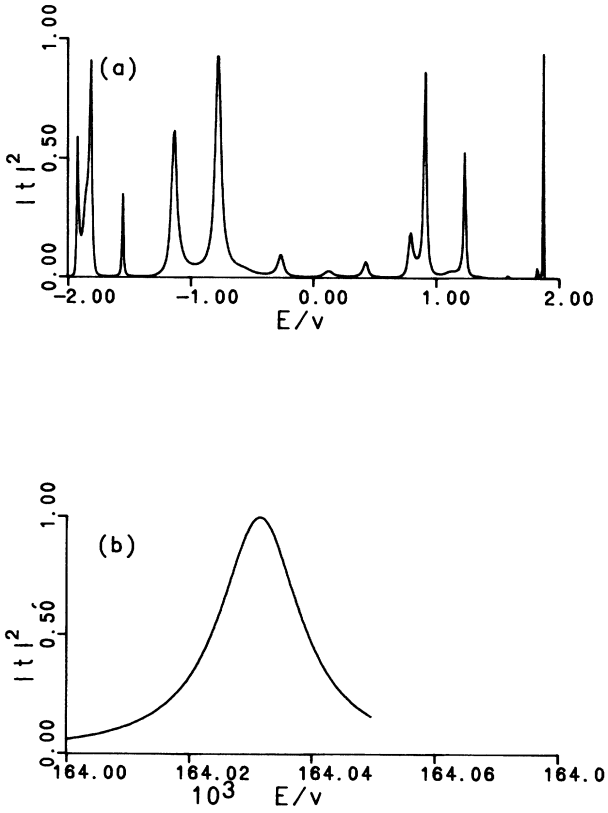

FIG. 2. Transmittance of two disordered wires as a function of energy for $w/v=2$. (a) The full band for a chain 20 sites long. (b) A narrow region of the band for a chain 180 sites long, showing a sharp resonance.

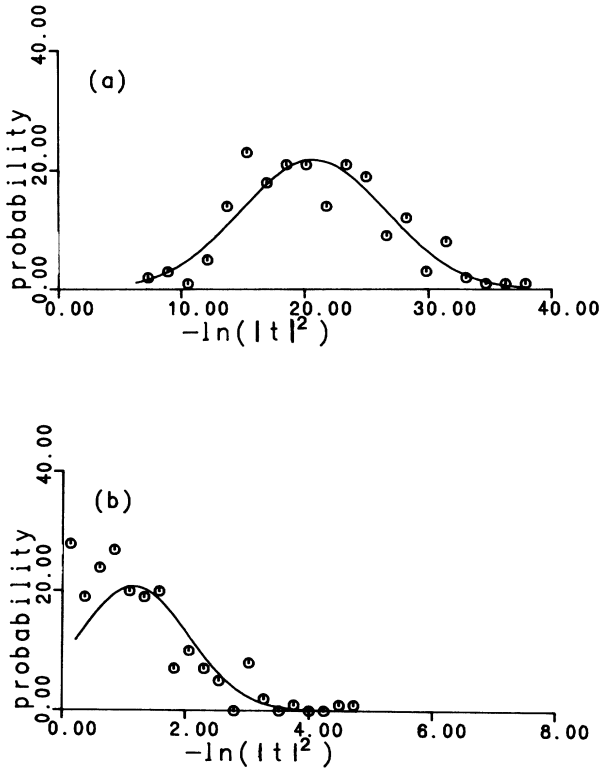

FIG. 3. Relative probability density distribution for finding a chain with a given transmittance at fixed disorder, length, and incident wave energy in the following limits. (a) Low transmittance (240 sites, $w/v=2$, $E/v=0.5$). The probability histogram (circular data points) is well fitted by a Gaussian (solid line). (b) High transmittance (200 sites, $w/v=0.5$, $E/v=0.5$). The histogram is skewed and is not well fitted by a Gaussian.

know of no authors who have quantified the relative likelihood of the existence and strength of different types of resonances in a given Anderson model; such a calculation remains an open problem. It has also been observed[15,31] that large fluctuations in transmittance occur near band edges in samples with random δ-function (vacancy) defects.

The statistical variance of $|t|^2$ for a given length and disorder was calculated by generating 200 chains with this length and disorder and calculating $|t(E)|^2$ at a few selected energies for each. One would expect that in the limit of long chains with weak disorder the distribution of $|t|^2$ would be log-normal by the following argument[8] which follows the ideas of Thouless:[32] In the weak-disorder limit the leading term in t will be the product of the forward-scattered component of a propagating wave at each site. If this component at site i is t_i, then $t \approx \prod_i t_i$. This is because in a system of many random scatterers multiply backscattered waves interfere with random phase. The interference is therefore destructive, and these components do not contribute to the transmitted wave. It can be shown that in this limit the t_i equal $\varepsilon_i^2/(8v^2\sin^2\theta)$ so that

$$\ln t \approx (8v^2\sin^2\theta)^{-1}\left[\sum_{i=1}^{2N}\varepsilon_i^2\right], \tag{16}$$

which for large N is distributed normally. We observe this in the appropriate limit (Fig. 3). In fact, even for stronger disorder ($w/v \geq 2$), for chains more than a few localization lengths long, the first eight moments of the distribution of $|t|^2$ at a given energy agree to those of an appropriately fitted log Gaussian to within the standard error of each moment. This is in agreement with the results of Economou and Soukoulis.[23]

The frequency distribution cannot have this form in the limit of shorter chains, of course, since mathematically the range of $|t(E)|^2$ is between 0 and 1 so its log cannot range over all real numbers, and physically because backscattering is more important when the wave has fewer lattice sites to randomize the phase of the multiply backscattered components. In this limit we observe a significant skew [Fig. 3(b)] which can result in a most probable value significantly different from the average. This is in qualitative agreement with results for isolated chains,[13] and for randomly spaced δ-function barriers.[19]

It is tempting to ask whether the resonances can be understood as the "tail end" of this distribution. This cannot be the case, however, since (16) tells us that in this approximation a resonance where $t \approx 1$ ($\ln t \approx 0$) corresponds to a lattice where all the ε_i are zero. The conclusion is that for long chains resonances occur for exceptional energies at which the approximation of incoherent backscattering breaks down. At these energies the backscattering is strongly coherent and interferes destructively to give a transmittance that is nearly unity.

The scaling of $|t|^2$ with the length of the sample can be shown by taking statistics at the same energy and disorder for several different lengths. We expect that $|t|^2 \approx e^{-L/\xi}$, where ξ is the localization length and L is the length of the sample, so that a plot of $\ln|t|^2$ against L would give a straight line of slope $1/\xi$. Figure 4(a) shows that this is true for the mean at all length scales we have examined, but *not* the most probable value of $\ln|t(E)|^2$ when $2N \leq \xi$ [Fig. 4(b)]. (There is, of course, considerable departure from this average behavior when one looks at individual chains.) The error bars in Fig. 4 for the mean are standard errors of the mean and those for the most probable value represent an estimate of the uncertainty based on the width of the histogram classes we used in calculating distributions functions for $\ln|t|^2$.

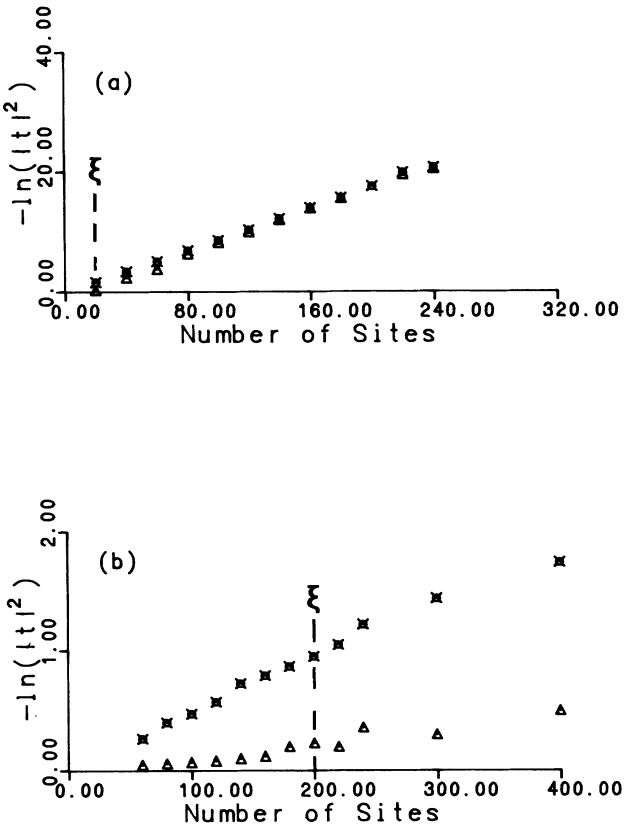

FIG. 4. Scaling behavior of the mean (crossed-circle data points) and most probable value (triangular data points) of $\ln|t|^2$ for fixed disorder and incident energy in two regimes. Except for most probable values in (*b*), error-bar sizes are comparable to data-marker sizes. (a) $2N > \xi$ ($w/v = 2$, $E/v = 0.5$). The average localization length ξ is about 10 sites. (b) $2N \approx \xi$ ($w/v = 0.5$, $E/v = 0$). Here, ξ is about 200 sites.

We can find an "average" localization length for these systems using the method of Thouless[32] and the approximation of $\ln t$ given in (16). The inverse of the localization length $1/\xi$ will approximately equal $(1/2N)\ln t^2$ or $(1/N)\ln t$. The right-hand side of (16) can be approximately summed by taking $2N$ times $\langle\varepsilon_i^2\rangle$, where this average over all the ε_i equals

$$\langle\varepsilon_i\rangle = (1/w)\int_{-w/2}^{w/2} x^2 dx = (\tfrac{1}{96})(w/v)^2 ,$$

giving a localization length

$$\xi \approx 47(v/w)^2(1/\sin^2\theta) . \tag{17}$$

This agrees with the slopes of the lines we have plotted to within one or two standard errors of the slope in each case.

Figure 4 demonstrates an interesting result. For $N < \xi$ the resonances dominate the statistics of the transmittance, as can be seen in Fig. 3. It is therefore not obvious that a scaling law of the form $t \approx e^{-N/\xi}$ should be obeyed in this regime, since the nearly transparent states are becoming more significant in the average (Fig. 2). The mean, however, does obey this scaling law exceptionally well; it is the most probable value that does not. This is the opposite of what one would naively expect.

It should be pointed out that Pichard[14] observed a localization length that varied with the sample size in transfer-matrix calculations for $\xi \gg 2N$. Specifically, he observed $\xi \propto N^{1/2}$. We do not observe such a dependence. $\langle \ln | t |^2 \rangle$ appears linear at all length scales. If we *literally* take $| t |^2 \equiv e^{-L/\xi}$ and use the most probable value of $\ln | t |^2$, we get an approximate power law for $\xi(N)$ of the form $\xi \propto N^{\gamma}$, where γ is somewhere between 1 and 3 in the few cases we have examined. Whether we are not using chains with $2N$ sufficiently smaller than ξ to see this effect or the effect is really not present in an Anderson model is not clear to us.

V. CONCLUSION

We have introduced a new method for calculating the transmission properties of an arbitrary disordered system. This calculation is more stable than previous methods when applied to systems of dimension greater than 1. This method involves attaching the disordered system to ordered, elemental leads and transforming the matrix into a block-tridiagonal form that allows calculation of the scattering (S) matrix by means of a stable three-term recurrence and a straightforward matching of boundary conditions. We have applied this to the statistics of disordered 1D systems. We observe highly transparent resonances even for long chains with strong disorder. The average localization lengths in our chains are in close agreement with those predicted by the analytic method of Thouless and seem to be independent of the chain length.

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