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The localization length and density of states of 1D disordered systems

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Abstract. We present a simple and fast method for calculating the localization length and density of states of disordered one-dimensional systems. The method is based on a multiple-scattering picture of transport in disordered media and draws from transfer matrix theory. We use our new method with the tight-binding model to demonstrate its convergence for both discrete and continuous distributions of disorder. We also demonstrate its use in investigating the weak disorder limit.

1. Introduction

The propagation of waves in one-dimensional (1D) disordered systems has been studied extensively. The motivation for such studies is not only their academic interest but also an increasing need due to the development of a wide range of quasi-1D materials. The localization length is one of the most important quantities in describing the wave function of a disordered system, and for 1D systems, both numerical simulation (Mackinnon and Kramer 1983, Pichard and Sarma 1981, Azbel 1980) and analytic approaches (Landauer 1970, Theodorou and Cohen 1976, Kappus and Wegner 1981, Pendry 1982a,b, Kirkmann and Pendry 1984 a,b, Derrida and Gardner 1984, Slevin and Pendry 1988) are well developed. There are also a large number of publications in the literature that investigate the density of states (or eigen-energy spectra) of disordered chains (Schmidt 1957, Halperin 1965; for a review of earlier works see Dean 1972, Butler 1973, Goncalves da Silva and Koiller 1981, Koiller *et al* 1983, Kirkmann and Pendry 1984a, Slevin and Pendry 1988, Tan and Yang 1988, Nieuwenhuizen and Luck 1985).

The transport properties of a disordered system are determined by its reflection and transmission coefficients. The transmission coefficient is usually considered to be the most useful of the two due to its simple relation to important physical quantities, such as the localization length, conductivity and density of states. However, the reflection coefficient is a more tractable quantity (Pendry and Barnes 1989, Barnes and Luck 1990). In the long-length limit its moments become stationary and are easily calculated. Hence, we may expect that analysis of the properties of 1D disordered systems can be much simplified if expressed in terms of the reflection coefficient of the system.

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In this paper, we prove that the inverse localization length (Lyapunov exponent) and the integrated density of states may be expanded in terms of the stationary moments of the reflection coefficient of a disordered chain, and show how these moments may be found exactly using the reflection transfer matrix introduced by Pendry and Barnes (1989). The localization length is the reciprocal of the Lyapunov exponent and the density of states can be found by numerical differentiation of the integrated density of states. Hence, we obtain a new method for calculating the localization length and density of states of disordered 1D systems.

Although approaches already exist for calculating the localization length and density of states we believe that our new method is a useful contribution to this field. Firstly, the moment expansion provides us with a simple picture for the make-up of the localization length and density of states in terms of elementary multiple-scattering paths. Secondly, the new method has a good convergence rate. Convergence is a vital factor in the study of disordered systems. For example, near the weak disorder limit, the localization length is very large and it is impossible to obtain accurate results by numerical simulation because chains much longer than the localization length must be considered. Finally, the method provides a new basis for exact numerical calculation and can be used to give analytic results in limiting cases.

The paper is arranged as follows. In section 2, we present the formalism for our new method. In section 3, we discuss its convergence for the tight-binding model and calculate the localization length and the density of states for both discrete and continuous distributions of disorder. In section 4, we use the new method to investigate the weak disorder limit of the tight-binding model. A brief conclusion is given in section 5.

2. Formalism

Consider a one-dimensional disordered chain sandwiched between two semi-infinite ordered leads capable of supporting propagating waves. If the amplitude of a wave incident on the disordered chain is v_i then the amplitudes of the transmitted and reflected waves, v_t and v_r, are related through the reflection and transmission coefficients: $v_r = Rv_i$ and $v_t = Tv_i$. Suppose that the disordered chain further decomposes into L statistically independent units. If we add an $(L+1)$th unit to the disordered chain we may use the multiple-scattering picture shown in figure 1 to find the reflection and transmission coefficients of the composite system. For the reflection coefficient we find

$$\begin{aligned} R_{L+1} &= r^+_{L+1} + t^+_{L+1}R_L t^-_{L+1} + t^+_{L+1}R_L(r^-_{L+1}R_L)t^-_{L+1} + \dots \\ &\quad + t^+_{L+1}R_L(r^-_{L+1}R_L)^n t^-_{L+1} + \dots \\ &= r^+_{L+1} + t^+_{L+1}t^-_{L+1}\sum_{n=1}^{\infty}(r^-_{L+1})^{n-1}(R_L)^n \end{aligned} \tag{2.1}$$

and for the transmission coefficient we find

$$T_{L+1} = T_L t^-_{L+1}\sum_{n=0}^{\infty}(r^-_{L+1}R_L)^n \tag{2.2}$$

where the superscript + indicates that a wave has been scattered in the positive direction and the superscript − indicates that a wave has been scattered in the negative direction as indicated in figure 2. Both series here are convergent for

$$|r^-_{L+1}R_L| < 1. \tag{2.3}$$

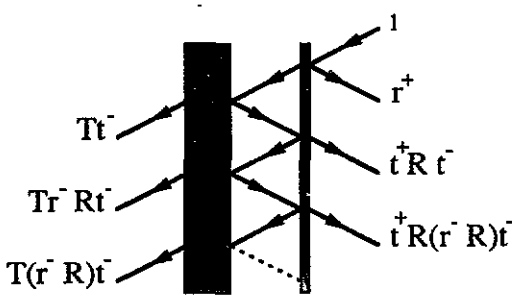

Figure 1. Multiple scattering between a single unit and L units.

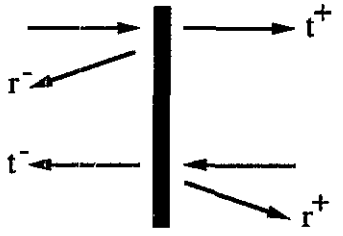

Figure 2. Scattering from a single unit.

The complex Lyapunov exponent of a disordered semi-infinite chain $= -\gamma(E) + i\pi N(E)$ has real part $\gamma(E)$ which is the Lyapunov exponent and imaginary part $N(E)$ which is the integrated density of states. It is well known that this quantity is related to the transmission coefficient of a disordered chain through

$$-\gamma(E) + i\pi N(E) = \lim_{L\to\infty} \frac{1}{L} \ln(T_L) = \lim_{L\to\infty} \frac{1}{L} \sum_{n=1}^{L} \ln \frac{T_n}{T_{n-1}}. \tag{2.4}$$

If we now consider an ensemble of disordered systems in which the complex Lyapunov exponent self-averages we may rewrite this expression in the form

$$-\gamma(E) + i\pi N(E) = \lim_{L\to\infty} \langle \ln T_L/T_{L-1} \rangle \tag{2.5}$$

where the notation $\langle\ \rangle$ denotes an ensemble average. Substituting equation (2.2) into (2.5) we find

$$\begin{aligned} -\gamma(E) + i\pi N(E) &= \lim_{L\to\infty} \left\langle \ln\Big(t^-_L \sum_{n=0}^{\infty} (r^-_L R_{L-1})^n \Big) \right\rangle \\ &= \langle \ln t^- \rangle + \lim_{L\to\infty} \sum_{n=1}^{\infty} \frac{\langle r^{-n} \rangle \langle R^n_{L-1} \rangle}{n}. \end{aligned} \tag{2.6}$$

In the limit $L \to \infty$ the moments of the reflection coefficient $\langle R^n_L \rangle$ become stationary:

$$\lim_{L\to\infty} \langle R^n_L \rangle = \langle R^n_\infty \rangle. \tag{2.7}$$

This is because the important length scale for the reflection coefficient is the localization length or penetration depth not the total length. Hence, taking the limit $L \to \infty$ in equation (2.6) we find

$$-\gamma(E) + i\pi N(E) = \langle \ln t^- \rangle + \sum_{n=1}^{\infty} \frac{\langle r^{-n} \rangle \langle R^n_\infty \rangle}{n}. \tag{2.8}$$

In equation (2.8) we now have a simple expression for the Lyapunov exponent and the integrated density of states in terms of a convergent series. The first term on the left-hand side of equation (2.8) gives the contribution due to forward scattering (Roberts and Pendry 1990) and subsequent terms give contributions due to higher-order multiple scattering.

What we must do now is to show how the moments $\langle R_\infty^n \rangle$ may be found. Pendry and Barnes (1989) have provided a simple way to do this. Following their work, we define a vector whose elements comprise all integer powers of R_L:

$$v_L = \begin{pmatrix} 1 \\ R_L^1 \\ R_L^2 \\ R_L^3 \\ \vdots \end{pmatrix}. \tag{2.9}$$

By expanding each integer power of R_{L+1} as a power series in R_L, we can derive the transfer matrix relation (see Pendry and Barnes 1989)

$$v_{L+1} = \mathbf{m}_{L+1} v_L. \tag{2.10}$$

The elements of $\mathbf{m}_L$ are easily calculated from the recursion relation

$$(\mathbf{m}_L)_{n+1,m} = \sum_{i=1}^{m} \mathbf{m}_{n,m-i} \mathbf{m}_{1,i} \tag{2.11}$$

using the initial conditions

$$(\mathbf{m}_L)_{1,0} = r_L^+ \qquad (\mathbf{m}_L)_{1,n} = t_L^+ t_L^- (r_L^-)^{n-1} \tag{2.12}$$

derived from equation (2.1). We will refer to $\mathbf{m}$ as the reflection transfer matrix.

Taking the ensemble average of equation (2.9) and letting $L \to \infty$

$$\lim_{L\to\infty} \langle v_{L+1} \rangle = \lim_{L\to\infty} \langle \mathbf{m}_{L+1} v_L \rangle \tag{2.13}$$

we find the stationary equation

$$\langle R_\infty^n \rangle = \sum_{m=0}^{\infty} (\langle \mathbf{m} \rangle)_{n,m} \langle R_\infty^m \rangle. \tag{2.14}$$

The elements of the ensemble average matrix $\langle \mathbf{m} \rangle$ may be found from the distribution of the reflection and transmission coefficients of a single unit. It may be done either analytically or numerically depending on the complexity of the distribution. For the symmetric exponential alloy the matrix is particularly simple; equation (2.14) reduces to a five-term recursion relation (Barnes and Luck 1990). In order to solve for $\langle R_\infty^n \rangle$ we truncate $\langle \mathbf{m} \rangle$ to an $N \times N$ matrix and solve the set of N linear equations:

$$\sum_{m=1}^{N} (\langle \mathbf{m} \rangle_{n,m} - \delta_{n,m}^c) \langle R_\infty^m \rangle = -\langle r^{+n} \rangle \qquad \text{for} \quad n = 1, 2, \ldots, N \tag{2.15}$$

using a standard numerical package. The notation $\delta_{n,m}^c$ used here denotes a Kronecker delta. The moments of the reflection coefficient $\langle R_\infty^n \rangle$ converge rapidly with increasing n and we choose N to be sufficiently large that we may calculate the complex Lyapunov exponent from equation (2.8) to desired accuracy.

3. Numerical results for the tight-binding model

In this section, we use our new method to obtain the density of states and localization length for the tight-binding model.

We consider a chain of atoms in which the wave function amplitudes are given by the tight-binding Hamiltonian

$$V\psi_{n+1} + V\psi_{n-1} = (E - \epsilon_n)\psi_n. \tag{3.1}$$

The chain consists of a central disordered region, in which the orbital site energies ϵ_n are statistically independent with distribution $P(\epsilon_n)$, and semi-infinite leads, in which the site energies are constant with $\epsilon_n = \epsilon_0$. Solving equation (3.1) in the leads gives

$$E = \epsilon_0 + 2V\cos k \qquad k = [0, \pi]. \tag{3.2}$$

In the disordered region we define a single disordered unit to consist of a single site and a single bond to its left. Such units have reflection and transmission coefficients of the form

$$r^+ = \frac{i\delta}{1 - i\delta} \qquad r^- = e^{2ik}r^+ \qquad t^\pm = e^{ik}\frac{1}{1 - i\delta} \tag{3.3}$$

where

$$\delta = (\epsilon - \epsilon_0)/2\sin k. \tag{3.4}$$

In this model the convergence criterion equation (2.3) is only guaranteed if the incident wavevector k is real since this ensures $r_{L+1}^- < 1$ from equations (3.3)–(3.4) and $R_L \leqslant 1$ from unitarity. Hence, from equation (3.2) for any particular value of ϵ_0 convergence is only guaranteed in the band of energies $|E - \epsilon_0| < 2V$. Therefore at any particular energy we must pick a value of ϵ_0 that ensures convergence. We can do this because both the density of states and localization length are inherent properties of the disordered system and therefore independent of the value of ϵ_0.

We have calculated the density of states and localization length using the new method for both continuous and discrete distributions of site energies. As an example of a continuous distribution, we consider the Anderson distribution

$$P(\epsilon) = \begin{cases} 1/W & \text{if} \quad |\epsilon| \leqslant W/2 \\ 0 & \text{otherwise} \end{cases} \tag{3.5}$$

with $W = 1$. For this distribution we average the reflection transfer matrix numerically. We then solve the linear equations (2.15) for the stationary moments of the reflection coefficient and use them to sum equation (2.8). The localization length is then the inverse of the Lyapunov exponent and the density of states found by numerically differentiating the integrated density of states. This differentiation is complicated for weak disorder by the existence of anomalies. Section 4 deals with this problem. Figure 3 shows how the density of states for this model converges with increasing $N = 5, 20, 50$ in equation (2.15). Figure 4 shows the convergence of the localization length with $N = 3, 5, 20$. We see that both the localization length and the density of states converge very rapidly with increasing N. However, the density of states converges less rapidly than the localization length, so we may conclude that

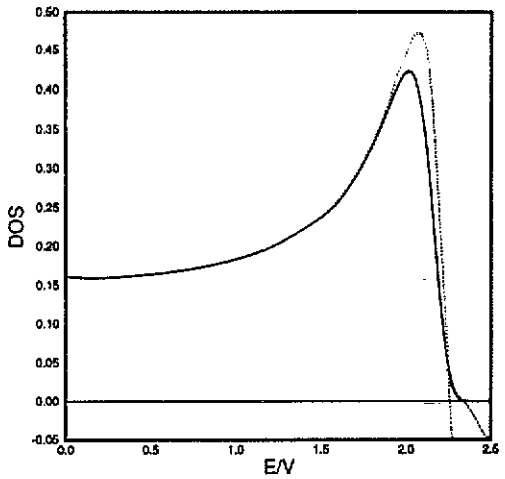

Figure 3. Plot of the density of states of the Anderson model with $W=1$. The curves show the convergence of our method with increasing dimension of the ensemble average transfer matrix: $N = 5$, dotted curve; $N = 10$, broken curve; $N = 50$, full curve.

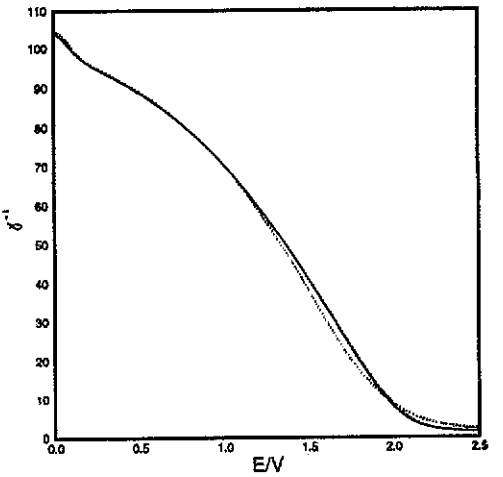

Figure 4. Plot of the localization length of the Anderson model with $W=1$. These curves show the convergence of our method with: $N = 3$, dotted curve; $N = 5$, broken curve; $N = 20$, full curve.

it has a stronger dependence upon multiple scattering. It can also be seen that the convergence rate of our theory has a strong dependence on energy for both the density of states and the localization length. The convergence is slowest within the band tail. This is easy to understand since scattering near a band edge is always very strong even for weak disorder.

As an example of a discrete distribution of disorder, we consider a random binary alloy with distribution function defined by

$$P(\epsilon) = \begin{cases} \frac{1}{2} & \epsilon = +\Delta \\ \frac{1}{2} & \epsilon = -\Delta \end{cases} \tag{3.6}$$

with $\Delta = 2$. The random binary alloy has been studied extensively. Numerical simulation and analytical work show that the integrated density of states and Lyapunov exponent of these systems have a very rich structure (Halperin 1965, Butler 1973, Koiller *et al* 1983, Makler *et al* 1985, Nieuwenhuizen and Luck 1985, Tan and Yang 1988). Both quantities contain power law singularities of the form $N(E+x)-N(E) \sim |x|^{\alpha}$ with $\alpha > 0$ at a dense set of energies. Clearly this has the consequence that, at or near these energies, the density of states and localization length are not well represented by a finite truncation of the moment expansion (2.8), particularly in the circumstance that $\alpha < 1$. However, away from these points our method converges very well and near these points the detail of the structure begins to appear as we look on a finer energy scale and increase N. We have used figures 5, 6 to demonstrate this point. The convergence of the density of states is complicated by the appearance of unphysical negative values for small N. However, these only appear at energy gaps and disappear with increasing N.

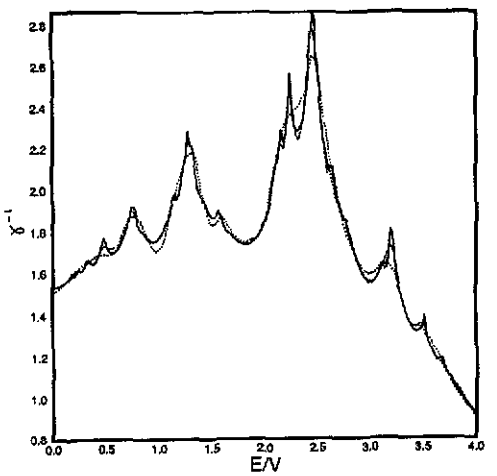

Figure 5. The localization length of a random binary alloy with: $\Delta = 2$ calculated using our theory with $N = 10$, dotted curve; $N = 20$, broken curve; $N = 50$, full curve.

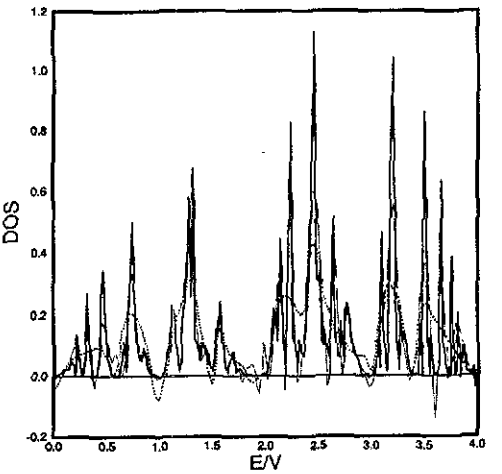

Figure 6. The density of states of a random binary alloy with $\Delta = 2$ calculated using our method with: $N = 10$, dotted curve; $N = 20$, broken curve; $N = 80$, full curve.

4. The weak disorder limit

In this section we will look at the weak disorder limit of the tight-binding model. This limit has been studied extensively and it is known that the complex Lyapunov exponent contains anomalies at special energies (Kappus and Wegner 1981, Pendry 1982a, Lambert 1984, Derrida and Gardner 1984, Bovier and Klein 1988). However, in this section we hope to show that our new method can give these weak disorder results in a simple and transparent manner.

We split the ensemble average reflection transfer matrix into two parts: a zero-disorder part and a perturbing part due to the disorder

$$\langle \mathbf{m} \rangle = \mathbf{m}^{(0)} + \mathbf{m}'. \tag{4.1}$$

In the tight-binding model, the zero-disorder part has the diagonal form

$$\mathbf{m}^{(0)}_{n,m} = \mathrm{e}^{2ikn}\delta^c_{n,m}. \tag{4.2}$$

Hence, substituting equations (4.1), (4.2) into the stationary equation (2.14) and using first-order perturbation theory we find

$$\langle R^n_\infty \rangle \approx \frac{\mathbf{m}'_{n,0}}{1 - \mathrm{e}^{2ikn}} \approx \frac{\langle r^{-n} \rangle}{1 - \mathrm{e}^{2ikn}} \tag{4.3}$$

If we assume that we have a symmetric distribution of site potentials then moments $\langle r^{-n} \rangle$ take the form

$$\langle r^{-2n} \rangle \approx (-1)^n \langle \delta^{2n} \rangle \mathrm{e}^{2ik(2n)} \qquad \langle r^{-2n-1} \rangle \approx (-1)^n (2n-1) \langle \delta^{2n} \rangle \mathrm{e}^{2ik(2n-1)} \tag{4.4}$$

to leading order from equations (3.3) and (3.4).

Now we can substitute these values for the moments of the reflection coefficient into our expression for the complex Lyapunov exponent equation (2.8). To leading order this gives

$$-\gamma(E)+\mathrm{i}\pi N(E)\approx -\langle\delta^2\rangle/2+\mathrm{i}k \tag{4.5}$$

which is simply the result of Thouless (1979). An important point to note here, in terms of the physical interpretation of this result, is that it is the result we would have obtained had we used only the forward scattering term in equation (2.8).

In carrying out the perturbation theory method here we have clearly ignored the fact that the wavevector k may be rationally related to π, e.g $k=q\pi/u$. If it is, then the zero-disorder reflection transfer matrix will contain degeneracies that we must take into account. Using degenerate perturbation theory yields the general result that, to leading order at a point $k=q\pi/u$ in the band, the moments with $n=$ integer $\times\, u$ are anomalously larger than their value at neighbouring points not rationally related to π. This fact, in conjunction with the moment expansion for the complex Lyapunov exponent, equation (2.8), explains the occurrence of anomalies in the complex Lyapunov exponent at all points in the band for which the wavevector is rationally related to π. The most striking occurrence of this type of anomaly occurs at the band centre $k=\pi/2$ where the eigenvalues of $\mathbf{m}^{(0)}$ are degenerate on either 1 or -1. The degenerate subspace with eigenvalue -1 gives $\langle R_\infty^{2n-1}\rangle=0+\mathcal{O}(\langle\delta^2\rangle)$ and that with eigenvalue 1 yields the three-term recursion relation

$$(2n-1)\langle R_\infty^{2n-2}\rangle+12n\langle R_\infty^{2n}\rangle+(2n+1)\langle R_\infty^{2n+2}\rangle+\mathcal{O}(\langle\delta^2\rangle)=0. \tag{4.6}$$

Solving this equation numerically we find that $\langle R_\infty^2\rangle$ converges quickly to $0.0861068...+\mathcal{O}(\langle\delta^2\rangle)$. It does not become zero in the limit of zero disorder as it does at neighbouring irrational points. Hence, substituting this value into equation (2.8) the complex Lyapunov exponent at the band centre takes the form

$$-\gamma(E=0)+\mathrm{i}\pi N(E=0)=-\frac{\langle\delta^2\rangle}{2.188\,44}+\mathrm{i}\pi/2 \tag{4.7}$$

to order $\langle\delta^2\rangle$. For the Anderson model this gives $\gamma(E=0)=W^2/105.045$ in exact agreement with the published results for this anomaly (Czycholl *et al* 1981, Kappus and Wegner 1981, Kirkmann and Pendry 1984a,b, Derrida and Gardner 1984)

5. Conclusion

In this paper we have presented a new method for calculating the localization length and density of states of disordered one-dimensional chains which we feel makes a useful contribution to this field. The method uses an expansion for the complex Lyapunov exponent in terms of the stationary moments of the reflection coefficient. It has a simple conceptual basis in multiple-scattering theory. For continuous distributions of disorder our method is exact and highly convergent. For discrete distributions such as the binary alloy the method has good convergence away from singular points in the band. At or near these points, however, the structure and weight of the singularities is approximated.

We look at the weak disorder limit of the tight-binding model and show how simple first-order perturbation theory applied to the reflection transfer matrix demonstrates the existence of anomalies in the complex Lyapunov exponent at all points in the band where the wavevector is rationally related to π. In particular we retrieve the band centre anomaly.

Finally, we mention that it is possible to consider our method for any dimension since it is easy to translate equations (2.1), (2.2), (2.5) to higher dimensions.

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