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Reflection of waves from disordered surfaces

J B Pendry and C Barnes

The Blackett Laboratory, Imperial College, London SW7 2BZ, UK

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Abstract. The transmission of waves through disordered media has received much attention in the context of electrical conduction, and numerous techniques have been brought to bear on the problem. Here we focus on the reflection coefficient, a closely related quantity. The change in reflectivity on adding a new element to a disordered chain can be calculated by a recursion formula. This in turn suggests a novel formulation of the problem in terms of transfer matrices. These new matrices can be calculated explicitly and, although in principle of infinite dimensions, can be approximated by a truncated form. Using this tool we show how some problems can be solved exactly and how an accurate perturbation expansion can be made for others.

1. Introduction

The general question of wave motion in disordered media is a difficult one which has not been fully resolved. The crucial point that emerges in these systems is that fluctuations in quantities, such as the transmission coefficient, grow without bound as the sample becomes longer, in contrast to simpler problems in disorder where increasing size brings with it better behaved statistics. Where waves are concerned statistics are always with us.

The reflection coefficient offers prospects of a somewhat more tractable quantity. We expect that for a very thick sample waves will be reflected from the surface with nearly 100% probability, which leaves only the question of with what phase they are reflected. We shall show that for a simple one-dimensional model of a surface both numerical and analytical work confirms this to be the case. The distribution of phases converges to a limit with increasing length of sample. Somewhat paradoxically, this distribution grows broader as the disorder is decreased.

Our analytical approach to the problem is a novel one which contrasts with other approaches in its simplicity. We have succeeded in finding a generalised transfer matrix for the reflection coefficient of a disordered medium. The matrix, though infinite, can be approximated by a finite truncation, and is amenable to perturbative treatments, and in some cases to analytical solution.

Previous work has concentrated on the problem of electrical conduction (Landauer 1957, 1970, Anderson 1958, Anderson *et al* 1980, Thouless 1972) which has to do with the transmission coefficient of the disordered sample. Progress has been seen in analytical work (Imry 1986, Pichard 1986, Pichard and Sarma 1981a, b), the invariant embedding method (Bellman and Wing 1975), and in numerical simulations (Mac-Kinnon and Kramer 1981, 1983). We have developed the transfer matrix approach



Figure 1. A region of disordered material partly reflects an incident wave.

(Kirkman and Pendry 1984a, b, Pendry 1982a, b, c, 1984, 1986, 1987, Pendry and Kirkman 1984, 1986, Pendry *et al* 1986, Pendry and Castaño 1988a, b, Slevin and Pendry 1988).

First we assume a one-dimensional system which consists of two ordered regions sandwiching a region of disorder; figure 1 shows what we have in mind. We suppose that we can further decompose the disordered region into statistically independent units. For example, in the electron case these units might be atoms in a substitutionally disordered alloy. In the case of sound waves in a rod they might be randomly placed imperfections in the rod. Each of these units is in turn characterised by a reflection and transmission coefficient, as shown in figure 2. This is the simplest formulation of the problem we can



Figure 2. A single unit of impurity partly reflects an incident wave.

make. All manner of embellishments may be imagined, but the model already contains the essence of the problem and presents a major challenge to theorists. A review of 1D work can be found in Erdos and Herndon (1982). Related work on the reflection coefficient can be found in Heinrichs (1988), Lambert and Thorpe (1982), Stone *et al* (1983), Sulem (1973).

In earlier studies of waves in disordered media, transfer matrices have played an important role. The transfer matrix is a function only of the reflection and transmission coefficients of the system and has the property that it is the ordered product of the individual transfer matrices for the component units:

$$\mathbf{M}_L = \prod_{n=1}^L m_n. \tag{1}$$

This linear relationship offers a tremendous advantage in that, for a system of statistically independent units, \mathbf{M}_L can be averaged exactly simply by averaging the individual components. The problem is that in its elementary form the transfer matrix contains functions of R and T that are not closely related to observable. It was the achievement of our earlier work to generalise \mathbf{M}_L to contain more relevant functions of R and T.

In this work we seek a transfer matrix for the reflection coefficient and have been lucky enough to find one which takes a simple form. In contrast with the conventional transfer matrix, the new transfer matrix is a function only of R, not of T. We derive it as follows.

Suppose we have a system comprising *n* random units, reflection coefficients R_n . We now put in place the (n + 1)th random unit and ask what is the new R_{n+1} . We obtain a

simple expression by summing the multiple scattering between the new unit and the old units:

$$R_{n+1} = r_{n+1} + t_{n+1}R_n t_{n+1} + t_{n+1}R_n r_{n+1}R_n t_{n+1} \dots$$

+ $t_{n+1}(R_n r_{n+1})^s R_n(t_{n+1} + \dots$
= $r_{n+1} + t_{n+1}R_n t_{n+1}/(1 - r_{n+1}R_n)$ (2)

where we have assumed for simplicity that the transmission coefficient of the unit is symmetrical. In our quest for a transfer matrix it is the series that interests us, not the closed expression for the sum. It is essentially a series in powers of R_n :

$$R_{n+1} = r_{n+1}R_n^0 + t_{n+1}^2R_n^1 + t_{n+1}^2r_{n+1}^1R_n^2 + \ldots + t_{n+1}^2r_{n+1}^{s-1}R_n^{s+1} + \ldots$$
(3)

Define a vector whose elements comprise all the powers of R_n :

$$v_n = [R_n^1, R_n^2, R_n^3, R_n^4, R_n^5 \dots]$$
(4)

then we can write equation (2) in matrix form:

$$\boldsymbol{v}_{n+1} = \boldsymbol{m}_{n+1} \boldsymbol{v}_n. \tag{5}$$

where m_n is our new transfer matrix,

It has the fundamental property of the old transfer matrix

. .

$$\mathbf{M}_{L} = \prod_{n=1}^{L} m_{n} \tag{7}$$

and

Thus we can average any power of R_L using the result

$$\langle \boldsymbol{M}_L \rangle = \prod_{n=1}^L \langle \boldsymbol{m}_n \rangle = \langle \boldsymbol{m}_1 \rangle^L \tag{9}$$

provided that all the units are independently distributed according to the same statistics.

These transfer matrices have infinite dimensions, but we shall show that truncating to finite dimensions in a systematic manner will enable us to calculate quantities of interest to the desired accuracy.

In the long length limit when R nearly always has modulus unity,

$$R_L = |R_L| \exp(i\Theta_L) = \exp(i\Theta_L).$$
⁽¹⁰⁾

Then because we can calculate

$$\langle R_L^N \rangle = \langle \exp(iN\Theta) \rangle = \int \exp(iN\Theta) P(\Theta) \,\mathrm{d}\Theta$$
 (11)

we have the Fourier transform of $P(\Theta)$, from which we can reconstruct $P(\Theta)$ itself.

Obviously $\langle m_n \rangle$ is required to have eigenvalues

$$|\mathbf{e}_i| \le 1. \tag{12}$$

We can see from equation (8) that there is always one eigenvalue

$$e_0 = 1 \tag{13}$$

corresponding to a left-hand eigenvector of

$$v_0^1 = [1, 0, 0, 0, \dots]. \tag{14}$$

This eigenvalue gives the asymptotic behaviour of the system. Although at first sight this would appear to give asymptotic properties independent of the details of the disorder, this is not the case, because the right-hand eigenvector v_0^r , corresponding to e_0 is more complex and involves details of the distribution:

$$\langle R_L^N \rangle = (v_0^1)_N e_0^L (v_0^1)_0.$$
 (15)

2. Derivation of the full transfer matrix

Having defined our new transfer matrix and indicated the form which it takes, we need to give a prescription for its construction. We start from the recursion formula

$$R_{n+1} = r + t^2 R_n / (1 - rR_n)$$
(16)

where we have written r and t in place of r_{n+1} and t_{n+1} for clarity. Raising each side of equation (16) to the *i*th power gives

$$(R_{n+1})^{i} = [r + t^{2}R_{n}/(1 - rR_{n})]^{i}$$
(17)

which may be expanded binomially:

$$R_{n+1}^{i} = r^{i} + \sum_{j=1}^{\infty} (c)_{i,j} R_{n}^{j}$$
(18)

where

$$(c)_{i,j} = \sum_{k=1}^{\min(i,j)} \frac{i!(j-1)!}{(i-k)!k!(k-1)!(j-k)!} r^{i+j} (t^2/r^2)^k.$$
(19)

This series converges under all physical circumstances because of the unitarity condition

$$|rR_n| \le 1. \tag{20}$$

Hence we can find the general element of m_n :

$$(\boldsymbol{m}_{n})_{0,j} = \delta_{0j}$$

$$(\boldsymbol{m}_{n})_{i,0} = \delta_{i0}r^{i}$$

$$(\boldsymbol{m}_{n})_{i,j} = \sum_{k=1}^{\min(i,j)} \frac{i!(j-1)!}{(i-k)!k!(k-1)!(j-k)!} r^{i+j}(t^{2}/r^{2})^{k}.$$
(21)

3. Solutions for special cases

Suppose we have a binary distribution of units in the disordered region such that unit 1 is identical with those occurring in the ordered regions, and further suppose that for this unit the energy is such that

$$t = -1 \qquad t^2 = 1$$

then the transfer matrix for unit 1 is the unit matrix, which commutes with the transfer matrix for unit 2. Thus for a system with x unit 2s and L - x unit 1s in the disordered region, the reflection coefficient is that of a single continuous slab of x unit 2s and can be calculated by conventional means of matching Bloch waves. The probability distribution of reflectivities is given simply by the statistical probability of finding x unit 2s in the disordered region. In the limit of a large system there will always be a large number of unit 2s and the distribution of reflection coefficients will converge on a single value of the reflection coefficient.

The same result holds as in the case for unit 1:

$$t = +1$$
 $t^2 = 1.$ (22)

For our second example take unit 1 to be identical with the units in the ordered regions. Therefore once more its reflection coefficient is zero, but now we allow its transmission coefficient to have a phase

$$t_1 = \exp(i\alpha) \qquad r_1 = 0. \tag{23}$$

Unit 2 is taken to have unit reflection coefficient

$$t_2 = 0 \qquad r_2 = \exp(i\beta)$$

so that on constructing m_1 and m_2 we find

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If unit 1 and unit 2 occur with probabilities P_1 and P_2 respectively, then

Intuitively we can see what the result must be: the wave travels into the disordered region passing through all unit 1s, let us say x of them, until it meets a unit 2 and is then reflected. The total reflection coefficient is zero unless the wave meets a unit 2, otherwise it takes the value

$$R(x) = \exp(2i\alpha x + i\beta)$$

It only remains to calculate the probability of encountering x unit 1s before a unit 2, which can be done from simple statistics:

$$P(x) = P_2(1 - P_2)^x = P_2 P_1^x \qquad x \le L.$$
(27)

The probability of zero reflection coefficient is

$$P_0 = P_1^L. (28)$$

In the limit of $L = \infty$ this gives for the moments

$$\langle R_{\infty}^{N} \rangle = P_{2} \sum_{x=0} P_{1}^{x} \exp(2Ni\alpha x + Ni\beta)$$

= $P_{2} \exp(Ni\beta) / (1 - P_{1} \exp(2Ni\alpha)).$ (29)

Alternatively we can diagonalise $\langle m \rangle$ and verify that the moments of R which we obtain are consistent with this probability distribution. The right-hand eigenvector of $\langle m \rangle$ corresponding to unit eigenvalue is by inspection

$$\boldsymbol{v}_0^r = [1 \dots P_2 \exp(si\beta) / (1 - P_1 \exp(2si\alpha)) \dots].$$
(30)

Therefore in the long-length limit, from the e = 1 eigenvector of $\langle m \rangle$,

$$\langle R_{\infty}^{N} \rangle = P_{2} \exp(Ni\beta) / (1 - P_{1} \exp(2Ni\alpha))$$
(31)

which agrees with equation (29).

4. Perturbation theory

In this section we show that our new transfer matrix can be treated by perturbation theory in the weak scattering limit. For simplicity we consider the discrete model of disordered systems described by an Anderson Hamiltonian with diagonal disorder only:

$$V\varphi_{n+1} + V\varphi_{n-1} + \varepsilon_n \varphi_n = E\varphi_n. \tag{32}$$

This is the tight-binding approximation with one orbital per site, nearest-neighbour hopping assumed constant independent of site and two-centre integrals V only. φ_n represents the amplitude of the orbital on the *n*th site in the total wave function, ε_n the site energy of the orbital at the *n*th position and E the energy of the wave incident from the perfect leads. In the leads

$$\varepsilon_n = 0$$
 (33)

$$E = 2V\cos(k)$$
 $k = [0, \pi].$ (34)

For these systems we derive the reflection and transmission amplitudes of individual units as

$$r_n = i\delta_n \exp(-ik)/(1 - i\delta_n) \qquad t_n = \exp(-ik)/(1 - i\delta_n)$$
(35)

where

$$\delta_n = -\varepsilon_n / (2V \sin(k)). \tag{36}$$

These obey the general requirements of unitarity and current conservation. Substituting these definitions in the recursion relation (2) for R, we get the expression

$$R_{L+1} = \frac{\exp(-ik)}{1 - i\delta_L} \left[i\delta_L + \frac{\exp(-ik)R_L}{1 - i\delta(1 + \exp(-ik)R_L)} \right].$$
(37)

In practice our equations simplify if we work with a reflection matrix with shifted phase

$$R'_L = \exp(+\mathrm{i}k)R_L.$$

Equation (6) for the transfer matrix shows that diagonal elements are of order unity, and each successive off-diagonal element contains one further power of the reflection coefficient r. Since r is first order in our small parameter δ , this means that the transfer matrix has a banded form. Each band removed by n elements from the diagonal is of order δ^n . From equation (37) we can derive the ensemble average transfer matrix $\langle m_s \rangle$ as a series in the moments of the distribution of disorder $\langle |i\delta^n| \rangle$. This series is convergent if

$$\langle \delta^n \rangle < 0.5^n. \tag{38}$$

The coefficients in this series are matrices with 2n + 1 bands. In this paper we consider symmetrical distributions of disorder only, so that $\langle m_s \rangle$ may be written in the form

$$\langle \boldsymbol{m}_{s} \rangle = \sum_{n=0}^{\infty} \langle (\mathrm{i}\delta_{s})^{2n} \rangle \boldsymbol{D}^{(n)}$$
(39)

where

$$\boldsymbol{D}_{i,j}^{(n)} = \exp(-2ikj)\mathbf{i}(2n)! \sum_{m=a}^{b} \frac{(2n+i-m-1)!}{(2n-j+i-m)!(j-i+m)!m!(n-m)!(i-m)!}$$
(40)

and

 $a = -\min(0, j - i) \qquad b = \min(2n - j + i, \min(2n, i)). \tag{41}$

The reflection coefficient and its moments can be found from equations (8) and (9). The prescription is a simple one: the transfer matrix is raised to the *L*th power by diagonalising, and then raising each of the eigenvalues to the *L*th power. Expressed more formally, we must evaluate the expression:

$$\langle R_L^{\prime n} \rangle = \sum_{p=0}^{\infty} (\boldsymbol{v}_p^{\mathrm{r}})_n \boldsymbol{e}_p^L (\boldsymbol{v}_p^{\mathrm{l}})_0$$
(42)

where $(v_p^r)_n$ is the *n*th component of the right eigenvector of $\langle m_s \rangle$ corresponding to the eigenvalue e_p , and $(v_p^1)_0$ is the zeroth component of the left eigenvector. In this paper we evaluate these eigenvectors and eigenvalues to first-order Rayleigh Schrödinger perturbation theory. We write the eigenvalue equation

$$(D^{(0)} + D')v_p^r = e_p v_p^r$$
(43)

where from equation (40)

$$\boldsymbol{D}' = \sum_{n=1}^{\infty} \langle (\mathrm{i}\delta_s)^{2n} \rangle \, \boldsymbol{D}^{(n)} \tag{44}$$

and develop the perturbation expansion in D'.

One point to note is that at certain values of the wavevector k the zeroth-order diagonal elements $\exp(-2ijk)$ have degeneracies, explicitly when

$$k = q\pi/r$$
 (q and r integer). (45)

The most extreme instance of degeneracy occurs at the band centre, where every other diagonal element is degenerate.



Figure 3. (a) Loci of the first moment of the distribution of reflected amplitudes for wavevector k between 0.52π and 0.95π , for a random substitution alloy ensemble of length 10 units and disorder parameter $\delta = 0.1$. The full curve is the first-order perturbation theory result; the broken curve is the exact numerical result. (b) Loci of the second moment of the distribution of reflected amplitudes. Other details as for (a).

When we are near a degeneracy the moments series for $\langle m_s \rangle$ is truncated at some maximum moment order,

$$n_{\max} < r/2. \tag{46}$$

This reduces the problem to non-degenerate perturbation theory, and equation (42) becomes

$$\langle R_L^{\prime n} \rangle = \sum_{p=0}^{2n_{\max}} (\boldsymbol{v}_{p0}^r)_n e_{p0}^L (\boldsymbol{v}_{p0}^1)_0.$$
(47)

The loci of the first two moments with k are shown in figure 3 for a substitutionally disordered alloy ensemble of length ten units.

A symmetrical distribution of disorder implies two simple symmetries for the moments of the distribution of reflection amplitudes. First, under the transformation $k \rightarrow -k$ the ensemble average matrix $\langle m_s \rangle \rightarrow \langle m_s \rangle^*$ and hence

$$\langle R_L^{\prime n}(k) \rangle = \langle R_L^{\prime n}(-k) \rangle^*. \tag{48}$$

Second, if we define $k' = (\pi/2) - k$ the same symmetry exists if we put $k' \rightarrow -k'$, that is:

$$R_{L}^{\prime n}[(\pi/2) + k']\rangle = \langle R_{L}^{\prime n}[(\pi/2) - k']\rangle^{*}.$$
(49)

Due to this symmetry the plots need show only one-half of the band.

The band centre, where every other zeroth-order diagonal element is degenerate, is a special case since the truncation method described above is not possible without cutting the disorder out of the problem. That is, there are only two different zeroth-order eigenvalues at the band centre and the first term in the series for $\langle m_s \rangle$ has five diagonals. Hence the condition for the approximation to be possible

$$r > 2n_{\max}$$

is not satisfied. However, if we truncate the series at the first matrix, the secular equation

is tri-diagonal and we find a non-zero limit for each moment of the distribution as the disorder tends to zero. This same anomaly was found at the band centre by Kappus and Wegner (1981) for the density of states.

Turning now to the long-length limit, we assume that the unit eigenvalue determines the asymptotic behaviour of the moments. This is borne out by direct evaluation to first order of the eigenvalues determining the form of $\langle R_L^{\prime n} \rangle$ for any small disorder. Hence

$$\langle R_L^{\prime n} \rangle = \langle \exp(\mathrm{i}n\Theta) \rangle = (U_{00}^{\mathrm{r}})_n.$$
⁽⁵⁰⁾

The negative moments may be found by taking the complex conjugate of equation (50). These moments may be used to evaluate the distribution of reflection phases in the following way. By definition:

$$\langle \exp(in\Theta) \rangle = \int_{-\pi}^{\pi} \exp(in\Theta) P(\Theta) d\Theta.$$
 (51)

If we multiply both sides of this equation by $\exp(-in\Theta')$ and sum over n from $-\infty$ to ∞ we derive the Fourier series for $P(\Theta)$ in terms of the moments $\langle \exp(in\Theta) \rangle$:

$$P(\Theta) = (1/2\pi) \sum_{n=-\infty}^{\infty} \langle \exp(in\Theta) \rangle \exp(-in\Theta).$$
(52)

We show in figure 4 plots of $P(\Theta)$ at different positions in the band including the band centre. We include only those for half the band since the symmetry gives rise in this limit to

$$P(k = (\pi/2) + k':\Theta) = P(k = (\pi/2) - k':-\Theta).$$
(53)

5. Monte Carlo calculations

From the reflection coefficient found using the recurrence relation (2), or an adaptation of it, we can calculate quantities of interest for a large random selection of chains in the ensemble, and either average them or place them in a histogram to obtain a distribution. The statistical fluctuations diminish as $1/N^{1/2}$ for average quantities and as $(B/N)^{1/2}$ for distributions, where *B* is the bin number in the histogram and *N* is the number of chains randomly chosen from the ensemble.

For a random substitutional alloy ensemble of short chains, length L, the statistical fluctuations in the moments $\langle R_L^{\prime n} \rangle$ calculated by the Monte Carlo technique are still significant, even after the number of trials exceeds the size of the ensemble. So it is faster simply to evaluate the reflection coefficient of each chain in the ensemble and calculate the moments $\langle R_L^{\prime n} \rangle$ directly. This we did by iterating relation (2) directly to the required length, with the boundary condition $R_0^{\prime} = 0$.

The distribution of reflection phases $P(\Theta)$ obeys a limit theorem, that is it converges to a given form in the limit of long chains. Practically this limit is achieved when the length of the chain is very much greater than the localisation length. Hence in principle we could find $P(\Theta)$ using the Monte Carlo technique with relation (2). Whilst undoubtedly it gives the correct form for $P(\Theta)$ this technique is not practical in the weak-disorder limit, where we have done our perturbation theory, for a combination of two reasons. Firstly, the distributions are almost flat, meaning that we have to look at a very large number of chains in the ensemble in order to iron out the fluctuations introduced by the Monte



Figure 4. Distribution of the reflection phases for a random substitutional alloy ensemble in the long-length limit with disorder parameter $\delta = 0.1$. The full curve is the first-order perturbation theory result, the crossed line is the Monte Carlo numerical result for 10^9 data points for (a) $k = \pi/8$; (b) $k = \pi/4$; (c) $k = 3\pi/8$; (d) $k = \pi/2$.

Carlo technique. Secondly, the localisation length is large and hence each chain must be made very long.

Instead we assume that the limiting distribution may be found by taking an arbitrary section of chain which has a pure phase reflection amplitude and randomly adding units of either type to it, placing successive phases in a histogram. An iterative relation for such a system may be derived from equation (2) by assuming |R'| = 1:

$$t_{L+1} = 2\delta_{L+1} + (t_L - \tau)/(1 + t_L \tau)$$
(54)

where

$$t_L = \tan(\Theta_L/2) \qquad \tau = \tan k. \tag{55}$$

By running very long simulations using the first technique and comparing them with results from iterating (54), we have been able to satisfy ourselves that the assumptions above are justified and that in fact the statistics are even improved.

6. Conclusions

We have developed a new transfer matrix applicable to calculation of the reflection coefficient of a disordered system. The matrix has a simple form and can be applied either to analytical or to numerical studies. We give examples of each type of application and show the accuracy of the method by comparison with numerical simulations.

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