ELECTRON LOCALISATION IN 1 DIMENSION

By

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ABSTRACT

Various models of a disordered chain of atoms are presented for noninteracting electrons at zero temperature. Localisation of the electrons occurs in all but a few pathological cases giving rise to electrical resistance. The problem of calculating physically important quantities is complicated by the fact that the distribution of resistance gets broader as the length of chain increases making a full treatment of the statistics essential. The state of existing knowledge of the system is presented, paying particular attention to exact results and promising analytical techniques.

The approach of using direct products of transfer matrices to calculate any integral power of the resistance $\langle R^N \rangle$ is presented in detail. In limiting cases sufficient information can be extracted from these quantities to find the distribution of resistance P(R) and thence physically important quantities such as $\langle \ln R \rangle$ and $\langle R^{-1} \rangle$ are obtained.

Numerical investigation of the form of $\langle R^N \rangle$ in some cases of general disorder shows that the first 10 or 15 moments, which we can calculate, contain insufficient information to permit a reliable calculation of $\langle R^{-1} \rangle$ or $\langle \ln R \rangle$.

The problem is ultimately solved by generalising the transfer matrix expression for $\langle R^N \rangle$ to all N, not necessarily real or positive. In fact I define R as proportional to $|t|^{-2}$ where t is the amplitude transmission coefficient of the chain and am able to

calculate $\langle t^x \rangle$ and $\langle |t|^x \rangle$. The former quantity is used to extract $\langle \ln R \rangle$ and the density of states, the latter to obtain the conductance and its moments. The expressions involve "generalised transfer matrices" which are of infinite dimension and are valid for all distributions of disorder and all lengths of chain. Various limiting results are obtained. A simple numerical implementation is developed and results presented for various distributions of disorder.

"In this work, when it shall be found that much
is omitted, let it not be forgotten that
much likewise is performed"

Samuel Johnson

(Preface to Dictionary)

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Synopsis

In this work I am concerned with the distribution of electrical resistance, P(R), and averages of physical quantities, for a disordered 1D chain. Following the review of previous work in Chapter I, an averaging technique based on taking direct products of transfer matrices is presented in Chapter II which gives $\langle R^N \rangle$ for N = 0, 1, 2 --- ∞. In Chapter III I consider what may be extracted from these moments by numerical techniques, which seems a natural way to proceed but I find fundamental difficulties with this approach. The main advances of this work are presented in Chapters IV and V where the techniques of Chapter II are extended by analytic continuation in the variable N. This is a difficult task for any case but it is easier to obtain $\langle \ln R \rangle$ and the density of states as is done in Chapter IV than the averaged conductance which is treated in Chapter V.

I. REVIEW

1. Introduction

The propagation of waves in 1D disordered systems has been the subject of much interest, particularly in the case of electrons on chains of atoms. Reviews in this field include Erdos and Herndon (1982), Thouless (1979), Ishii (1973) and Lieb and Mattis (1966). The motivation is that wave propagation is at the heart of many fundamental quantities of solid state physics, for example the density of states, the spread of the eigenfunctions, and the conductivity. In a disordered system we must consider the distribution of all these quantities in an ensemble of different chains whose composition is described statistically.

In the next section I present models of disorder in 1D for which the Schrodinger equation reduces to a 2x2 transfer matrix equation which relates the wave function at the n+1th site to that at the nth site through the properties of the atom at site n. We may imagine, for example, that the disordered section of length L is connected to infinite ordered sections at each end. This defines boundary conditions which enables the density of states to be defined. Alternatively, if a current emerges from the disordered section into an ordered section we can solve the Schrodinger equation (in principle) to find the wave function in the other ordered section and deduce the resistance. The precise definition of resistance chosen varies from author to author and is

often a compromise between physical reality and what is easily calculated. I defer the discussion of what is physically correct until section 7 but the two most reasonable possibilities are

$$R = \frac{\pi\hbar}{e^2}\,|t|^{-2} \quad \text{or} \quad R = \frac{\pi\hbar}{e^2}\,\frac{|r|^2}{|t|^2} \qquad (1)$$

where r, t are the amplitude reflection and transmission coefficients for the disordered section. The remarks of this chapter will apply to either definition if not otherwise specified.

Early work (Mott and Twose 1961, Borland 1963, Casher and Lebowitz 1971) showed that in 1D the average resistance of the chain, $\langle R \rangle$, scales exponentially in the length

$$\langle R \rangle \propto \exp[\alpha L] \qquad (2)$$

and that this phenomenon occurs due to the fact that all eigenfunctions are 'localised' in a given region in the sense that the wavefunction decays exponentially away from that region. However it is only comparatively recently that the importance of the distribution of resistance, P(R), has been appreciated.

Pendry (1982) and Erdos and Herndon (1982) showed that the average deviation of R from its mean grows exponentially with the length of the chain which means that $\langle R \rangle$ is not typical of the distribution P(R). This contrasts with thermodynamic quantities whose distributions get narrower as the size of the

system increases and has the important physical consequence that

$$\langle R^{-1} \rangle \neq \langle R \rangle^{-1}$$

$$\langle \ln R \rangle \neq \ln \langle R \rangle \qquad (3)$$

etc.

The problem of obtaining information about P(R) or alternatively finding averages of the conductance, density of states, and extent of eigenfunctions, given the distribution of disorder is extremely complex. In later chapters the problem is solved in a fairly general manner by developing the method based on taking direct products of transfer matrices which is described in detail in Chapter 2. In the present chapter I review various other techniques which have shed some light on these questions.

A major simplification to the problem occurs for ln R and the density of states, $\varrho(E)$. This is that

$$\frac{\ln R}{L} \quad \text{and} \quad \frac{\varrho(E)}{L} \qquad (4)$$

calculated for any given chain converge to the ensemble average value for long lengths of chain. That is to say that these quantities self average.

The justification for saying this lies in theorems which show that these quantities obey the central limit theorem and which state that they are asymptotically log normally distributed for large lengths. It is pointed out that these theorems are sufficiently weak that the averages of R, R^{-1}, and ln R are not consistent with a log normal distribution even for very long lengths.

Naturally we cannot be content with these general descriptions of the system, we must be able to calculate the physical quantities. Only in this way, when the models are made more realistic, will rigorous contact with experiment be made.

It is instructive to divide the discussion into those techniques which rely on the self averaging result and those which do not. It is clear that the self averaging technique, whilst permitting great simplification for those quantities for which it applies, is intrinsically limited, since it does not apply to the powers of resistance and conductance, and so will never solve the full problem.

The final section contains a brief review of the application of the theory of 1D localisation to experiment and indicates some of the remaining challenges in the field which are outside the scope of the rest of this work.

2. Models of Disorder in 1D

Introduction of disorder into an otherwise trivial Hamiltonian generates the completely new physical effect of localisation and

prevents analysis in anything like the degree of completeness which has been achieved in the ordered case. In this work I will be concerned with improving our understanding of this effect so, in common with many authors, I have chosen very simple models which leave out many possible terms in the Hamiltonian due to effects such as electron-electron interaction, electron-phonon interaction, electric fields magnetic fields. There is a great deal of interest in including all these effects but naturally less can be achieved in these areas.

The model I consider most is the tight binding model with one orbital per site. The Schrodinger equation reduces to

$$E\, a_n = E_n\, a_n + V_n\, a_{n+1} + V_{n-1}\, a_{n-1} \qquad (5)$$

where a_n is the amplitude of the wave function on the n th site, E_n is the site energy, V_n is the hopping integral, and E is the energy of the electron. Disorder in the E_ns is referred to as diagonal, whereas disorder in the V_ns is off diagonal. In later chapters I mostly treat the case of purely diagonal disorder where the E_ns are independent random variables with a given probability distribution. Some results for mixed off diagonal and diagonal disorder according to independent distributions are presented in Chapter 2. We will often use the fact that the Hamiltonian can be written in transfer matrix form

$$\begin{pmatrix} a_{n+1} \\ a_n \end{pmatrix} = M_n \begin{pmatrix} a_n \\ a_{n-1} \end{pmatrix}$$

$$\text{where} \quad M_n = \begin{pmatrix} (E - E_n)/V_n & , & -V_{n-1}/V_n \\ 1 & , & 0 \end{pmatrix} \qquad (6)$$

The wavefunction on the Lth site of a given chain can be found if a_0 and a_{-1} are specified

$$\begin{pmatrix} a_L \\ a_{L-1} \end{pmatrix} = \prod_{i=1}^{L} M_i \begin{pmatrix} a_0 \\ a_{-1} \end{pmatrix} \qquad (7)$$

from which the transmission and reflection coefficients of the chain can be deduced and hence the resistance of the chain is obtained through (1).

The other model considered is that of electrons on a chain of localised random potentials. This model is discussed extensively by Erdos and Herndon (1982) and is illustrated in Fig. 1.

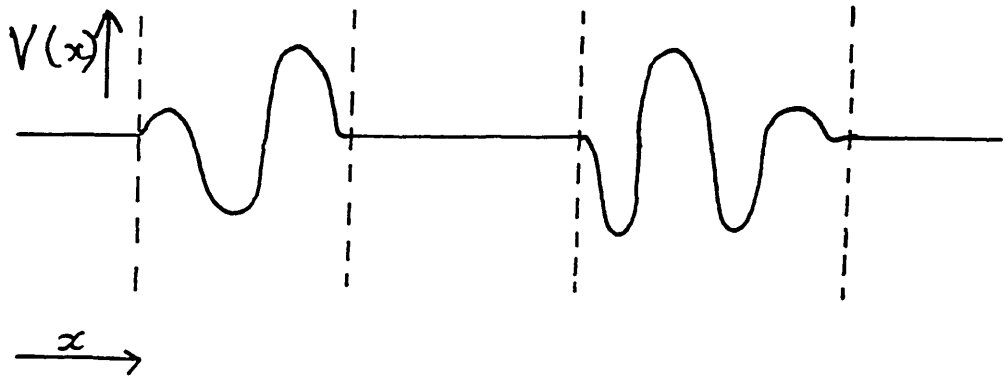


Figure 1

The wave function between the potentials is a linear combination of waves travelling forwards and backwards, $e^{\pm ikx}$, and the amplitudes at one side of the scatterer are related to those on the other side by a transfer matrix. Denoting wavefunction in the nth interpotential region by ψ_n we have

$$\psi_n = A_n e^{ikx} + B_n e^{-ikx}$$

$$\psi_{n+1} = A_{n+1} e^{ikx} + B_{n+1} e^{-ikx}$$

where $$k = \frac{\sqrt{2mE}}{\hbar}$$

and $$\begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = T_n \begin{pmatrix} A_n \\ B_n \end{pmatrix} \qquad (8)$$

The transfer matrix, T_n, depends on the form of the potentials but has the following general form

$$T = \begin{pmatrix} 1/t & r/t \\ (r/t)^* & 1/t^* \end{pmatrix} \qquad (9)$$

where $$|r|^2 + |t|^2 = 1$$

Thus T depends on at most three real parameters. If the potential has a line of symmetry, e.g. Fig. 2,

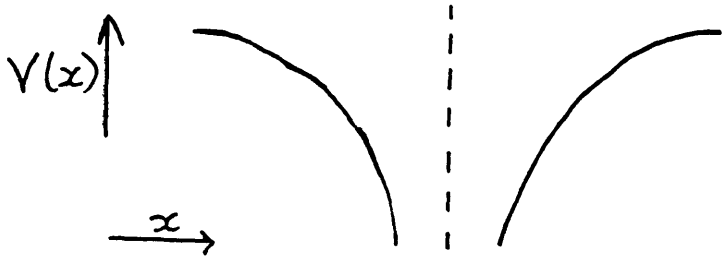


Figure 2

and spacing is regular along the chain, the transfer matrix is a function of only two parameters. A specific model is obtained by

specifying the distributions of potential positions and shapes and deriving a joint distribution function for the parameters of T. A common choice for the potentials is delta functions of random weights and/or positions and is known as the Kronig Penney model.

As in the case of the tight binding model, the wavefunction on the Lth site can be related to the wave function on the first site

$$\begin{pmatrix} A_L \\ B_L \end{pmatrix} = \prod_{i=1}^{L} T_i \begin{pmatrix} A_0 \\ B_0 \end{pmatrix} \tag{10}$$

Since we are working in a wave basis we can obtain expressions for t^{-1} and rt^{-1} for the chain directly.

$$t^{-1} = (1, 0) \prod_{i=1}^{L} T_i \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{11}$$

$$rt^{-1} = (1, 0) \prod_{i=1}^{L} T_i \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{12}$$

Thus the resistance can be calculated for either definition (1).

It is a simple matter to transform the transfer eqn. (6) for the tight binding Hamiltonian to a wave basis where the transfer matrix, $T_n \equiv T\ (E_n, V_n, V_{n-1})$, has the same form as (9) so equations (11) and (12) apply. For this reason the mathematics of the models is very similar and although I do most work on the

tight binding model the formalism can easily be applied to the disordered potential model.

It is interesting to notice that the mathematics of these models can be applied quite directly to a wide variety of cases in which a wave propagates in a disordered 1D medium. The waves can be electromagnetic, acoustic, or water (see e.g. Azbel 1982). Indeed in many cases the models may apply better to these cases since the complications we have decided to ignore in the electronic case are not present.

A model which has attracted much attention is that of a frictionless chain of masses connected by springs. Eqn. (6) applies where a_n are the displacements of the masses and M_n becomes

$$M_n = \begin{pmatrix} \frac{2k_n - m_n\omega^2}{k_n} & -\frac{k_{n-1}}{k_n} \\ 1 & 0 \end{pmatrix} \qquad (13)$$

where m_n is the mass and k_n is the spring constant. I include work on this problem in the review.

3. Limit Theorems for ln R

From eqns. (11) and (12) we see that the problem of finding the distribution of resistance in our models amounts to finding the distribution of elements in T^L where

$$T^L = \prod_{i=1}^{L} T_i \qquad (14)$$

and T_i is the site to site transfer matrix for either the disordered potential model or the tight binding model in a wave basis.

Let us consider the simpler problem of a product of L real random scalar variables

$$X = \prod_{i=1}^{L} x_i \tag{15}$$

where the x_i are chosen at random from a distribution $P(x_i)$. Taking logs we have

$$\ln X = \sum_{i=1}^{L} \ln x_i \tag{16}$$

In the limit $L \rightarrow \infty$ the usual central limit theorem applies and we have

$$\ln X = L \langle \ln x_i \rangle \tag{17}$$

and it is often stated that (LnX)/L is asymptotically log normally distributed.

In the case of a product of random matrices as in eqn. (14) the mathematics is much more complicated but similar theorems do exist. Most recently these theorems were applied by Johnston and Kunz (1983) to show that, for the tight binding model at least, every element of T^L satisfies

$$\lim_{L\to\infty} \frac{\ln |T_{ij}^{L}|}{L} - \gamma = 0 \quad , \quad i,j = 1,2 \qquad (18)$$

where γ is strictly positive and is known as the Lyapunov exponent. The theorems also state that the modulus of every element of T^L is asymptotically log normally distributed about γL. The problem was treated in its most abstract form by Furstenberg (1963), Oseledec VI (1968), Tutubalin (1968). O'Connor (1975) applied these theorems to the disordered harmonic chain. One of the problems associated with the application of these theorems is to show that matrices of the type T_i are of a form covered by the theorems. This was shown to be the case for the tight binding model by Johnston and Kunz and it is doubtless also the case for the disordered potential model.

A "physicist's argument" which leads to the same conclusion (18) as the abstract mathematical arguments was given by Anderson, Thouless, Abrahams and Fischer (1980) but relies on an assumption that the phase of the wavefunction becomes uniformly distributed for long lengths. Lambert and Thorpe (1982) have criticised this assumption but phase randomisation is not an explicit requirement of the mathematical theories so the conclusions are unaffected. The theorems have been demonstrated to hold in numerical simulations by Andereck and Abrahams (1980).

Clearly a considerable insight into the distribution, P(R), is obtained through these theorems although they provide no method for calculating the two parameters which determine the log normal distribution, $\langle \ln R \rangle$ and $\langle (\ln R)^2 \rangle - \langle \ln R \rangle^2$.

Apart from this obvious short comming there has been a tendency in some quarters to consider the problem of 1D localisation to be solved, at least in the long length limit, since the theorems tend to give the impression that P(R) is known exactly. The precise meaning of the statement "each element of T^L is asymptotically log normally distributed for large lengths" is lost in the obscure formalism of the mathematical papers and is not treated thoroughly in the physical ones which use the mathematical result. The question is however very important, because if the statement were taken to mean that P(R) was exactly log normal for long lengths, one would only need to know two independent parameters of the distribution such as $\langle R \rangle$ and $\langle R^2 \rangle$ to be able to specify the distribution and thus all physically important quantities would be known.

An understanding of the limitations of these limit theorems can be obtained using the approach of Anderson et al.. Their argument is that ln R for the whole chain is derived from the sum of a large number of ln R_i for sections of chain (the section being sufficiently long that phase randomisation occurs). Thus eqn. (16) and (17) apply. The authors argue that ln R is distributed "like" a gaussian and point out the limitations under consideration. Developing their argument we may use the central limit theorem to state that ln R is asymptotically log normally distributed. (In fact the law of large numbers does not always hold and many counter examples can be constructed, however in view of Tutubalin et al.'s theorems we may take it

that it is appropriate). More precisely the law gives

$$P(x) = \left\{ 1 + A \frac{d^3}{dx^3} + B \frac{d^4}{dx^4} + \cdots \right\} \times \frac{1}{\sqrt{\pi L}\, 6} \exp\left[\frac{(x - \mu L)^2}{6^2 L} \right] \qquad (19)$$

where $x = \ln R$ and A is the largest correction term and of order $L^{-\frac{1}{2}}$. For the average powers of ln R the formula shows that

$$\langle (\ln R)^n \rangle = a_n L^n + O(L^{n-\frac{1}{2}}) \qquad (20)$$

where a_n is what would be obtained if P(x) were exactly gaussian. Thus the average powers of ln R obtained using P(x) given in (19) are the same as would be obtained from a gaussian to leading order in L. However the contribution to the average positive powers of R from each term in the expansion (19) grows exponentially with L thus it is meaningless to say that the contribution from the term in A is reduced by a factor of order $L^{-\frac{1}{2}}$ compared to the leading term. We see that when the central limit theorem applies for ln R it is sufficiently weak that the average powers of R are not gaussian like no matter how great the length of the chain. The same result applies for $\langle R^{-N} \rangle$.

In the next chapter a formalism is presented which gives expressions for all the average positive integer powers of R. In the weak disorder case the distribution is found to be log normal for large lengths in a stronger sense than is given by

the central limit theorem. That is the average powers of R do agree with the log normal form. In the strong disorder case it is shown explicitly that the average powers of R are not consistant with P(R) being log normal. For general disorder the expression for $\langle R^N \rangle$ depends on the first 2N moments of the disorder. Since one can alter these quantities over a wide range while keeping say $\langle R \rangle$ and $\langle R^2 \rangle$ fixed it seems implausible that P(R) is in general log normal in the strong sense.

To conclude one may say that although eqn. (18) holds, the central limit theorem approach leaves many questions about P(R) unanswered. There seems to be no theoretical justification for supposing the average powers of R are consistent with P(R) being log normal and results in the next chapter show that in general they are not.

4. Application of Theorems on Long Length Behaviour of ln R

The notion that $\ln |T_{ij}^L|$ is a statistically well behaved quantity was established in the previous section. A consequence of this is that $\gamma(L)$, defined for a member of the ensemble as

$$\gamma(L) = \frac{1}{2} \frac{\ln R_L}{L} \tag{21}$$

will approximate the average value in the ensemble for long enough chains. That is to say $\gamma(L)$ "self averages". Taking the long length limit of (21) we define ξ_o^{-1} as

$$\xi_o^{-1} = \frac{1}{2} \lim_{L\to\infty} \frac{\ln R_L}{L} = \frac{1}{2} \lim_{L\to\infty} \frac{\langle \ln R_L \rangle}{L} \qquad (22)$$

ξ_o is known as the localisation length and from (18) we see that it is equal to the reciprocal of the Lyapunov exponent. The important point about ξ_o is that it is a characteristic length for every chain in the ensemble, in contrast to other lengths one can define such as

$$\left[\lim_{L\to\infty} \frac{\ln \langle R \rangle}{L} \right]^{-1}$$

which have a purely statistical meaning. The localisation length is a measure of the spread of the wavefunction.

From basic statistical mechanics one would expect that the density of states per site would also self average, since it is related to thermodynamic quantities such as the specific heat. For the tight binding model the density of states per site is given by

$$\rho(E) = \frac{-1}{\pi} \frac{\partial}{\partial E} \operatorname{Im} \frac{\ln 1/t}{L} \qquad (23)$$

where the phase of t is defined to be monatonicly increasing along the chain rather than being defined in the range 0 - 2π for example. The self averaging of $\ln \frac{1}{t}$ and $\rho(E)$ are clearly

related since they are respectively related to the real and imaginary parts of $\ln \frac{1}{t}$. Thouless (1972) derived a relation between ξ_o and $\varrho(E)$ based on this

$$\xi_o^{-1} = \int \ln |E-E'| \, \varrho(E') \, dE' - \langle \ln |V| \rangle \quad (24)$$

The fact that $\varrho(E)$ and ξ_o can be found by self averaging forms the basis of some important methods of calculating these quantities.

A simple numerical technique is to interate the recurrence relation for the model eqn. (6) or (8) choosing the random variables according to a certain distribution using a random number generator. The recurrence can be executed so quickly that chain lengths of the order of 10^5 can be obtained even on micro computers. The algorithm would estimate the desired quantity, ξ_o or D(E) where

$$D(E) = \int_{-\infty}^{E} \varrho(E') \, dE' \quad (25)$$

at various intervals along the chain and therby obtain an estimate of the error. The self averaging property ensures that the error drops as the length increases so the iteration proceeds until the desired accuracy is obtained.

To find ξ_o^{-1} one can use the fact that the same limit exists for each element of T^L so any convenient basis may be used. For

the tight binding model the real space basis with a real starting vector provides a completely real recurrence relation. The estimate of ξ_o^{-1} at any length is

$$\frac{\ln |a_L|}{L} \qquad (26)$$

The method has been used by MacKinnon and Kramer (1984) though the bulk of their work is in higher dimensions. I use the method in Chapter 4.

The density of states may be found in the tight binding model using the theorem that in 1D the eigenfunction corresponding to the Nth eigenvalue (measured in ascending order) has precisely (N-1) nodes. A node is a change of sign between one site and the next when the wavefunction is real. The estimate of D(E) at any length is then

$$\frac{\text{Number of nodes}}{L} \qquad (27)$$

The node counting and self averaging ideas were combined in an analytical theory by Schmidt as long ago as (1957). His formalism is equivalent to that of Dyson (1953) but is considerably simpler. Taking the transfer equation for the tight binding model (6) and choosing a starting condition so that the amplitudes a_i are real he defines a phase ϕ_n by

$$\tan \tfrac{1}{2} \phi_n = \frac{a_{n-1}}{a_n} \tag{28}$$

Eqn. (6) implies a continuous relationship between ϕ_n and ϕ_{n+1} which can be made unique in such a way that $\phi_L(E)$ is a monatonic function of E. When

$$\phi_L(E) = 2\pi h, \quad h = 0, 1, 2 \cdots$$

the boundary condition $\psi_L = 0$ is satisfied and E is an eigenvalue. Hence by the node counting argument

$$L\, \rho(E) = \frac{1}{2\pi} \frac{\partial \phi_L}{\partial E} \tag{29}$$

When M_n is disordered he derives an expression for the probability distribution of $\phi_L(E)$, $W_L(\phi)$ which turns out to be periodic with period 2π. $W_L(\phi)$ can be simply related to $W_{L-1}(\phi)$ through the distribution of disorder

$$W_L(\phi) = F\{W_{L-1}(\phi)\} \tag{30}$$

He argues that for very long lengths $W_L(\phi)$ tends to a limit distribution $W(\phi)$ which is defined by the functional equation

$$W(\phi) = F\{W(\phi)\} \tag{31}$$

From the distribution $W(\phi)$ obtained by solving this equation the average of (29) can be found. Since $W(\phi)$ may be a highly singular function it is convenient to work in practice with its integral

$$\Omega(\phi) = \int_{-\infty}^{\phi} w(\phi')\, d\phi' \qquad (32)$$

Agacy (1964) used a numerical implementation of this technique to calculate the spectrum of normal modes for the infinite disordered chain. The method can be applied to other models with suitable extensions.

5. The Saxon Hutner Theorem

Saxon and Hutner (1949) conjectured that energies which are in the gap of both ordered chains of pure A and pure B type atoms will be in the gap of the disordered chain formed from a mixture of A and B type atoms. Their investigation was confined to the Kronig Penney Model and was not conclusive. Since there are very few completely general statements about disordered systems, the result is of some importance and the reviews of Erdos and Herndon (1982) and Lieb and Mattis (1966) gave a detailed consideration of whether the conjecture is correct. Luttinger (1951) proved the theorem for the Kronig Penney Model with random strengths of potential but perfect spatial order. The proof was extended by Hori and Matsuda (1964) to include any number of types of atom

and a wide class of model hamiltonians which can be described in the transfer matrix formalism. The Saxon Hutner theorem is found to be valid for the tight binding hamiltonian (6) with purely diagonal disorder and the conditions under which it holds in other cases were stated. Erdos and Herndon appear to have misunderstood the terms of the theorems in the paper although they are well defined in the text and consequently underestimate the conclusiveness of this work.

6. Techniques in which an Ensemble Average is made

We have seen that the localisation length and the density of states in the long length limit may be found by calculating the quantity for a single chain. This permits both analytical and numerical approaches which do not involve ensemble averaging or any detailed analysis of the distribution. However to find $\langle \ln R \rangle$ or $\langle \varrho(E) \rangle$ for finite chains, or $\langle R \rangle$ and $\langle R^{-1} \rangle$ for any length of chain including infinite, a proper average must be taken.

In the next chapter I review the powerful transfer matrix technique which permits averages to be made in a straightforward way and is the technique developed in subsequent chapters. Here I will present some other techniques.

Eqn. (24) shows that if the density of states is known for the tight binding model the localisation length can also be calculated. The density of states can be found from the diagonal elements of the Green's function operator since in the basis of

eigenstates

$$G_{ij} = \frac{\delta_{ij}}{E - \epsilon_i} \tag{33}$$

where ϵ_i is an energy eigenvalue. Thus (24) becomes

$$\xi_o^{-1} = Re \int_{-\infty}^{\epsilon} \sum_i G_{ii}(E')\, dE'$$

Thouless (1979) made an expansion of G in the case of weak diagonal disorder

$$N^{-1} \sum_i G_{ii} = N^{-1} \Big[\sum_i G^o_{ii} + \sum_{ij} G^o_{ij}\, \delta E_i\, G^o_{ji} + \sum_{ijk} G^o_{ij}\, \delta E_j\, G^o_{jk}\, \delta E_k\, G^o_{ki} \Big] \tag{34}$$

where δE_i is the departure of the ith site energy from the average value. The term in δE_i averages to zero, thus the leading contribution is proportional to $\langle \delta E_i^2 \rangle$. The final result is

$$\xi_o^{-1} = \frac{1}{2} \frac{\langle \delta E^2 \rangle}{4 - (E - \langle E \rangle)^2} \tag{35}$$

For the Lloyd model where the site energies have a lorentzian distribution and there is no off diagonal disorder, the density of states was found exactly by Lloyd (1969), and Thouless (1972) derived an expression for the localisation length.

$$\cosh \xi_0^{-1} = 4V^{-1}\left[\left\{(2V+E)^2+\gamma^2\right\}^{1/2}+\left\{(2V-E)^2+\gamma^2\right\}^{1/2}\right] \quad (36)$$

however this distribution of disorder has some very pathological properties, such as the fact that all its moments are infinite except the zeroth, which may make it a poor model of reality.

A technique due to Abou Chacra, Anderson and Thouless (1973) involved calculation of the diagonal elements of G by a self consistency equation for the distribution of self energies. The paper was mainly trying to tackle the 3D localisation problem but the theory was exact for a Bethe lattice and a 1D chain is a special case of one of these. The resulting equations were very complicated and no progress has been made on the 1D problem by this technique, none the less it could be an interesting approach.

Abrikosov and Ryzhkin (1977) studied localisation in a model where the random potential is modelled by gaussian random fields which are uncorrelated from point to point and scatter the electron either from one side of the fermi surface to the other or leave it where it is. They show that this model is equivalent to the Born approximation for scattering and Thouless and Kirkpatrick (1981) have argued that this model corresponds to the models we are considering in the weak disorder limit.

Ultimately Abrikosov (1981) obtains an expression for the probability distribution of resistance, which amounts to a complete solution of their model, and is able to extract all important quantities from it. The solution shows the exponential increase (decrease) of the resistance (conductance) with length and that the relative variation of these quantities increases exponentially with the length. The approximately log normal form of P(R) is also evident. We will refer to these results in Chapter 4.

A general technique for taking ensemble averages was developed by Kappus and Wegner (1981). The method has its origins in work by Schmidt (1957), I have already mentioned and, like the transfer matrix method, is based on taking averages of powers of the wavefunction. A phase is defined in terms of the wavefunction on successive sites which, being a scalar can be analysed more simply than the full transfer matrix equation. Applications and developments include works by Halperin (1965), Wegner (1975) and Gorkhov and Dorokhov (1976). One end of the chain is considered fixed, $\phi_0 = 0$. For any energy the probability distribution of site energies, E_n, can be converted to a distribution of ϕs

$$P(\phi_r, \phi_{r-1} \cdots \phi_1)\, d\phi_r \cdots d\phi_1 = \prod_{l=1}^{r} \left(P(E_l)\, dE_l \right) \qquad (37)$$

provided the disorder is purely diagonal.

Hence

$$P(\phi_r, \phi_{r-1} \cdots \phi_1)\, d\phi_r \cdots d\phi_1$$
$$= \prod_{l=1}^{r} \left(P(E_l)\, d\phi_l \right) \left| \frac{\partial(E_1, \cdots E_r)}{\partial(\phi_1, \cdots \phi_r)} \right| \tag{38}$$

The Jacobian takes a very simple form due to the fact that ϕ_i only depends on energies E_i less than or equal to i.

$$P(\phi_r, \phi_{r-1}, \cdots \phi_1)\, d\phi_r \cdots d\phi_1$$
$$= \prod_{l=1}^{r} P(E_l) \left| \frac{\partial E_l}{\partial \phi_l} \right| d\phi_l \tag{39}$$

This fact is precisely what is used by the transfer matrix technique of the next chapter. Kappus and Wegner develop a transfer operator for ϕ which is valid for any distribution of disorder. They succeed in finding an expression for the moments

$$\left\langle \left(\frac{a_0}{a_r} \right)^n \right\rangle \tag{40}$$

Since this is not a physical quantity they are limitted in what can be extracted. However their formulae are automatically valid for all n, not just integral. They obtain expressions for the localisation length using

$$\xi_0^{-1} = \lim_{r \to \infty} \frac{\partial}{\partial n} \left\langle \left(\frac{a_0}{a_r} \right)^n \right\rangle \tag{41}$$

and the density of states. They only analyse the weak disorder limit although their technique is exact for any disorder. In particular they discovered an anomaly in the localisation length at E = 0 which gives a departure from the Thouless result (35). The anomaly is due, in their formalism, to degeneracies amongst the eigenvalues of the integral operator which make simple perturbation theory inapplicable. I will often refer to this anomaly in later work since it provides a good check of any theory.

7. Definition of Resistance

Landauer (1970) put forward a definition of resistance based on simple physical arguments. One imagines a current j_o incident on the left of the disordered section. The particle density on the left is due to both the incident and the reflected waves

$$n_o = (j_o + j_r)/ve \qquad (42)$$

The excess electron density on the right is due to just the transmitted current, j_t

$$n_t = j_t / ve \qquad (43)$$

Using the amplitude reflection and transmission coefficients

for the whole chain we have

$$j_r = |r|^2 j_0 \quad , \quad j_t = |t|^2 j_0 \tag{44}$$

Hence

$$\delta n = n_0 - n_t = 2 \frac{|r|^2}{|t|^2} \frac{j_t}{ve} \tag{45}$$

On the other hand the density difference is related to the potential difference through

$$\delta n = \frac{dn}{dE} \delta E = \frac{dn}{dE} e \delta V \tag{46}$$

but

$$\frac{dn}{dE} = \frac{dn}{dk} \Big/ \frac{dE}{dk} = \frac{2}{\pi \hbar v} \tag{47}$$

where the factor 2 comes from spin.

Hence

$$\delta V = \frac{\pi \hbar}{e^2} \frac{|r|^2}{|t|^2} j_t \tag{48}$$

This provides a definition of resistance through Ohm's Law

$$R = \frac{\delta V}{j_t} = \frac{\pi \hbar}{e^2} \frac{|r|^2}{|t|^2} \tag{49}$$

Pendry has proposed an alternative definition. In this case we imagine two boxes of length L, which at a given instant in time are connected by the 1D resistance. The states of the electrons in the boxes which have not yet scattered off the resistance are unchanged by its presence, so we may work out the initial current incident on the resistor from the states in the boxes before the resistance is connected.

If the fermi levels of the boxes are equal, no current flows. However, if the fermi level of one of the boxes is raised by Ve, the number of states which may contribute to the current is

$$Ve \frac{dN}{dk} = Ve \frac{2L}{\pi\hbar} \frac{dk}{d\omega} \tag{50}$$

Each state contributes a current towards the resistor of

$$e \frac{d\omega}{dk} \frac{1}{2L} \tag{51}$$

so the total current incident on the resistor is

$$I = \frac{Ve^2}{\pi\hbar} \tag{52}$$

At the instant the resistor is connected the fraction of the current transmitted is $|t|^2$, thus our definition of the resistance is

$$R = \frac{V}{I} = \frac{\pi\hbar |t|^{-2}}{e^2} \tag{53}$$

The difference between the two results appears to stem from the fact that the models on which both are based are so abstract that it is not clear which "thought experiment" corresponds most closely to a real experiment. More precisely the difference comes about by assuming in the Landauer argument that the flow of the current changes the equilibrium particle densities of both reservoirs. This can only be true if there is some way for the electrons to come to equilibrium and in our model there is no such mechanism, although physically this could be achieved through electron-electron interactions. In phonon and photon systems, where non interaction of wavepackets is a much better approximation, a definition of resistance proportional to $|t|^2$ is clearly the more appropriate.

There have been attempts to derive the formulae for the definition of resistance by more formal mathematical arguments, but it is not clear whether the results obtained can claim any special relevance to physical reality. The technique used in approaches by Economou and Soukoulis (1981), Fischer and Lee (1981), Langreth and Abrahams (1981) is to apply the Kubo-Greenwood formula for the conductivity in the system of a disordered section connected to infinite ordered wires. The formula is given by

$$\sigma = \lim_{\gamma \to 0} \frac{2e^2\hbar}{\pi m_e^2} \frac{1}{L a} \times \mathrm{Tr}\left\{ p \, \mathrm{Im}\, G(E+i\gamma)\, p \, \mathrm{Im}\, G(E+i\gamma) \right\} \qquad (54)$$

and comes about through calculating the current generated by a perturbing electric field in the hamiltonian using linear expanse theory. Problems associated with the application of this technique

appear to have been resolved by the latter authors who find agreement with (49).

The two definitions presented, (49) and (53) are clearly closely related since they are both moduli of elements of the transfer matrix for the chain and Eqn. (11) and (12) show that the difference between them is purely an end effect. One would expect that theoretical techniques capable of calculating one quantity, could be applied to the other. For large resistances the definitions are equivalent, thus averages dominated by large R will be similar for either definition. This is the case for $\langle R^N \rangle$, N = 0, 1 --- and $\langle \ln R \rangle$. For the moments of the conductance the two definitions could give significantly different results but it is clear that knowledge of either quantity would contribute to our understanding of the system.

Rather than focussing on the differences between the two definitions, I prefer to focuss on how similar they are and view the Kubo Greenwood formula as giving support to the concepts used in the physical arguments rather than discriminating between them.

8. Numerical Application of the Kubo Formula for the Conductivity

I have mentioned that only the localisation length and the density of states can be found by self averaging, however the Kubo formula for the conductivity can be modified so that it does self average. The only change in definition needed is to

fix γ in (54) to some finite value rather than taking the limit as it approaches zero. This is equivalent to introducing an inelastic relaxation process with a relaxation time $\hbar/2\gamma$. MacKinnon (1980) and Thouless and Kirkpatrick (1981) used this approach to make simulations of the conductivity so defined and found that it does self average.

The models I have discussed so far do not have an inelastic relaxation time in them so the results obtained in this way are not applicable to them, on the other hand the existence of a relaxation time may well be more physically realistic. Thouless and Kirkpatrick mention that the relaxation time they have introduced is uncorrelated which may not be entirely realistic.

Both sets of authors demonstrate that results for g for various widths of disorders as a function of γ can be scaled onto a universal curve. My work, to be presented in the final chapter, shows that the conductance is sensitive to the precise form of the distribution of site energies so it is hard to see how a scaling involving just one parameter of the distribution comes about. I find that the conductance is a smooth featureless function of disorder for smooth distributions of site energies and this may be the reason behind the apparent validity of the scaling hypothesis. A more severe test of the hypothesis would be to use a chain made up of just two types of atom with equal probability since I have found that this case gives more structure.

9. Other Current Topics in 1D Localisation

In this section I will give a brief outline of some important topics in 1D localisation which are outside the scope of the later chapters but are attracting attention in the literature.

The problem of applying the theory of 1D localisation to experiment has two aspects, one is to discover a system which is effectively 1 dimensional in some regime, the other is to make appropriate additions to the model to describe effects we have so far left out, such as inelastic lifetimes, finite electric fields etc.

Thouless (1977) argued that in the absence of temperature effects, a wire of any cross section and resistance greater than $10K\Omega$ will have a resistance which scales exponentially with its length. He argued that the apparent conflict with normal experience can be resolved by considering the electron states to have a finite lifetime due to inelastic scattering. In Thouless (1981) a length, L_T, is introduced which is the distance an electron wavepacket can diffuse before inelastic scattering. It is essential that L_T be greater than the width of the wire for the behaviour to be one dimensional. In the limit where elastic scattering occurs much more rapidly than inelastic scattering L_T is given by

$$L_T = \lambda \left(\tau_i / \tau_e \right)^{1/2} \qquad (55)$$

where τ_i, τ_e are the inelastic/elastic lifetimes and λ is the mean free path.

Apel and Rice (1983) use the alternative definition

$$L_T = (l_e\, l_i)^{1/2} \qquad (56)$$

where l_e, l_i are the elastic/inelastic scattering lengths. If the length of the system is less than L_T we have

$$R = \exp\left[\frac{L}{l_e}\right] \qquad (57)$$

If the length is greater than L_T one can imagine the resistance is due to a sum of short lengths L_T

$$R = \frac{L}{L_T}\exp\left[\frac{L_T}{l_e}\right] = \frac{L}{L_T}\exp\left[\left(\frac{l_i}{l_e}\right)^{1/2}\right] \qquad (58)$$

Estimates of l_i and l_e suggest that localisation could be observed in very fine wires at low temperatures and fields. The inelastic scattering time, τ_i, can be increased by lowering the temperature, thus a manifestation of localisation will be an increase in resistance as the temperature is lowered. The observed increase in the resistance is only 2% and proportional to $T^{\frac{1}{2}}$. In Thouless' arguments, τ_i is the only temperature dependent quantity and this result suggests $\tau_i \propto T^{-1}$ which is not easy to explain as being due to electron-electron or electron-phonon interaction. In the Apel and Rice formulation both l_i and l_e are functions of temperature which depend on the electron-electron coupling constant.

They argue that if the electron-electron coupling is sufficiently strong, no effect of the localisation will be seen even at low temperatures.

Other 1D systems include polymer chains but it seems that interest is mainly focussed on other effects such as charge density waves and solitons.

Azbel (1983) showed that for the simple models of Section 2 ln R as a function of energy has some very sharp troughs. His work used a simulation technique on individual chains of short lengths. A consequence of this may have been observed experimentally in work on mosfets by Hartstein Webb Fowler and Wainer (1983) where 1D behaviour was obtained by electric field pinching of the 2D electron gas present in normal mosfets. They find an abundance of structure in the conductance as a function of gate voltage. Gate voltage alters both the width of the channel and the fermi level. The structure is reproducible for one sample but not reproducible from sample to sample.

From the point of view of my work the fact that the behaviour is not reproducible from sample to sample is consistent with the distribution of conductances being broad but the structure as a function of energy is not found to be present in the ensemble averaged quantities. The explanation must be that the structure in ln R as a function of energy for a given chain is completely washed out when an ensemble average is taken. This effect could be examined by calculating the correlation function

$$\frac{\langle \ln R(E)\ \ln R(E+\Delta E)\rangle}{\langle (\ln R(E))^2 \rangle} \qquad (59)$$

which should be possible with some extension to the formalism to be presented.

Modern lithographic techniques used in the semiconductor industries have made it possible to construct a large number of thin self supporting filaments connecting two blocks of substrate (M.J. Kelly 1982). It is hoped that it will be possible to observe phonon localisation in these systems. Since about 100 filaments are measured in parallel it may be possible to measure an averaged conductance. I hope it will also be possible to find evidence of the breadth of the distribution.

The frequency dependence of the conductivity is also of great interest. This is especially difficult to handle because it does not depend on ballistic transport of electrons from one end of the system to the other and the current need not be the same everywhere in the chain. Thus the Kubo formula cannot be simplified in the way that was done for the DC case and more detailed knowledge of states in the disordered chain is needed to evaluate it. Abrikosov and Ryzhkin have evaluated the conductivity for their model and found

$$\sigma(\omega) = \omega^2 \ln^2 \omega \qquad (60)$$

This form is in agreement with physical arguments due to Mott (1970).

The resistance of non interacting electrons in a finite electric field has been investigated by Soukoulis, José, Economou and Ping Sheng, mainly using a simulation technique for the Kronig Penney model. The results indicate that the states become less strongly localised and decay only as a power of the length. Their formulae can at least be used to deduce the conditions under which the electric field, F, can be neglected. It is when

$$\frac{L_T |F|}{E} \ll 1 \qquad (61)$$

where E is the energy of the electron.

II. CALCULATION OF THE MOMENTS OF P(R)

1. Introduction

In Chapter 1 I reviewed some of the approaches to the problems caused by disorder in the 1 dimensional Hamiltonian. Amongst early achievements in this area were theorems which gave the forms of the long length behaviour of $\langle R \rangle$ and $\langle \ln R \rangle$ but did not give any method for evaluating the parameters in the theory. The average of ln R could be found by the methods of Schmidt (1957) or Dyson (1953), or by numerical simulation but the restriction to long lengths remains. Numerical simulation for other quantities can be very expensive in computer time since the relative fluctuation of all moments of $P(R)$ increases with length. In addition to this results were available only in some special cases of disorder e.g. weak, strong or lorentzian.

These works all left unsolved the rather fundamental theoretical problem of how to analyse the properties of systems of any length in which the disorder does not correspond to a special case or limit. This fact can probably be attributed to the apparent difficulty of the problem, an electron wave will be reflected from an obstacle and reflected back to it many times with all sorts of correlations in amplitudes and phases.

In this chapter I will discuss the use of site to site transfer matrices which propagate moments of the wavefunction along the chain. The beauty of the technique is that a simple averaging procedure can be used to obtain moments of the resistance $\langle R^N \rangle$ at integer N for any length of chain and any distri-

bution of disorder whose moments are finite. This yields a wealth of information about the system which enables some analytical results to be extracted.

My own contribution, to be presented in later chapters consists of extending these techniques to apply to all N to give $\langle R^N \rangle$ where N can take any value not necessarily integral or positive.

Contemporary with the transfer matrix approach was the paper by Kappus and Wegner (1981) described in Chapter 1. They used an integral operator, which has essentially the same averaging properties as the transfer matrices to be described, to calculate

$$\left\langle \left(\frac{a_0}{a_r} \right)^n \right\rangle$$

for the tight binding model. Their operator could readily be generalised to all N but unfortunately this does not completely solve the problem since the quantity they were averaging was not a physical one. As we have seen, their formalism is quite simple but, perhaps because of that, it is not clear how to extend it. The transfer matrix approach, on the other hand, can be developed steadily and logically to give the average positive integer powers of a physically meaningful resistance but it is less clear how to use these quantities or how to analytically continue in N.

The transfer matrix technique was used by Abrahams and Stephen (1980) to obtain $\langle R^N \rangle$ for integer N. They were able to show that the fluctuations in the resistance grow more quickly with length than the average resistance and extracted a strong disorder limit. Stone, Joannopoulous and Chadi (1981) used the technique for the first moment, $\langle R \rangle$, only.

The ingredient of symmetry reduction of the transfer matrix was added by Pendry (1982) and by Erdos and Herndon (1982). In the latter work the symmetry reduction is only accomplished for $\langle R \rangle$ and $\langle R^2 \rangle$. Although it was appreciated that extension to higher moments was possible in principle, their formalism makes this a complicated procedure. Pendry chose to define resistance in a slightly unphysical way which departs from both the physically meaningful definitions described in the introduction only when the resistance is small. The resistance so defined has the advantage that it evolves according to a single subspace of the full transfer matrix and hence a full treatment of the symmetry reduction was avoided and an explicit expression for all the average positive integer powers of this resistance was obtained. It was pointed out that the average positive integer powers of the physically meaningful definitions of resistance could be obtained by reducing the full transfer matrix by use of the symmetric group and in Chapter V I perform this reduction and obtain an explicit expression for the average positive integer powers of $|t|^{-2}$. The subspaces of the transfer matrix that I find are of the same dimensionality as those predicted by Erdos and Herndon but the formulae are simpler than would be obtained by their prescription.

The objective of this chapter is to show how Pendry's expression for $\langle R^N \rangle$ at positive integer N was obtained and to indicate the results which follow. Following that author I restrict attention to the tight binding model since this model is as realistic as any of the models under consideration and generalisation to other cases is straight forward. It is also conve-

nient to treat diagonal disorder first, since this is the case I develop in Chapters III to V, and then indicate how the results for positive integer N may be extended to include off diagonal disorder. It is widely believed that purely diagonal disorder provides a reasonably good model of reality but that purely off diagonal disorder has some unphysical features.

2. Application of Transfer Matrices to Disorder Averages

In the case of purely diagonal disorder in the tight binding hamiltonian the hopping matrix elements V_n in (I.5) are all the same and we can drop the subscript. The site to site transfer Eqn. (I.6) reduces to

$$\begin{pmatrix} a_{n+1} \\ a_n \end{pmatrix} = M_n \begin{pmatrix} a_n \\ a_{n-1} \end{pmatrix}$$

where

$$M_n = \begin{pmatrix} \Delta_n & -1 \\ 1 & 0 \end{pmatrix} \tag{1}$$

and

$$\Delta_n = \frac{E - E_n}{V}$$

Since E_n is a random variable according to some distribution independent of the site index, so is Δ_n.

The amplitude of the wavefunction at the Lth site can be found if the amplitudes a_o and a_{-1} are given.

$$\begin{pmatrix} a_L \\ a_{L-1} \end{pmatrix} = \prod_{i=1}^{L} M_i \begin{pmatrix} a_0 \\ a_{-1} \end{pmatrix} \tag{2}$$

This equation can be simply averaged due to the fact that M_i is statistically independent of the vector on which it acts. This is a key step in the transfer matrix formalism so it is worth labouring it. The wave amplitude pair (a_j, a_{j-1}) depends on (a_o, a_{-1}) and Δ_i for $i \leq j$. To find (a_{j+1}, a_j) we apply M_{j+1} which by definition depends only on Δ_{j+1} and hence is statistically independent of $(a_j\ a_{j-1})$. When the M_i are averaged in (2) each one is equal to <M>, independent of the site index. We therefore have

$$\left\langle \begin{pmatrix} a_L \\ a_{L-1} \end{pmatrix} \right\rangle = \langle M \rangle^L \begin{pmatrix} a_o \\ a_{-1} \end{pmatrix} \qquad (3)$$

This is not a directly useful result since the wave function is not an observable quantity. The definition of resistance chosen by Pendry is equal to the modulus squared of the wavefunction on the Lth site when a current of unit amplitude is flowing through the chain. Since the current is the same all the way along the chain it can be set to unity by a suitable choice of (a_o, a_{-1}) however we cannot extract the modulus squared of the wavefunction at the Lth site from (3).

If we denote

$$v_i = \begin{pmatrix} a_i \\ a_{i-1} \end{pmatrix} \qquad (4)$$

then the doubly subscripted quantity e_i may be defined as

$$e_{i\,j\,j'} = v_{ij}\, v^{*}_{ij'} = \begin{bmatrix} a_i\, a_i^{*} & , & a_i\, a_{i-1}^{*} \\ a_{i-1}\, a_i^{*} & , & a_{i-1}\, a_{i-1}^{*} \end{bmatrix} \qquad (5)$$

It is clear that the transfer equation for e_i is just

$$e_{n+1\,i\,j} = \sum_{j'=1}^{2} \sum_{i'=1}^{2} m_{n\,i\,i'}\, m_{n\,j\,j'}\, e_{n\,i'\,j'} \qquad (6)$$

where use has been made of the fact that M_n is real. This equation can be interated down the chain and averaged in the same way as (2) to give

$$\langle e_L \rangle = \chi^L e_o \qquad (7)$$

where

$$\chi_{\substack{i\ i' \\ j\ j'}} = \langle m_{ii'}\, m_{jj'} \rangle \qquad (8)$$

To calculate the resistance we need to know the matrix e_o which corresponds to unit current. One imagines that the disordered section is connected to an infinite ordered section for which $\Delta_n = \Delta_o$, n = 0, -1 --- $-\infty$. The wavefunction corresponding to a unit current going away from the disordered section towards n = $-\infty$ is

$$a_n = e^{-ikn} \tag{9}$$

where $e^{\pm ik}$ are the eigenvalues of the transfer matrix in the ordered section

$$\begin{pmatrix} \Delta_o & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} e^{\pm ik} \\ 1 \end{pmatrix} = e^{\pm ik} \begin{pmatrix} e^{\pm ik} \\ 1 \end{pmatrix}$$

$$\cos k = \frac{\Delta_o}{2} \qquad 0 < k < \pi \tag{10}$$

From (5) and (9) we have

$$e_o = \begin{pmatrix} 1 & e^{-ik} \\ e^{ik} & 1 \end{pmatrix} \tag{11}$$

We select the component of $\langle e_L \rangle$ in (7) which gives $a_L\, a_L^*$ to find

$$\langle R \rangle = \langle a_L\, a_L^* \rangle = u\, \chi^L\, e_o \tag{12}$$

where $u_{ii'} = \delta_{i1}\, \delta_{i'1} \qquad i, i' = 1, 2$

It is clear that the choice of Δ_o only affects the definition of resistance through an effect at the end of the chain. Originally the choice $\Delta_o = \langle \Delta \rangle$ was made.

In more formal language, χ is the direct product of the M_s

$$\chi = \langle M \otimes M \rangle \tag{13}$$

and e_o is a direct product of V and V* and in this language (12) becomes

$$\langle R \rangle = (1,0) \otimes (1,0) . \langle M \otimes M \rangle^L . \begin{pmatrix} 1 \\ e^{ik} \end{pmatrix} \otimes \begin{pmatrix} 1 \\ e^{-ik} \end{pmatrix} \quad (14)$$

In this notation the extension to higher powers of R is clear

$$\langle R^N \rangle = [(1,0)^{\otimes 2N}] . \langle M^{\otimes 2N} \rangle^L \times \left[\begin{pmatrix} 1 \\ e^{ik} \end{pmatrix} \otimes \begin{pmatrix} 1 \\ e^{-ik} \end{pmatrix} \right]^{\otimes N} \quad (15)$$

where $x^{\otimes r}$ means r direct products of x with itself.

This is the final result of this section. In view of the complexity of the problem being tackled, (15) is a remarkably simple equation. The disorder average is achieved simply by integrating $M^{\otimes 2N}$ over the probability distribution of site energies $P(\Delta)$. The dimension of $M^{\otimes 2N}$, in the form of a matrix with two subscripts, is 2^{2N} which grows very rapidly with increasing N.

$\langle M^{\otimes 2N} \rangle$ can be block diagonalised by symmetry considerations and the choice of projection vectors at the ends of the chain in (15) means that only one of the subspaces is significant and very greatly simplifies the problem. Erdos and Herndon chose a more physically reasonable definition of the resistance

$$R = |r\, t^{-1}|^2 \quad (16)$$

(as discussed in Section I.7) but were only able to obtain $\langle R \rangle$ and $\langle R^2 \rangle$. In the final chapter I obtain all the averages of positive integer powers of (16) and it is clear from the form of this expression that the dominant length dependence for large lengths is the same as for the definition chosen by Pendry.

3. Symmetry Reduction

The symmetry we employ holds for every chain in the ensemble we are averaging over thus the reduction can be performed before or after the average of $M^{\otimes 2N}$ is taken.

Suppose

$$V_{n\, j_1 j_2 \cdots j_{2N}} \tag{17}$$

is a vector in the space of $M^{\otimes 2N}$ which is symmetric under interchange of any pair of subscripts i.e. in the case of N=1

$$V_{n\, j_1 j_2} = V_{n\, j_2 j_1} \tag{18}$$

We form the vector at site n+1 by applying $M^{\otimes 2N}$

$$V_{n+1\, i_1 i_2 \cdots i_{2N}} = \sum_{\{j_i\}} M_{n\, i_1 j_1} M_{n\, i_2 j_2} \cdots M_{n\, i_{2N} j_{2N}} V_{j_1 j_2 \cdots j_{2N}} \tag{19}$$

Interchainging a pair of i s, for definiteness i_1 and i_2

we have

$$V_{n+1\, i_2 i_1 \cdots i_{2N}} = \sum_{\{j_i\}} M_{n\, i_2 j_1} M_{n\, i_1 j_2} \cdots M_{n\, i_{2N} j_{2N}} \times V_{n\, j_1 j_2 \cdots j_{2N}} \qquad (20)$$

which using the symmetry of V_n gives

$$V_{n+1\, i_2 i_1 \cdots i_{2N}} = \sum_{\{j_i\}} M_{n\, i_2 j_1} M_{n\, i_1 j_2} \cdots M_{n\, i_{2N} j_{2N}} \times V_{n\, j_2 j_1 \cdots j_{2N}} \qquad (21)$$

Now j_1 and j_2 on the right are just summation variables so they may be interchanged. We find

$$V_{n+1\, i_2 i_1 \cdots i_{2N}} = V_{n+1\, i_1 i_2 \cdots i_{2N}} \qquad (22)$$

The same result holds for any pair of subscripts chosen in place of i_1 i_2. We see that if V_n is symmetric under interchange of all pairs of subscripts so is V_{n+1} due to the special form of $M^{\otimes 2N}$. This means that vectors with this symmetry evolve according to a subspace of $M^{\otimes 2N}$. To exploit the symmetry we must choose a set of basis vectors in the subspace and derive an operator which gives the effect of $M^{\otimes 2N}$ on them. The set originally chosen

were $u^{J,\,2N}$ where

$$u^{J,2N}_{j_1 j_2 \cdots j_{2N}} = \left(\frac{2N!}{J!\,(2N-J)!}\right)^{1/2} \quad \text{if there are J 2s amongst the subscripts } j_1 j_2 \cdots j_{2N}$$

$$= 0 \quad \text{otherwise} \qquad (23)$$

$$J = 0, 1, \cdots 2N$$

The basis set is orthonormal, that is

$$u^{J,2N} \cdot u^{J',2N} = \delta_{JJ'} \qquad (24)$$

The symmetry reduced form for $M^{\otimes 2N}$ is an operator χ^{2N} in the space of u^J

$$\chi^{2N}_{I,J} = u^{I,2N} \cdot M^{\otimes 2N} \cdot u^{J,2N} \qquad (25)$$

or explicitly

$$\chi^{2N}_{i,j} = \langle \Delta^{i+j-2N} \rangle (-1)^j \frac{\Theta(i+j-2N)}{(i+j-2N)!} \times \left[\frac{i!}{(2N-i)!}\,\frac{j!}{(2N-j)!}\right]^{1/2} \qquad (26)$$

where the Θ function is zero for negative values of the argument and 1 otherwise.

The right projection vectors of (15) can be projected onto the symmetric vectors as follows

$$e_{oJ}^{S\,N} = u^{J,\,2N} \cdot \left[\begin{pmatrix} 1 \\ e^{ik} \end{pmatrix} \otimes \begin{pmatrix} 1 \\ e^{-ik} \end{pmatrix} \right]^{\otimes N}$$

$$= \sum_{j_+=0}^{N} {}^{N}C_{j_+}\, {}^{N}C_{j_-}\, \exp\left[i\,(j_+ - j_-)\,k \right] \qquad (27)$$

where

$$j_+ + j_- = J \qquad J = 0, 1, 2 \cdots 2N$$

and

$${}^{N}C_{r} = \frac{N!}{(N-r)!\,r!}$$

The left projection vector is simple since it is exactly equal to $u^{0,\,2N}$, that is

$$u^{0,\,2N} = (1, 0)^{\otimes 2N} \qquad (28)$$

It is due to the fact that the left projection vector is entirely within the symmetric subspace that other subspaces of $M^{\otimes 2N}$ are not required. The symmetry reduced version of (15) is therefore

$$\langle R^N \rangle = s \cdot \left(\chi^{2N}\right)^{L} \cdot e_{o}^{S,\,N} \qquad (29)$$

where $\qquad s_j = \delta_{j,0} \qquad j = 0, 1, \cdots 2N$

As we see from (25) the matrix χ^{2N} has dimension 2N+1 which for large N represents a considerable reduction from the dimension

of $M^{\otimes 2N}$ which is 2^{2N}. This yields advantages for the use of (29) analytically and makes numerical calculation of a much greater number of moments of P(R) possible.

4. Extension of Formalism to Include Off Diagonal Disorder

Only in the case of diagonal disorder does M_n take the simple form (1) in which the Δ_ns are not correlated from one site to the other. If the Vs are disordered as well as the site energies, E_n, in Eqn. I.6 it is clear that the same V_n occurs in M_n and M_{n+1} which implies a correlation between adjacent transfer matrices. This problem is solved by splitting M into a product of two statistically independent parts as was shown by Pendry (1982b)

Writing

$$\Delta_n = \frac{E - E_n}{V} \tag{30}$$

we consider a product of M_s

$$\begin{aligned} &\cdots M_{n+1} M_n M_{n-1} \cdots \\ &= \begin{pmatrix} \Delta_{n+1} V / V_{n+1} & , & -V_n / V_{n+1} \\ 1 & , & 0 \end{pmatrix} \\ &\times \begin{pmatrix} \Delta_n V / V_n & , & -V_{n-1} / V_n \\ 1 & , & 0 \end{pmatrix} \\ &\times \begin{pmatrix} \Delta_{n-1} V / V_{n-1} & , & -V_{n-2} / V_{n-1} \\ 1 & , & 0 \end{pmatrix} \end{aligned} \tag{31}$$

which can be rearranged to give

$$M_{n+1} M_n M_{n-1} = \begin{pmatrix} V V_{n+1}^{-1} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \Delta_{n+1} & -1 \\ 1 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} V V_n^{-1} & 0 \\ 0 & V^{-1} V_n \end{pmatrix} \begin{pmatrix} \Delta_n & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} V V_{n-1}^{-1} & 0 \\ 0 & V^{-1} V_{n-1} \end{pmatrix} \begin{pmatrix} \Delta_{n-1} & -1 \\ 1 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} 1 & 0 \\ 0 & V^{-1} V_{n-2} \end{pmatrix} \qquad (32)$$

Defining

$$U_n = \begin{pmatrix} V V_n^{-1} & 0 \\ 0 & V^{-1} V_n \end{pmatrix}$$

$$M_n = \begin{pmatrix} \Delta_n & -1 \\ 1 & 0 \end{pmatrix} \qquad (33)$$

and supposing that $V_L = V_0 = V$ we can form the generalisation of (15) straight away

$$\langle R^N \rangle = (1,0)^{\otimes 2N} \cdot \left(\langle M^{\otimes 2N} \rangle \cdot \langle U^{\otimes 2N} \rangle \right)^L$$

$$\times \left[\begin{pmatrix} 1 \\ e^{ik} \end{pmatrix} \otimes \begin{pmatrix} 1 \\ e^{-ik} \end{pmatrix} \right]^{\otimes 2N} \qquad (34)$$

Since M_n and U_n are statistically independent of each other. The symmetry reduction of the previous section can be applied to any operator which is the direct product of 2N 2x2 matrices, so $U^{\otimes 2N}$ can also be symmetry reduced analagously to (25) to give $U^{S,\,2N}$ given by

$$u_{ij}^{S,2N} = \left\langle \left(\frac{V_n}{V} \right)^{2i-2N} \right\rangle \delta_{ij} \qquad (35)$$

$$i, j = 0 \text{---} 2N$$

Multiplying $U^{S,2N}$ by the symmetry reduced $M^{\otimes 2N}$ given by χ^{2N} in Eqn. (26) we obtain the form for χ generalised to include off diagonal disorder

$$\chi^{2N}_{i,j} = \left\langle \left(\frac{N_n}{V}\right)^{2i-2N} \right\rangle \left\langle \Delta^{i+j-2N} \right\rangle (-1)^i \times \frac{\Theta(i+j-2N)}{(i+j-2N)!} \left[\frac{i!}{(2N-i)!} \frac{j!}{(2N-j)!}\right]^{1/2} \tag{36}$$

Expression (29) for $\langle R^N \rangle$ holds with this generalised form for χ^{2N}.

Erdos and Herndon's work was on the disordered potential model described in Section I.2. The transfer matrix Eqn.(I.9) factorises analogously to (33) into a part which depends on the two parameters describing the shape of the potential which is analogous to M_n and a part depending on a parameter which describes the asymmetry and position of the potential which is analogous to U. It is clear that an expression for all moments of P(R), $\langle R^N \rangle$, could be developed for this model and that it would closely parallel the formalism for the tightbinding model. The key features which a model must have for the formalism to be applicable reasonably directly are that the Schrodinger equation can be represented as a 2x2 transfer matrix equation where the transfer matrices are uncorrelated with each other or with their position in the chain.

5. Analytic Properties, Long Length Dependence of $<R>$ and $<R^2>$

To calculate the moments, $<R^N>$, from (29) we must diagonalise χ^{2N}. Thus we obtain

$$\langle R^N \rangle = S_o \left[\sum_{i=0}^{2N} \lambda_i^{(2N)L} | v_i^{2N} \rangle \langle v_i^{2N} | \right] e_o^{S,N} \qquad (37)$$

where $\lambda_i^{(2N)}$ are the eigenvalues and $| v_i^{2N} \rangle$, $\langle v_i^{2N} |$ are the associated right and left eigenvectors. Pendry discussed the analytic properties of these eigenvalues as a function of energy and disorder. Since R is a positive quantity the largest eigenvalue must be real and cannot collide with any other eigenvalue as a function of energy. The remaining eigenvalues are either real or complex conjugate pairs. It is possible for these eigenvalues to collide on the real axis giving rise to non analytic energy/disorder dependence for $<R^N>$. Only in the limit of weak disorder can the energies where this occurs be found explicitly. For large lengths the largest eigenvalue dominates and the moments of P(R) are asymptotically analytic.

The signature of localisation in 1D is that $<R>$ grows exponentially with the length which would correspond to the largest eigenvalue of χ^2 being greater than 1 in the present formalism. Pendry (1982) has shown that this is the case for any non zero amount of diagonal disorder when there is no off diagonal disorder with a graphical proof. For the case of pure off diagonal disorder

this result does not hold since there is at least the pathological case where

$$V_n = \pm V$$

with equal probability for the + and - signs. Since χ depends on an even power of V_n the moments of R are the same as in the ordered case.

A general result for the case of mixed off diagonal and diagonal disorder appears to be lacking. It seems obvious that the resistance must increase with the length of chain which gives

$$|\lambda^{(2)}_{max}| \geq 1 \qquad (38)$$

and I have shown that this is indeed the case with an analytical argument. It seems probable that the equality sign in (38) only holds in a few very special cases of disorder.

Next we turn to $\langle R^2 \rangle$. The theory of moments of positive definite functions gives

$$\begin{vmatrix} \langle R^0 \rangle & , & \langle R^1 \rangle \\ \langle R^1 \rangle & , & \langle R^2 \rangle \end{vmatrix} \geq 0 \qquad (39)$$

where the equality sign holds when P(R) is a delta function. Since

$\langle R^0 \rangle = 1$ we have

$$\langle R^2 \rangle \geqslant \langle R \rangle^2 \tag{40}$$

By considering the form (37) for $\langle R \rangle$ and $\langle R^2 \rangle$ we deduce

$$\lambda_{max}^{(4)} \geqslant \left(\lambda_{max}^{(2)}\right)^2 \tag{41}$$

The relative fluctuation of R is defined as

$$\frac{\left(\langle R^2 \rangle - \langle R \rangle^2\right)^{1/2}}{\langle R \rangle} \tag{42}$$

Provided the inequality sign holds in (41), as we believe it will except for when there is no disorder or in some pathological cases of off diagonal disorder, the relative fluctuation will increase exponentially with the length of the chain. This is a remarkable result. It contrasts strongly with the behaviour of thermodynamic quantities where the relative fluctuation gets smaller as the size of the system increases and is the first indication that a careful treatment of the statistics will be essential to a proper understanding of the system. The result shows that $\langle R \rangle$ is not a physically meaningful quantity for macroscopic systems since one would have to measure the resistance of a huge number of chains to calculate $\langle R \rangle$ properly. It was in anticipation of this result that we obtained an expression for all the moments of P(R) so that we can attempt to find the distribution.

6. Limiting Cases

In the case of no disorder χ^{2N} can be diagonalised analytically. Define Q^{-1} to be the matrix of eigenvectors of MU

$$Q^{-1} = \begin{pmatrix} 1 & 1 \\ e^{-ik} & e^{ik} \end{pmatrix} \tag{43}$$

then

$$\begin{pmatrix} e^{ik} & 0 \\ 0 & e^{-ik} \end{pmatrix} = Q\, m\, u\, Q^{-1} \tag{44}$$

The matrix of eigenvectors of $MU^{\otimes 2N}$ is just $(Q^{-1})^{\otimes 2N}$ and the symmetric projection may be taken as in (25) to give the eigenvectors of χ^{2N}. The zero disorder eigenvalues of χ^{2N} can be found by symmetry reducing

$$\begin{pmatrix} e^{ik} & 0 \\ 0 & e^{-ik} \end{pmatrix}^{\otimes 2N}$$

The result for the eigenvalues is

$$\lambda_j^{(2N)} = \exp[i 2kj] \cdot j = -N, -- 0, -- N \tag{45}$$

Provided these eigenvalues are not degenerate, simple perturbation theory can be applied. Degeneracy arises from two causes. Firstly the eigenvalues all lie on the unit circle so for large N they crowd together and the perturbation will eventually be large compared with their separation. Thus the perturbation

theory is always asymptotic. Secondly if

$$k = 2\pi \frac{p}{q} \qquad p, q = 0, 1, \cdots \tag{46}$$

the eigenvalues are degenerate for any N.

When there is no degeneracy amongst the eigenvalues for no disorder the eigenvalues for weak disorder may be found from the diagonal elements of the symmetric projection of

$$\left\langle \left(Q\, m_n\, u_n\, Q^{-1} \right)^{\otimes 2N} \right\rangle \tag{47}$$

where Q is chosen to minimise the perturbation. In the case of purely diagonal disorder one chooses

$$\cos k = \frac{\langle \Delta \rangle}{2} \tag{48}$$

and the perturbation may be expressed in terms of the quantity

$$\delta' = \frac{\Delta - \langle \Delta \rangle}{2 \sin k} \tag{49}$$

The largest eigenvalue is found to be

$$\lambda_{max}^{(2N)} = 1 + \langle \delta'^2 \rangle (N+1) N \tag{50}$$

The asymptotic nature of the perturbation is evident since the perturbation gets larger with increasing N. The moments of P(R) are given in this approximation by

$$\langle R^N \rangle = \exp\left[\langle \delta'^2 \rangle N(N+1)L\right] \qquad (51)$$

From this Pendry deduced the probability distribution

$$P(R) = \left[4\pi\langle\delta'^2\rangle R\right]^{-1/2} \times \exp\left[-\frac{\langle\delta'^2\rangle L}{4} - \frac{(\ln R)^2}{4\langle\delta'^2\rangle L}\right] \quad R>0$$

$$= 0 \qquad R \leq 0 \qquad (52)$$

This was a major achievement of the theory. The form of P(R) is log normal as would be expected by the limit theorems discussed in Chapter I. In fact it is more accurately log normal than those theorems predict since the moments (51) are consistent with the log normal form whereas the theorems do not prove that this will always be the case. The form of (52) is also consistent with the general comments about the width of the distribution in the previous section.

From (52) we immediately find

$$\langle \ln R \rangle = \langle \delta'^2 \rangle L \qquad (53)$$

which agrees with the result by Thouless (1979).

The average conductance can also be found but this quantity is sensitive to the definition of R since it is dominated by the very low resistance samples.

A qualitatively similar result for P(R) is obtained for weak purely off diagonal disorder. In addition to this some results for pure off diagonal disorder with $\Delta = 0$ were calculated, but as was mentioned previously these may not be of great physical importance.

The fact that this perturbation theory is inapplicable to cases where there is degeneracy in the zero disorder eigenvalues gives rise to interesting anomalies at the energies given by (46) and (48). The effect was analysed by Kappus and Wegner at the band centre and Lambert (1983) showed that this is the only anomaly to order $\langle \delta^2 \rangle$ everywhere except at the band centre.

Abrahams and Stephen derived a strong disorder limit without using any symmetry reduction. It is clear that if

$$\Delta \gg 1$$

for all atoms in the chain M is approximately scalar. Thus from (15) we can deduce that

$$\langle R^N \rangle \approx \langle \Delta^{2N} \rangle^L \qquad (54)$$

and

$$R \approx \prod_{i=1}^{L} \Delta_i^2 \qquad (55)$$

Taking the logarithm of (55) we find that ln R is the sum of independent random variables and therefore the central limit theorem may be used. The distribution of (ln R)/L tends to a gaussian

$$P(\ln R/L) \approx \left(\frac{L}{2\pi D^2}\right)^{1/2} \exp\left[-\frac{(\ln R - L\langle \ln \Delta^2\rangle)^2}{2D^2 L}\right]$$

where

$$D^2 = \langle(\ln \Delta^2)^2\rangle - \langle \ln \Delta^2\rangle^2 \qquad (56)$$

In section I.3 I showed that when the central limit theorem is obeyed by ln R the moments of P(R) are not necessarily consistent with a log normal distribution. This is shown explicitly by (56) and (54) since calculation of $\langle R^N \rangle$ from (56) gives

$$\langle R^N \rangle = f(N, \langle \ln \Delta^2 \rangle, D) \qquad (57)$$

where f is a function we do not need to determine but is the same for all P(Δ) provided the strong disorder limit applies. It is clear that by changing P(Δ) we can leave D and $\langle \ln \Delta^2 \rangle$ unchanged while changing (54) over a wide range. Thus (57) and (54) are contradictory as we should expect.

III NUMERICAL RECONSTRUCTION OF P(R) FROM ITS MOMENTS

1. Introduction

The transfer matrix formalism of the previous section has produced formulae for all the moments of the distribution of resistance, $\langle R^N \rangle$ N=0, 1 2 ---, which are valid for all disorders and all lengths. The formulae involve the χ^{2N} matrix raised to the power L, the length of the system, and evaluation of this requires diagonalisation. Only in a few limiting cases can sufficient information be extracted analytically from the χ^{2N} matrix to permit us to obtain explicit form for $\langle R^N \rangle$. Even when this is done it is not a simple matter to find a distribution function P(R) which is consistent with these moments. Numerical diagonalisation of the χ^{2N} matrices, which are real and of dimension 2N+1 will enable us to find $\langle R^N \rangle$ rather generally up to some N where restrictions of the computer force us to stop. It is natural to consider whether this information can be used to tell us anything about the physically important quantities for the system such as the conductance, $\langle \ln R \rangle$ or even P(R).

The problem of finding integrals of arbitrary functions over some positive definite distribution function is part of what is known as the Classical Moment Problem and was of great interest to mathematicians from the latter half of the nineteenth century onwards (Stieltjes, Chebyshev, Hamburger). Modern accounts are to be found in books by Akhiezer (1965) and Sohat and Tamarkin (1943). More recently the techniques have been

successfully applied to finding the density of states using the recursion method (Nex 1978, Haydock 1980) and the existence of a library of routines for this problem due to Nex greatly assisted my numerical work.

The standard techniques I will present are known to be usually difficult to implement in a numerically stable manner but in fact I will show that it is not this which limits them. The main limitation is that the form of the moments that occurs in our problem means that any practically realisable number of them contains very little information relative to the objectives mentioned. This contrasts strongly with the density of states case where 10 moments often produces good results. Only for very short chains, e.g. 10 atoms, would the techniques considered in this chapter be useful and this can in no way be considered a satisfactory conclusion to the work.

The reason for the poor performance of this approach can be understood in general terms. It is due to a very long, large R, tail on the distribution which we expect to be present from the weak disorder result. The large N moments, $\langle R^N \rangle$, are dominated by the large R dependence of P(R) and contain very little information about the small R region. In the density of states problem there is no long tail so we might expect the method to be better in that case. Clearly more quantitative arguments are required.

In view of the unsuitability of the methods of the Classical Moment Problem my treatment of them will be brief and just

enough to show up their limitations. My reason for including it is that it seems the most natural way to exploit the theory of the previous section and without the considerations of this chapter the successful techniques of subsequent chapters might seem unreasonably exotic.

2. Form of the Moments

The analytical work of the previous chapter produced two limiting forms for the moments, $\langle R^N \rangle$. For weak disorder there is Eqn. II.50 and for strong disorder Eqn. II.54

From the formula for χ^{2N} it may be seen that the bottom right hand corner of the matrix contains very large elements even in the case of weak disorder. We know that the moduli of the eigenvalues for no disorder are all 1 i.e. very much smaller than the largest elements in the matrix for large N. This presents a numerical instability which limits the number of moments we can actually calculate. An estimate of the error in an eigenvalue is

$$\Delta\lambda = \sum_{ij} |\chi_{ij}|^2 \times \text{macheps}$$

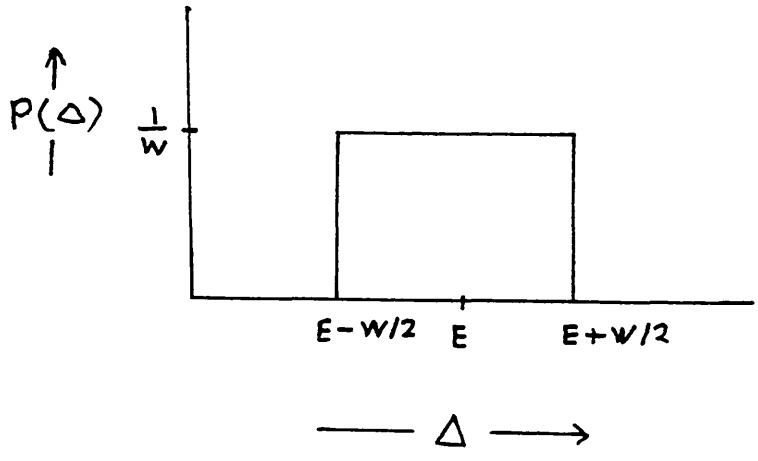
where in our case macheps is 10^{-14}. In practice this turned out to be approximately correct but slightly over cautious. The effect restricted our numerical diagonalisations to less than 20 moments and for higher moments only the larger eigenvalues are reliable. As we will see in later chapters, χ can

be transformed to a basis where it is diagonal in the case of no disorder and this may provide a more stable way of calculating the moments when there is disorder although this does have the disadvantage of making the matrix complex. In fact I find that the limitations of the subsequent processing of the moments would not be overcome if the number of moments available were increased.

The expression for the moments II.37 may be written

$$\langle R^N \rangle = \sum_{i=0}^{2N} c_i^{(2N)} \lambda_i^{(2N)\,L} \qquad (1)$$

where the $c_i^{(2N)}$ are formed from the projection of the initial and final vectors onto the eigenvectors of χ^{2N} and $\lambda_i^{(2N)}$ are the eigenvalues. Plots of $|c_i^{(2N)}|$ and $\ln|\lambda_i^{(2N)}|$ against N were obtained for the cases of diagonal disorder described by an Anderson top hat distribution as in the figure,



a gaussian distribution and the exponential distribution

$$P(\Delta) = \delta^{-1} \exp[-\Delta/\delta] \quad \Delta \geq 0$$

$$= 0 \quad , \Delta < 0 \qquad (2)$$

This last distribution is expected to show the strong disorder limiting behaviour for large δ. The results are presented in Figures 1-3. In the graphs of the cs the lines join c_is of equal i where the is are chosen to run in order of decreasing $|\lambda_i|$, i=0 being the largest eigenvalue.

The gaussian of Fig. 2 has a standard deviation of 3 which is quite strong disorder and causes the largest eigenvalue to be larger in the range plotted than that for the Anderson distribution with weaker disorder in Fig. 1. The upward curve of the largest eigenvalue in Fig. 1 suggests that for sufficiently large N it will be larger than that of Fig. 2 and a comparison of the weak and strong disorder limits also shows this effect. Fig. 3 shows the expected approximate separability of the χ matrix for large disorders since all the eigenvalues apart from the largest one can be ascribed to rounding errors.

It seems that for all the distributions we have considered the largest eigenvalue will give the dominant contribution to the moments even for quite short lengths of chain, due to the fact that the corresponding c is always of order 1 and that the next largest eigenvalue is not found to be pathologically close. In the range of N we have looked at the form of the moments can be considered to be approximately given by

$$\langle R^N \rangle = \exp[(\alpha N + \beta N^2)L]$$

$$\alpha, \beta \geq 0 \qquad (3)$$

where α and β could be determined from the largest eigenvalue. This form is supported by the weak disorder limit for all N. It should be noted that this form is not exact for any range of N and almost certainly is not very good for N well outside the range considered. The intention is merely to summarise our knowledge of the typical behaviour of the moments so that we can analyse the effectiveness of the CMP techniques on them.

3. Power Series Expansions

A technique one might think of using is to express quantities such as $(1+R)^{-1}$ and $\ln(1+R)$ as power series in R. These series can be averaged and the moments (3) substituted

$$\langle f(R) \rangle = \sum_{i=0}^{\infty} a_i \langle R^i \rangle \tag{4}$$

however for the series of interest to us these forms are not convergent.

In the same vein, we may expand the Fourier transform of P(R) in terms of the moments.

$$P(k) = \int P(R)\, e^{ikR}\, dR$$

$$= \sum_{r=0}^{\infty} \frac{\langle R^r \rangle}{r!} (ik)^r \tag{5}$$

This expansion cannot be applied for the same reason as before, it doesn't converge for moments of the form (3).

The non convergence of these expansions shows that a more subtle theory is needed so we now turn to the methods of the Classical Moment Problem.

4. Evaluation of Definite Integrals Over the Distribution Function

Given the first 2N moments, μ_0 -- μ_{2N-1} of a function $\sigma(x)$ where

$$\mu_i = \int_{-\infty}^{\infty} \sigma(x)\, x^i\, dx \qquad (6)$$

$$\sigma(x) \geq 0 \quad \text{for all } x$$

We can define a set of polynomials $P_n(x)$ n=0,1 -- N of degree n such that

$$\int_{-\infty}^{\infty} \sigma(x)\, P_i(x)\, P_j(x)\, dx = \delta_{ij}$$

$$i, j = 0, 1, -- N \quad \text{except} \quad i=j=N \qquad (7)$$

and the normalisation of $P_N(x)$ is arbitrary. Also define

$$P_n(x, \tau) = P_n(x) - \tau\, P_{n-1}(x) \qquad (8)$$

Then we can form the quantity

$$\int_{-\infty}^{\infty} \sigma(x)\, f(x)\, dx \qquad (9)$$

exactly if f(x) is a polynomial of degree $\leq$ 2N - 2 using

$$\int_{-\infty}^{\infty} \sigma(x) f(x)\, dx = \sum_{i=1}^{N} w_i f(x_i) \qquad (10)$$

where x_i are the roots of $P_N(x,\tau)$

and $$w_i = \left(\sum_{j=0}^{N-1} | P_j(x_i) |^2 \right)^{-1}$$

If $\tau=0$ the equations hold if f(x) is a polynomial of degree $\leq 2N-1$. Of course it is rather obvious that if we have the first 2N moments we can evaluate the average of any polynomial of degree 2N-1. If, however, f(x) is not a polynomial we can use (10) to <u>estimate</u> the integral of it over the distribution function. Equation (10) can be viewed as approximating $\sigma(x)$ by a distribution of delta functions in such a way that the first 2N moments are reproduced correctly. When f(x) is not a polynomial of degree $\leq 2N-1$ the theory spares us the trouble of making a polynomial approximation to it explicitly. Furthermore in trying to form the approximating polynomial how would we know where it was important to represent f(x) well and where it was not so important because $\sigma(x)$ is small? The procedure given in (10) always chooses a polynomial representation for f(x) which is exact at the positions of the delta functions which is as well as one can hope to do. Thus finding the x_i and w_i, by a procedure whose details we may skip over, yields an approximation for the integral which makes efficient use of the available information and which is rather easy to use.

5. Evaluation of Indefinite Integrals Over the Distribution Function

We are interested in integrals of the form

$$\int_{-\infty}^{x_0} 6(x)\, dx \tag{11}$$

This may be regarded as a definite integral over a step function

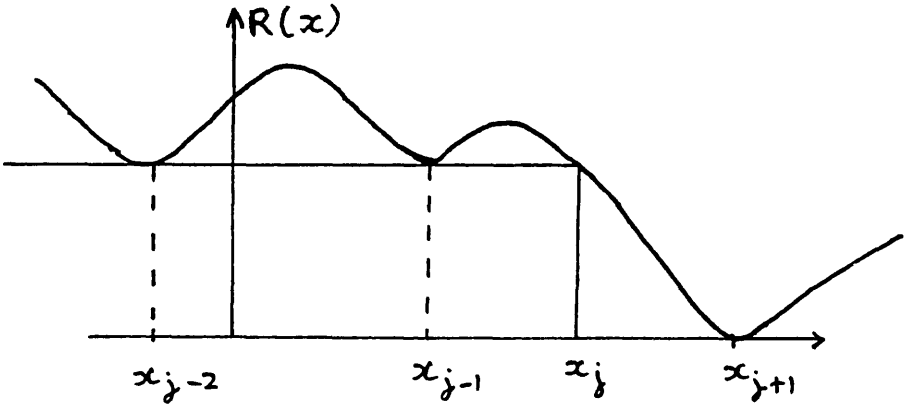
$$\begin{aligned} f(x) &= 1 \qquad x \leq x_0 \\ &= 0 \qquad x > x_0 \end{aligned} \tag{12}$$

Not only can we estimate the integral (11) but we can actually bound it.

First we choose τ in (8) so that one of the roots x_i of $P_n(x, \tau)$ lies at x_0. We then form the polynomial R(x) of degree 2N-2 which satisfies

$$\begin{aligned} R(x_i) &= 1 \qquad i \leq j \\ &= 0 \qquad i > j \\ R'(x_i) &= 0 \qquad i < j \text{ and } i > j \end{aligned} \tag{13}$$

as in the figure



Evaluating the integral of this polynomial using (10) gives the upper bound

$$\int_{-\infty}^{x_0} \sigma(x)\, dx \leq \sum_{i=1}^{j} w_j \tag{14}$$

The same procedure may be carried out for the polynomial of degree 2N - 2 which is always less than (12). we obtain

$$\int_{-\infty}^{x_0} \sigma(x)\, dx = \sum_{i=1}^{j-1} w_i + \tfrac{1}{2} w_j \pm \tfrac{1}{2} w_j \tag{15}$$

Thus this procedure has the great attraction of producing a rigorous bound for the integral. Nex developed a numerical differentiation procedure which extracts $\sigma(x_o)$ from (15) which has become a standard tool in the analysis of the density of states by the recursion method.

An alternative approximation for $\sigma(x)$ is given in terms of the continued fractions

$$\sigma(z) = \lim_{Im z \to 0} \cfrac{1}{z - a_0 - \cfrac{b_0^2}{z - a_1 - \cfrac{b_1^2}{\ddots \cfrac{}{z - a_n - f(z)}}}} \tag{16}$$

where the as and bs are chosen so that

$$\cfrac{1}{z-a_0-\cfrac{b_0^2}{z-a_1-\cfrac{b_1^2}{\ddots\;\cfrac{}{z-a_n-f(z)}}}} = \sum_{i=0}^{2N-1} \frac{\mu_i}{z^i} \qquad (17)$$

The usefulness of the continued fraction is that it guarantees that $\sigma(Z)$ is a positive definite function and permits one to terminate the continued fraction with f(Z) which should be Herglotz (that is everywhere analytic except possibly on the real axis). If f(Z) is chosen to be zero we obtain our previous formalism since $\sigma(Z)$ is N delta functions. However, if sufficient is known about σ a priori, an informed choice of f(Z) can be made and much better results can be extracted from a few moments. On the other hand there is always the danger that σ is wrongly influenced by the choice of f. My approach has been to use Eqns. (10) and (15) which are even handed in the sense that no "half baked" notions of what σ is like are used. I find in the next section that the information available from the form of the moments (3) is very small within this formalism which is an indication that $\sigma(Z)$ formed by (16) would be very sensitive to the choice of f(Z).

6. Application of C.M.P. Techniques to Moments, $\langle R^N \rangle$

In what follows I work through the theory of (10) with the

form (3) for the moments in mind. The explicit form for $P_n(x)$ (7) is

$$P_n(x) = \frac{1}{\sqrt{D_{n-1} D_n}} \begin{vmatrix} \mu_0 & \mu_1 & \cdots & \mu_n \\ \mu_1 & \mu_2 & \cdots & \mu_{n+1} \\ \vdots & & & \\ \mu_{n-1} & \mu_n & \cdots & \mu_{2n-1} \\ 1 & x & \cdots & x^n \end{vmatrix} \tag{18}$$

where

$$D_n = \begin{vmatrix} \mu_0 & \mu_1 & \cdots & \mu_n \\ \mu_1 & \mu_2 & \cdots & \mu_{n+1} \\ \vdots & & & \\ \mu_n & \mu_{n+1} & \cdots & \mu_{2n} \end{vmatrix}$$

We now find an approximate form for the c_i in the polynomial $P_n(x)$ where

$$P_n(x) = \frac{1}{\sqrt{D_{n-1} D_n}} \sum_{i=0}^{n} c_i x^i \tag{19}$$

From (18) we see that each c_i is the sum of products of μ_k but for large lengths the largest term in the sum dominates. For moments of the form (3) the largest term can be found by inspection and we have

$$c_0 = \mu_{2n-1}\,\mu_{2n-3} \cdots \mu_3\,\mu_1$$

$$c_1 = -\mu_{2n-1}\,\mu_{2n-3} \cdots \mu_3\,\mu_0$$

$$c_2 = \mu_{2n-1}\,\mu_{2n-3} \cdots \mu_2\,\mu_0$$

$$\vdots \qquad (20)$$

Thus each of the coeficients c_k scales exponentially with the length of the system.

The product of all the roots α_i of $P_n(x)$ is given by c_o by the simple theory of equations. Similarly c_1 is the sum of all possible products of n-1 roots. We suppose that the largest term in this sum dominates and show that the results are consistent with this assumption. We find the first root is given by

$$\alpha_1 = \frac{\alpha_1\,\alpha_2 \cdots \alpha_n}{\alpha_2 \cdots \alpha_n} \approx \frac{c_0}{c_1} = \frac{\mu_1}{\mu_0} \qquad (21)$$

similarly

$$\alpha_2 = \frac{\mu_3}{\mu_2}$$

$$\alpha_k = \frac{\mu_{2k-1}}{\mu_{2k-2}} \approx \exp\left[(\alpha + \beta(4k-3))L\right] \qquad (22)$$

where the form for the moments (3) has been substituted. We see that for large lengths the roots are indeed well separated which justifies our approximations.

This already shows the essence of why formula (10) does not work well for the functions we wish to average. The roots are well separated and at large values of R, so one can only make accurate averages of functions which are well approximated by a polynomial over a very wide range of R.

In evaluating the weights w_r from (10) we can take the contribution from those P_n for which $n \geq r$ to be zero approximately. Thus the weight at α_1 is all due to P_o which is 1. Clearly a more precise result would be

$$w_1 = 1 - e^{-\gamma L} \qquad \gamma > 0 \tag{23}$$

i.e. just less than 1 for large lengths. The other weights all tend exponentially to zero.

For both the functions we want to average, $\left(\frac{1}{R}\right)^n$ and $(\ln R)^n$, the contribution from the higher weights tends to zero for long lengths and we have

$$\int_{-\infty}^{\infty} \delta(x) f(x) dx \approx f\left(\frac{\mu_1}{\mu_0}\right) \tag{24}$$

This is an incorrect conclusion as may be seen from the form of P(R) in the weak disorder limit and shows that the approximation (10) is a very poor one for these functions.

Turning to expression (15) we see that the error in the

estimate of

$$\int_{-\infty}^{x_o} 6(x)\, dx$$

is equal to half the weight at x_o. If x_o happens to be a root with $\tau = 0$ the weights we have estimated are appropriate. The weights w_i are exponentially small for $i > 1$ so the function is accurately known. For $i = 1$ however the weight is 1 which means the function is almost completely unknown at this point. My numerical work shows, as one would expect, that the situation for $\tau \neq 0$ is that the tail of P(R) for large R is very well known but that the part close to R = <R> and lower is very badly known.

Within our approximate arguments increasing the number of moments available makes no difference to the convergence around R= <R> but in fact there will be small contributions from $P_n(x_i)$ which reduce the value of W_1 but these are so small that we would need vast numbers of moments to make any difference.

The results of this section were confirmed by direct numerical calculation. Eqn. (24) was verified and the results for the indefinite integral of P(R) are shown in Figs. 4 and 5 where the two bounds are plotted. The resulting reconstruction of P(R) is found to be quite unsatisfactory in regions where its integral is not tightly bounded.

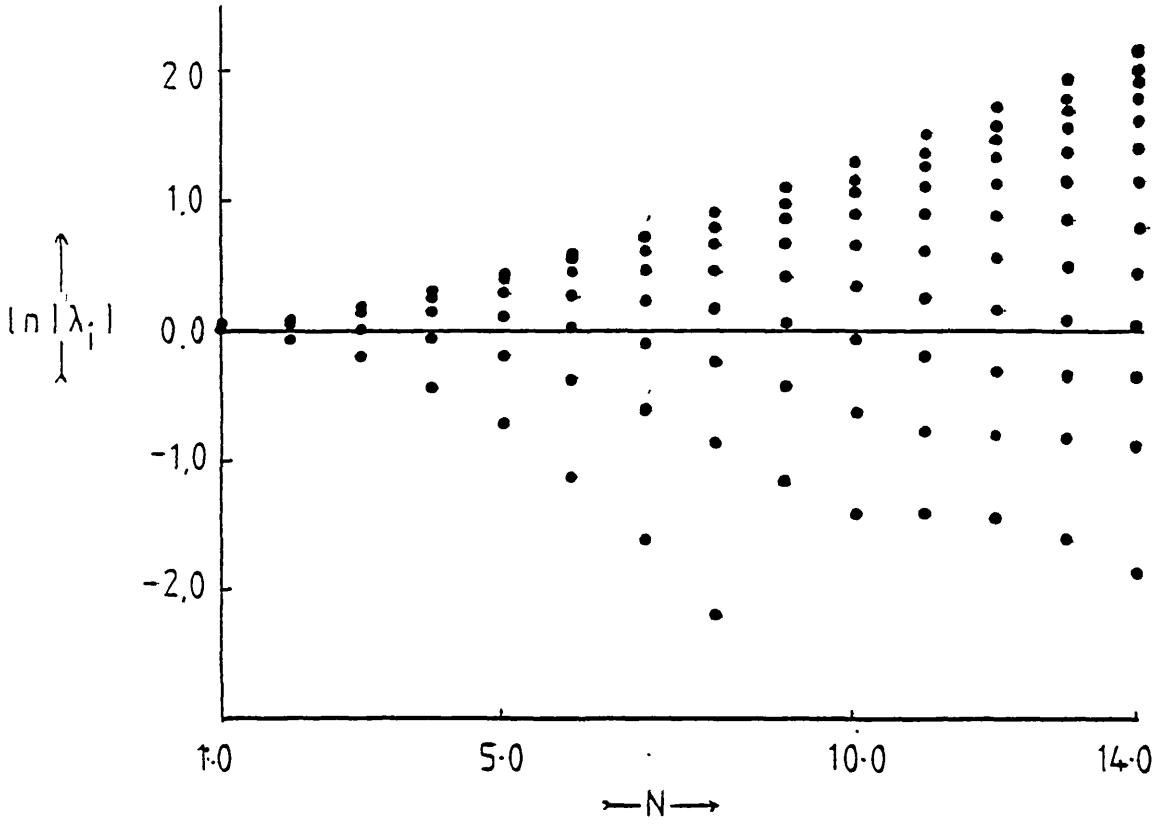


FIGURE 1a

Plot of logarithm of moduli of eigenvalues, λ_i, against N. (See Eqn. 1) for an Anderson distribution of diagonal disorder with E=1.0, W=0.75

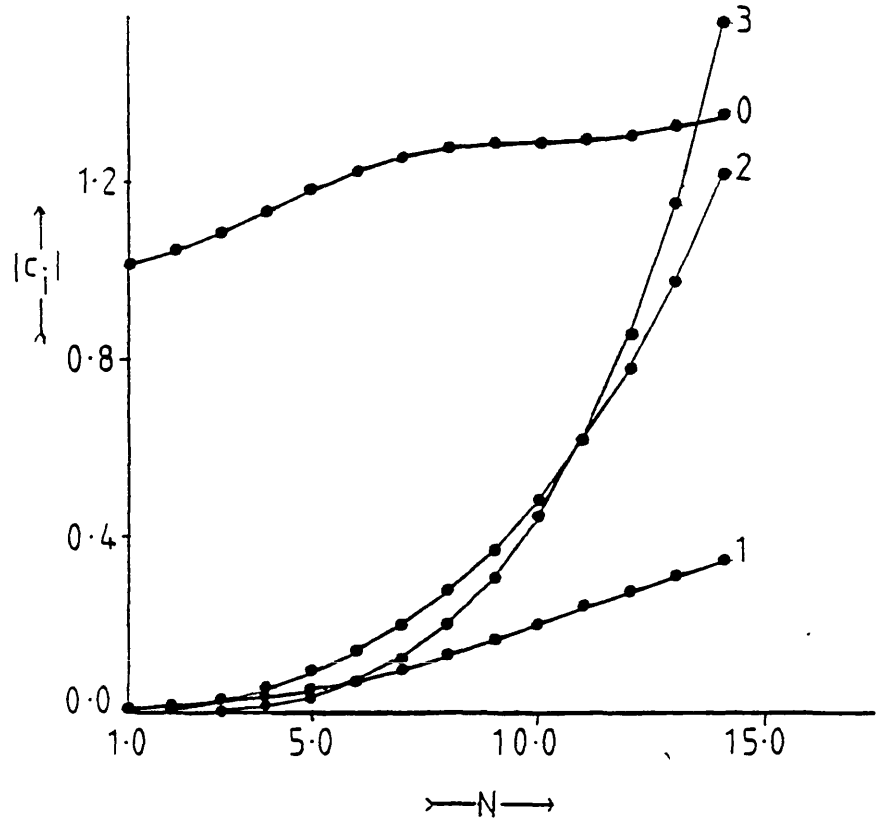


FIGURE 1b

Plot of modulus of C_i against N (see Eqn. 1) for an Anderson distribution of diagonal disorder with E=1.0, W=0.75. The curves are labelled with the subscript i.

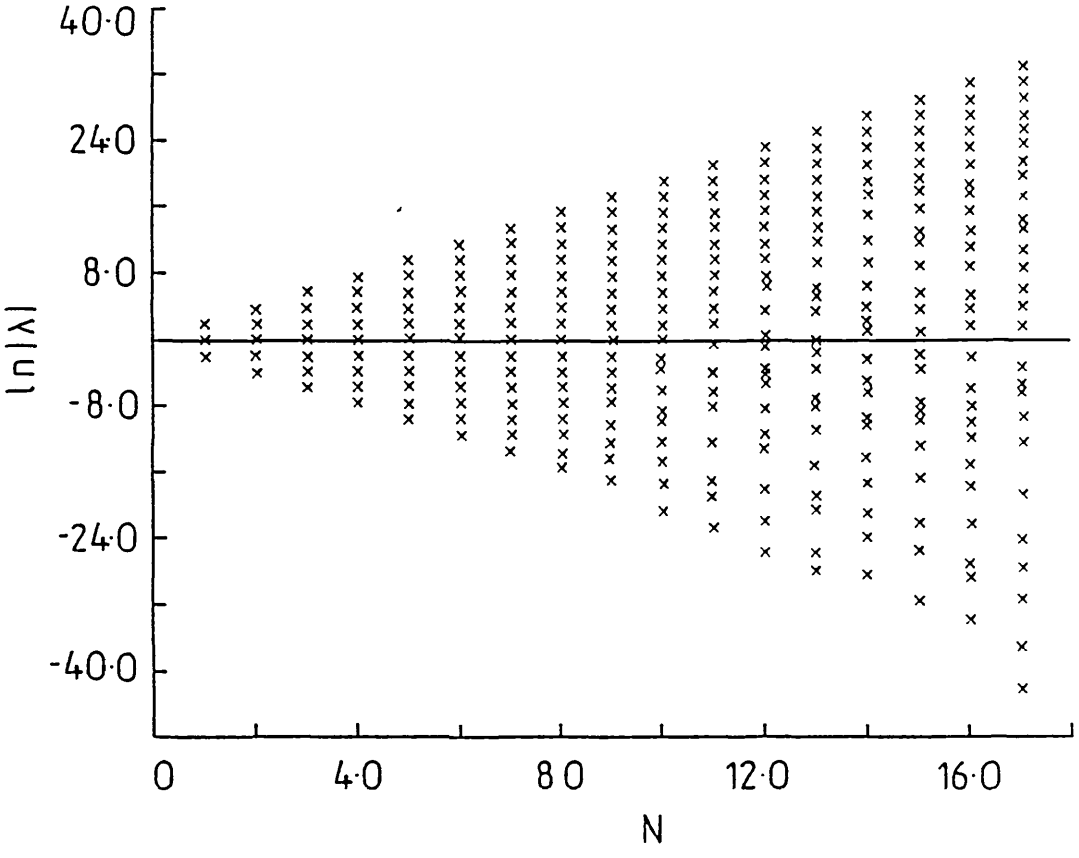


FIGURE 2a

Plot of logarithm of moduli of eigenvalues, λ_i, against N (see Eqn. 1) for a Gaussian distribution of diagonal disorder E=1.0, W=3.0. Numerical errors mean that for large N only the larger eigenvalues are reliably determined.

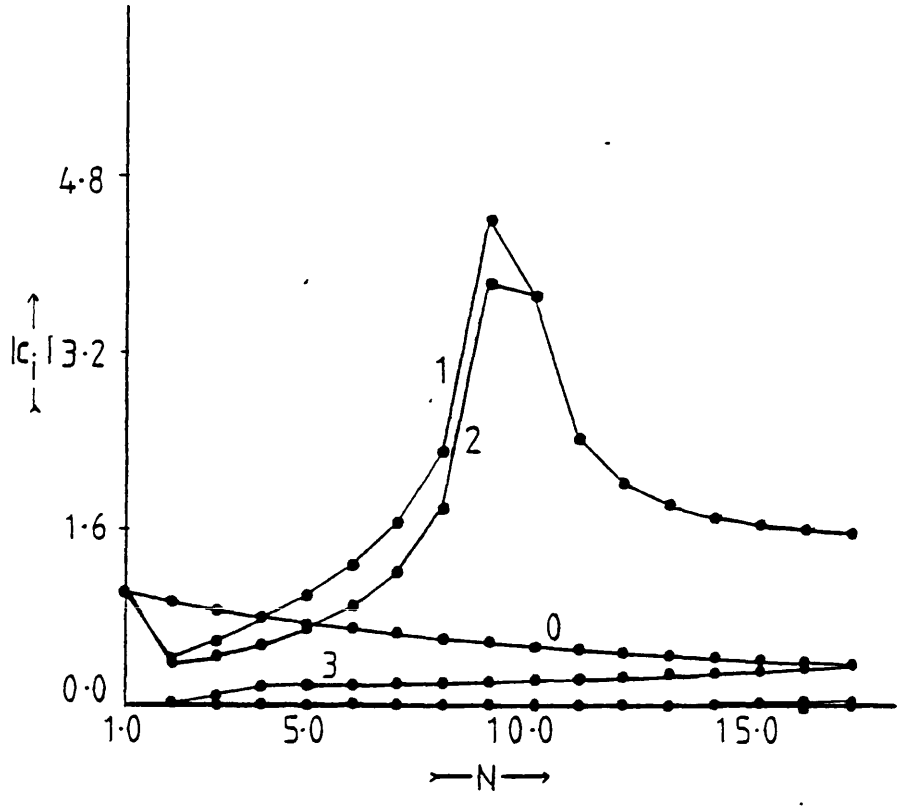


FIGURE 2b

Plot of modulus of C_i against N (see Eqn. 1) for a Gaussian distribution of diagonal disorder with E=1.0, W=3.0. The curves are labelled with the subscript i

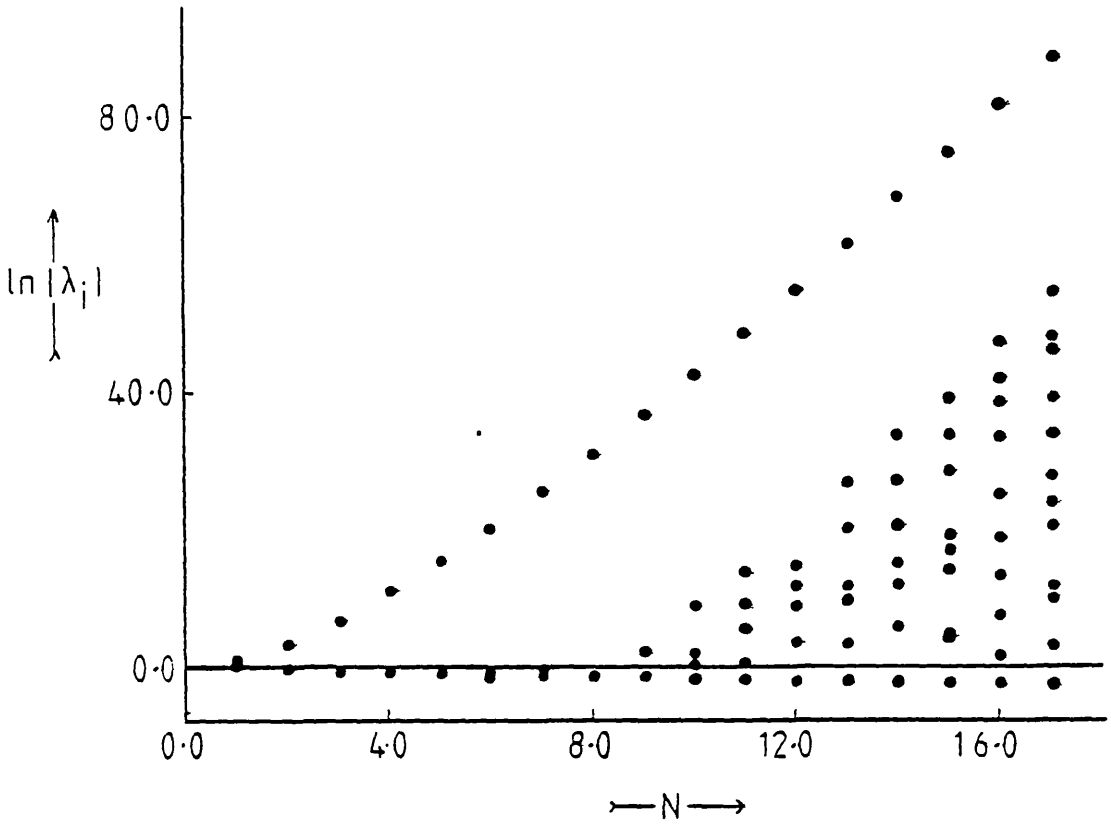


FIGURE 3

Plot of logarithm of moduli of eigenvalues, λ_i, against N (see Eqn. 1) for exponential distribution (Eqn. 2) of diagonal disorder with δ=10.0

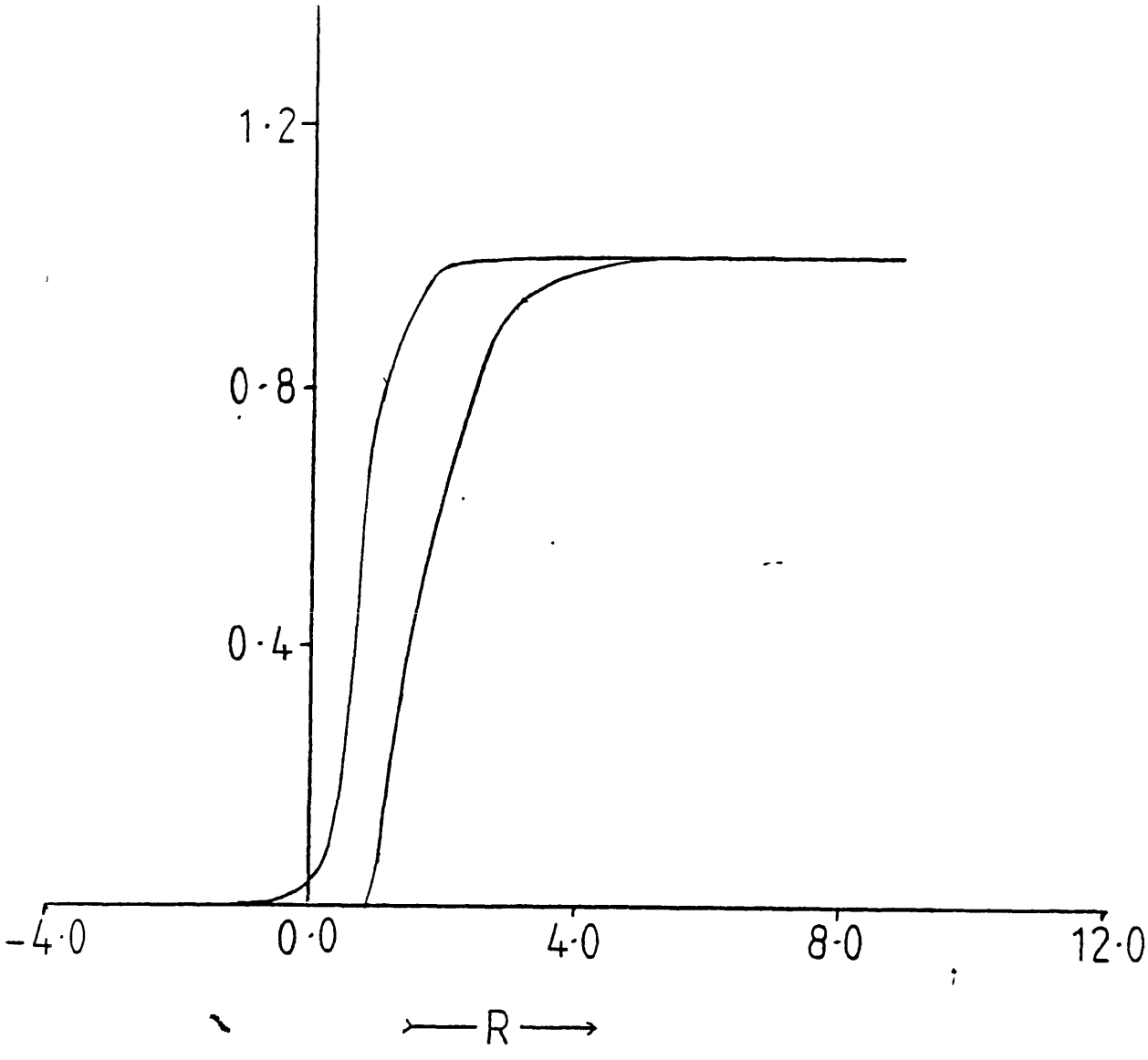


FIGURE 4

Bounds for the integral

$$\int_{-\infty}^{R} P(R')\, dR'$$

9 moments were used for a chain of length 10 with an Anderson distribution of diagonal disorder with E=1.5, W=0.5

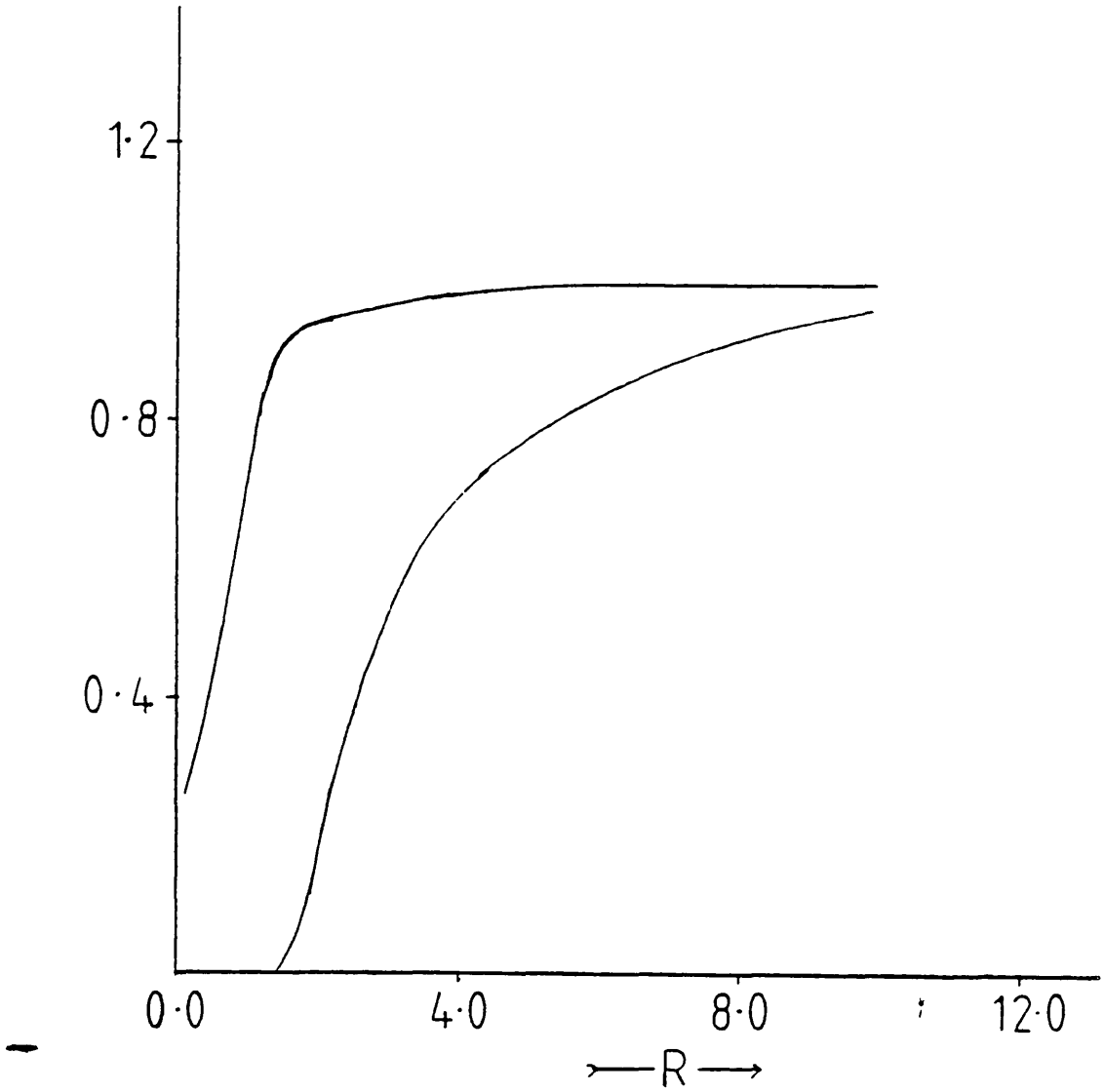


FIGURE 5

Bounds for the integral

$\int_{-\infty}^{R} P(R')\, dR'$

14 moments were used for a chain of length 50 with an Anderson distribution of diagonal disorder with E=1.0, W=0.5

IV CALCALCULATION OF <ln R > AND DENSITY OF STATES

BY ANALYTIC CONTINUATION

An exact expression for the moments of the resistance of a 1D chain of atoms $\langle R^N \rangle$ is obtained for positive integer N. We show how to analytically continue this result to all N and use this to calculate $\langle \ln R \rangle$ and the density of states. We compare our results for the localisation length with direct simulation work using a program generated by Mackinnon and derive some analytic results from our formulae.

1. Introduction

The propagation of waves in 1D disordered systems has been the subject of much interest, particularly in the case of electrons on chains of atoms. Erdos and Herndon (1982) have written an extensive review of the subject. The motivation is that wave propagation is at the heart of many fundamental quantities of solid state physics, for example the density of states, the spread of the eigenfunctions, and the conductivity. In a disordered system we must consider the distribution of all these quantities in an ensemble of different chains whose composition is described statistically.

It is well understood (Casher and Lebowitz 1971,Ishii 1973, Borland 1963) that in 1D the average resistance of the chain, $\langle R \rangle$, is exponential in the length, L,

$$\langle R \rangle \sim \exp(\alpha L)$$

which is due to the fact that all eigenfunctions are exponentially localised. Unfortunately $\langle R \rangle$ is not typical of the distribution P(R) so it is not a particularly useful quantity. Some light has been shed on the general form of the distribution by the theorems of Tutubalin (1968) and Oseledec (1968) which have been put to use by Pichard and Sarma(1981) and Johnston and Kunz (1982). The theorems show that although P(R) is rather unconventionally distributed, P(lnR) on the other hand converges for long chains to a normal distribution with

$$\begin{aligned} \langle \ln R \rangle &= 2L/\xi_0 \\ \langle (\langle \ln R \rangle - \ln R)^2 \rangle &\sim L \end{aligned} \qquad (1)$$

The arguments of Anderson et. al. (1980), which have been investigated by Lambert and Thorpe (1982) lead to the same conclusion. Equations (1) imply that $\langle \ln R \rangle$ is typical of the distribution and that the quantity ξ_0, known as the localisation length gives the typical extent of the eigenfunctions. However the conductivity and the average positive integer powers of resistance, $\langle R^N \rangle$, as well as other quantities of interest test the convergence of P(lnR) in its extreme tails because

$$\langle g \rangle = \langle R^{-1} \rangle = \int P(\ln R) \exp(-\ln R)\, d\ln R$$

and

$$\langle R \rangle = \int P(\ln R) \exp(\ln R)\, d\ln R \qquad (2)$$

are heavily weighted by the exponential for values of lnR which are very different from the typical value.

These theorems by themselves provide no way of calculating the localisation length, but if P were truly log normal a knowledge of say $\langle R \rangle$ and $\langle R^2 \rangle$ would be sufficient to determine the parameters of the distribution and the problem would be solved completely and trivially because these quantities are easily calculated. In fact it can be shown explictily that averages of powers of R are only consistent with a log normal distribution in the limit of of weak disorder. Thus for many quantities the theorem is of no help to us and the problem of calculating averages and distributions has still to be addressed.

This paper is part of a corpus of work aimed at discovering the form of the distribution function, the averages and statistical spread of the quantities mentioned. In two earlier papers one of us (Pendry 1982 and 1982b) showed how to average any integer power of the resistance for wires of any length. Certain distributions of disorder in the medium give rise to soluble models for P(R) and it is from these results that our statements about the convergence of P(R) follow.

In the present paper we work in terms of a transmission coefficient, t, defined in section 2, whose modulus squared we take to be proportional to the conductivity and whose phase will be used to extract the density of states (DOS). Using the concepts of Pendry (1982) we obtain an expression for the integer moments of

$1/t$, M_N, defined by

$$M_N = \langle t^{-N} \rangle \qquad (3)$$

The main development is to analytically continue this formula to all N. We then apply this to calculating

$$\langle \ln 1/t \rangle = \frac{\partial}{\partial N} \langle t^{-N} \rangle \Big|_{N=0} \qquad (4)$$

The real part of this gives the localisation length and we derive the DOS from the imaginary part.

The equations are sufficiently tractable to be solved analytically in the limits of weak and strong disorder and in the weak disorder case we reproduce the results of Kappus and Wegner (1981) for the anomaly in $\xi_0(E=0)$.

We have also developed a rapidly convergent numerical implementation of the theory which can calculate $\langle \ln 1/t \rangle$ for a wire of any length given the distribution of disorder characterising the wire. Comparison of our procedure with direct simulations of ξ_0 using a program provided by A. MacKinnon shows agreement to within the 1% accuracy of the simulations. We also present a calculation of the DOS.

2. Formalism for Integer N

We shall model our 1D wire with a tight binding Hamiltonian. This enables us to simulate any combination of group and phase velocity of the ordered system. Thus the amplitudes on successive sites, a_n, are related by

$$Ea_n = E_n a_n + Va_{n+1} + Va_{n-1} \tag{5}$$

or

$$a_{n+1} = \Delta_n a_n - a_{n-1} \tag{6}$$

where

$$\Delta_n = (E - E_n)/V \tag{7}$$

We shall deal with the case of diagonal disorder where the disorder is entirely confined to the Δ_n's. We expect that the off diagonal case can be treated in an analogous manner starting from the formalism introduced in an earlier paper (Pendry 1982b).

Eqn 6 can be rewritten as a transfer matrix

$$\begin{pmatrix} a_{n+1} \\ a_n \end{pmatrix} = \begin{pmatrix} \Delta_n & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a_n \\ a_{n-1} \end{pmatrix} \tag{8}$$

We transform to a wave basis defined by

$$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = Q \begin{pmatrix} a_n \\ a_{n-1} \end{pmatrix} \tag{9}$$

so that

$$\begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = T_n \begin{pmatrix} A_n \\ B_n \end{pmatrix} \tag{10}$$

where

$$T_n = Q \begin{pmatrix} \Delta_n & -1 \\ 1 & 0 \end{pmatrix} Q^{-1} \tag{11}$$

and

$$Q^{-1} = \begin{pmatrix} 1 & 1 \\ e^{-ik} & e^{ik} \end{pmatrix} \tag{12}$$

The real parameter k defines the wave basis and is arbitrary but we normally take it in the range $0-\pi$.

T has the form

$$T = \begin{pmatrix} t_+^{-1} & r_+ t_-^{-1} \\ r_- t_+^{-1} & t_-^{-1} \end{pmatrix} = \begin{pmatrix} (1-i\delta')e^{ik} & -i\delta' e^{ik} \\ i\delta' e^{-ik} & (1+i\delta')e^{-ik} \end{pmatrix} \quad (13)$$

where

$$\delta' = (\Delta - 2\cos k)/2\sin k \quad (14)$$

In the case of real Δ we have

$$T_n = \begin{pmatrix} t^{-1} & r t^{-1} \\ (r t^{-1})^* & t^{*-1} \end{pmatrix} \quad (15)$$

t_+ is the quantity we will be interested in and it has a simple physical interpretation for the system of a single scatterer embedded in an otherwise ordered chain. If a wave, e^{-ikn}, is travelling from $+\infty$ along an ordered chain for which $\Delta = 2\cos k$ and hits a scatterer, $\Delta \neq 2\cos k$ then the amplitude transmitted to the ordered section extending to $-\infty$ is t_+ (see fig 1). t_{+L} relates incident and transmitted waves in the same way when there are L consecutive scatterers and can be found from

$$t_{+L}^{-1} = (1, 0) \prod_{i=1}^{L} T_i \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad (16)$$

The definition of resistance has been discussed by Landauer(1970), Economou and Soukoulis (1981) and Langreth and Abrahams (1981). We define the resistance as

$$R = \frac{\pi \hbar}{e^2} |t|^{-2} = 12.89 \, |t|^{-2} \, k\Omega \qquad (17)$$

From the remarks of section 1 we find that the localisation length is given by

$$\xi_0^{-1} = \lim_{L \to \infty} \frac{Re \langle \ln t_L^{-1} \rangle}{L} \qquad (18)$$

where we have dropped the + sign on t.

We shall show that t is related to an element of the Green's function operator and thence we find the integrated DOS.

$$\int_{-\infty}^{E} \varrho(E') \, dE' = -\frac{1}{\pi} Im \langle \ln t_L^{-1} \rangle \qquad (19)$$

We now develop our averaging procedure.

The transfer matrix T is statistically independent of the vector

$$\begin{pmatrix} A_i \\ B_i \end{pmatrix}$$

on which it acts because this vector depends on scatterers with label less than i. This enables us to average the transfer equation (10) to obtain

$$\left\langle \begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} \right\rangle = \langle T_n \rangle \left\langle \begin{pmatrix} A_n \\ B_n \end{pmatrix} \right\rangle \qquad (20)$$

where

$$\langle T_n \rangle = \langle T \rangle = \int P(\Delta) \, T(\Delta) \, d\Delta$$

and $P(\Delta)$ is the probability distribution of Δ. Using eqn (16) and (20) we obtain the average reciprocal of the transmission coefficient for a chain of length L.

$$\langle t_L^{-1} \rangle = (1, 0) \langle T \rangle^L \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{21}$$

To obtain $\langle 1/t^2 \rangle$, however, we must use an outer product of two Ts as the transfer matrix

$$\langle t^{-2} \rangle = (1,0) \otimes (1, 0) \cdot \langle T \otimes T \rangle^L \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{22}$$

and in general, for any power of (1/t) we nave

$$\langle t^{-N} \rangle = [(1,0) \otimes (1, 0) \cdots (1,0)]$$
$$\times \langle T \otimes T \cdots T \rangle^L \cdot \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdots \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right] \tag{23}$$

in which the dots indicate that there are N identical entities in each group of direct products. The transfer matrix for each N is the direct product of N T matrices and so has dimension 2^N. However, this can be reduced to dimension N+1 by the use of the symmetric group. The symmetry we exploit is the symmetry of $T \otimes T \otimes \ldots T$ under interchange of subscripts.

Suppose a vector $v_{j_1 j_2 \cdots j_N}$ is symmetric under interchange of subscripts, then the vector $v'_{i_1 i_2 \cdots i_N}$ obtained when $T \otimes T \otimes \ldots T$ is applied to it is given by

$$V'_{i_1 i_2 \cdots i_N} = \sum_{j_1 j_2 \cdots j_N} T_{i_1 j_1} T_{i_2 j_2} \cdots T_{i_N j_N} V_{j_1 j_2 \cdots j_N} \qquad (24)$$

and is also symmetric. Since j takes the values 1 and 2 only, a symmetric vector may be indexed by the number of twos in the subscripts i.e. $v_j = v_{j_1 j_2 \cdots j_N}$ if there are j twos amongst the subscripts $\{j_1 j_2 \cdots j_N\}$. Hence we can write a symmetry reduced equation

$$v_i' = \sum_j \chi^N_{ij} \, v_j \qquad i,j = 0 \cdots N \qquad (25)$$

where

$$\chi^N_{ij} = \left\langle \sum^{*}_{j_1 j_2 \cdots j_N} T_{i_1 j_1} T_{i_2 j_2} \cdots T_{i_N j_N} \right\rangle \qquad (26)$$

where there are i twos amongst $\{i_1 i_2 \cdots i_N\}$ and the summation goes over all $j_1 \ldots j_N$ s.t. there are j twos amongst $\{j_1 \ldots . j_N\}$. All arrangements of the i's subject to the constraint are equivalent so we can choose one arrangement

$$\chi^N_{ij} = \left\langle \sum^{*}_{j_1 j_2 \cdots j_N} T_{2 j_1} T_{2 j_2} \cdots T_{2 j_i} T_{1 j_{i+1}} \cdots T_{1 j_N} \right\rangle \qquad (27)$$

This sum can be more conveniently expressed as

$$\chi^N_{ij} = \left\langle \sum_{p=0}^{\min(i,j)} {}^{i}C_p \; {}^{N-i}C_{j-p} \; T_{22}^{p} \, T_{21}^{i-p} \, T_{12}^{j-p} \, T_{11}^{N-i-j+p} \right\rangle \qquad i,j = 0 \cdots N \qquad (28)$$

χ^N is our symmetrically reduced transfer matrix and is related to the matrix of the same name in Pendry(1982b) by a similarity transformation. We note that since the projection vectors were symmetric they fall totally within the symmetry reduced space and

we obtain

$$\langle t_L^{-N} \rangle = (1, 0, 0 \cdots) (\chi^N)^L \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \qquad (29)$$

where the vectors and the matrix χ^N are of dimension N+1.

To examine the length dependence of $\langle 1/t^N \rangle$ one simply has to construct the matrix χ^N for a given $P(\Delta)$ through eqns (28), (13) and (14) and find the eigenvalues and eigenvectors. Fig 2 shows the moduli of the eigenvalues against N for a normal distribution of site energies. The largest eigenvalue is always is always real and the remaining eigenvalues come in pairs for which one is the complex conjugate of the other so each pair is represented by one point in the figure. The smooth behaviour of the largest eigenvalue is the motivation for the next section in which we find the path of the eigenvalues between the integer values of N.

3. Analytic Continuation to all N

Since the χ matrix's dimension is a function of the variable we wish to analytically continue we have an apparently hard task. Our approach is to recast the expression (29) in a form which is meaningful at all N and then to remove arbitrariness by demanding that our formulae reproduce known limits correctly.

In what follows we do not show the averaging of χ over site energies explicitly.

The Nth order transfer matrix equation

$$v_{n+1\,j} = \sum_{k=0}^{N} \chi^{N}_{jk}\, v_{n\,k} \quad , \quad j = 0 \cdots N \qquad (30)$$

may be rewritten in an integral form

$$\sum_{j=0}^{N} v_{n+1\,j}\, e^{-ijx} = \frac{1}{2\pi} \int_0^{2\pi} \left(\sum_{j,k=0}^{N} \chi^{N}_{jk}\, e^{i(ky - jx)} \right) \times \sum_{k'=0}^{N} v_{n\,k'}\, e^{-ik'y}\, dy \qquad (31)$$

identifying

$$\phi_n(y) = \sum_{k=0}^{N} v_{n\,k}\, e^{iky} \qquad (32)$$

and

$$\chi^{N}(x,y) = \sum_{j,k=0}^{N} \chi^{N}_{jk}\, e^{i(ky - jx)} \qquad (33)$$

we have

$$\phi_{n+1}(x) = \int_0^{2\pi} \chi^{N}(x,y)\, \phi_n(y)\, dy \qquad (34)$$

A remarkably simple form for $\chi^{N}(x,y)$ can be derived.

Substituting (28) and doing the k summation we have

$$\chi^{N}(x,y) = (2\pi)^{-1} \sum_{j=0}^{N} (T_{11} + T_{12}\, e^{iy})^{N-j} (T_{22}\, e^{iy} + T_{21})^{j}\, e^{-ijx} \qquad (35)$$

as can be verrified by expansion. We now do the j summation as a geometric progression

$$\chi^{N}(x,y) = (2\pi)^{-1} (T_{11} + T_{12}\, e^{iy})^{N} \frac{\left[1 - \left(\dfrac{T_{22}\, e^{iy} + T_{21}}{e^{ix}(T_{11} + T_{12}\, e^{iy})} \right)^{N+1} \right]}{1 - \left(\dfrac{T_{22}\, e^{iy} + T_{21}}{e^{ix}(T_{11} + T_{12}\, e^{iy})} \right)} \qquad (36)$$

So far we have only found a simple representation of χ, we have not changed anything but now the expression suggests an obvious

analytic continuation.

The ratio in the geometric progression was

$$\left(\frac{T_{22}\, e^{iy} + T_{21}}{e^{ix}\left(T_{11} + T_{12}\, e^{iy}\right)} \right)$$

which has modulus 1 . For the G.P. to converge at fractional N we must have this modulus less than unity which can simply be achieved by adding a small imaginary part to x. We then have

$$\phi_{n+1}(x) = \lim_{\eta \to 0} \int \chi^N(x - i\eta, y)\, \phi_n(y)\, dy \qquad (37)$$

The projection operators of eqn(29) correspond to integration over the function 1 so denoting by $\left(\chi^N(x,y)\right)^L$ the iterated kernel

$$\int \chi^N(x, z_{L-1})\, \chi^N(z_{L-1}, z_{L-2}) \cdots \chi^N(z_1, y)$$

$$dz_1\, dz_2 \cdots dz_{L-1} \qquad (38)$$

we have

$$\langle t_L^{-N} \rangle = \frac{1}{2\pi} \int_0^{2\pi} \left(\chi^N(x, y)\right)^L dy\, dx \qquad (39)$$

The expression we have found for the analytically continued χ^N is infact not the only one which gives the positive integer moments correctly. It sufficient for the moment to discriminate between the possible choices on the basis of the zero disorder limit though other limits are considered in the next section. The limit of interest is where the atoms of what would be the disordered section are all identical to the atoms of the two ordered sections and we

have

$$t_L^{-N} = e^{ikNL} \qquad (40)$$

We can see that our formula for t^{-N} is incorrect because, for example, it vanishes at N=-1.

These considerations lead us to consider the expression for $\langle t^{-N} \rangle$ given by (38) and (39) with χ' in place of χ where χ' is obtained by dropping the second term in square brakets in (36) to give

$$\chi'^{N}(x,y) = \frac{(2\pi)^{-1}\left(T_{11} + T_{12}\, e^{iy}\right)^{N}}{1 - \left(\dfrac{T_{22}\, e^{iy} + T_{21}}{e^{ix}\left(T_{11} + T_{12}\, e^{iy}\right)}\right)} \qquad (41)$$

In the ordered case we have

$$T_{12} = T_{21} = 0 \;, \quad T_{11} = e^{ik} \;, \quad T_{22} = e^{-ik}$$

and because of the simple form of χ' we can see that (40) holds.

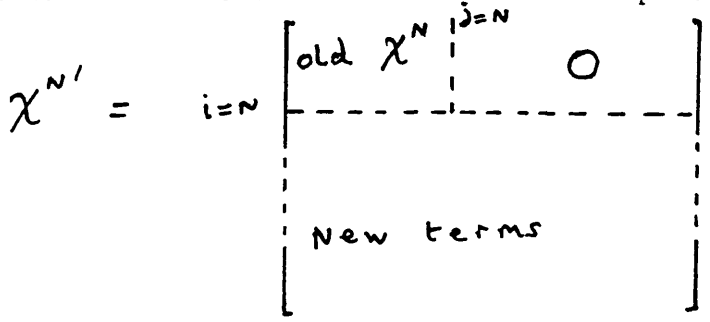
We must now show that using χ' does indeed give the correct form for the positive integer moments in the disordered case. This can most easily be seen if we represent $\chi'(x,y)$ as a matrix using the zero disorder eigenfunctions as a basis

$$\chi'^{N}_{jk} = (2\pi)^{-1} \int_0^{2\pi} \chi'^{N}(x,y)\, e^{i(jx - ky)}\, dx\, dy \qquad (42)$$

$$\Rightarrow \chi^{N}_{ij} = \sum_{p=0}^{\min(i,j)} {}^{i}C_{p}\; {}^{N-i}C_{j-p} \times T_{22}^{\,p}\; T_{21}^{\,i-p}\; T_{12}^{\,j-p}\; T_{11}^{\,N-i-j+p} \qquad (43)$$

$$i, j = 0, 1 \cdots \infty$$

We retrieve eqn(28) but now the matrix is infinite and defined for all N. We have also discovered along the way what to do with the p summation in the analytically continued form and that ${}^{N-i}C_{j-p}$ analytically continues in the same way as the binomial coefficients. The form of this matrix for positive integer N is



In the top left hand corner for i,j=0 to N is the old χ which we would have had if we had not analyticlly continued. For i=0 to N, j>N all the elements are zero. For i>N there are new "unphysical" terms in the matrix. In transforming eqn(38) to a matrix representation we obtain

$$\langle t_L^{-N} \rangle = u \left(\chi^{N'}\right)^L u^T \qquad (44)$$

where we define u as a vector of infinite dimension with components

$$u_j = \delta_{j,0}$$

At positive integer N the left hand projection vector remains of the form $v_j=0$, for j>N as it is propagated down the chain by χ' and never "feels" the unphysical part of the matrix. Consequently the expression for $\langle 1/t^N \rangle$ is the same as that obtained in section 2.

A generalisation of this argument to consider defining χ' with

an undetermined factor in front of the second term in square brakets in eqn(36) shows that we only get the correct answer in the ordered case if the factor is zero which is the χ' we have defined.

The expressions for $\langle 1/t^N \rangle$ given in matrix form by eqns (43) and (44), and equivalently in the integral form by using $\chi'(x,y)$ defined by eqn(41) in place of $\chi(x,y)$ in (38) and (39), are our final ones. We should remind the reader that eqns(41) and (43) for χ' are implicitly averaged over site energies , Δ, which enters through the definition of T eqns (13) and (14). We have shown that at positive integer N the expression agrees with those rigorously calculated for general disorder in section 2 and that it agrees with the known result for the ordered case for all N. At this stage we can only propose that our expresions are valid for all disorders and all N but in the remainder of the paper we accumulate such evidence for the proposal, by considering limiting cases and numerical results that we are lead to accept it. For the rest of this paper we will not need the χ' of eqn (36) so we can drop the primes on our analytically continued form in (41), (43) and (44).

Although we are interested in ensemble averaged quantities, further insight into (44) can be gained by considering one particular chain. Here we define a site transfer matrix χ_i^N, formed as given in (43) with T determined by the site parameter and we we do not ensemble average. We can show that

$$\chi^N(T.T') = \chi^N(T).\ \chi^N(T') \qquad (45)$$

By definition

$$t^{-N} = \chi^N_{oo} \qquad (46)$$

and we have

$$t_L^{-N} = u.\ \chi^N\left(\prod_{i=1}^{L} T_i\right) u^T \qquad (47)$$

and hence

$$t_L^{-N} = u.\left(\prod_{i=1}^{L} \chi^N_i\right) u^T \qquad (48)$$

which is just eqn (44) without averaging. We can see that $\chi^N_{(T_i)}$ is just a generalised site to site transfer matrix and the form of eqn (48) is such that averaging to obtain (44) is possible.

We now extract an expression for <lnl/t> which is the main objective of this work. For definiteness we proceed in the matrix representation. We write

$$\chi^N = \sum_{i=0}^{\infty} \lambda_i^N\ |v_i^N\rangle\langle v_i^N| \qquad (49)$$

where $|v_i^N\rangle, \langle v_i^N|$ are the right and left eigenvectors of χ^N and λ_i^N are the eigenvalues. Equation (44) becomes

$$\langle t_L^{-N}\rangle = u.\sum_i \lambda_i\ |v_i^N\rangle\langle v_i^N|\ .\ u^T \qquad (50)$$

Differentiating with respect to N we have

$$\langle t_L^{-N} \ln t_L^{-1}\rangle = \sum_{i=0}^{\infty} L\left(\lambda_i^N\right)^{L-1} \dot{\lambda}_i^N\ u\,|v_i^N\rangle\langle v_i^N|\,u^T$$

$$+\left(\lambda_i^N\right)^L u\,|\dot{v}_i^N\rangle\langle v_i^N|\,u^T + \left(\lambda_i^N\right)^L u\,|v_i^N\rangle\langle \dot{v}_i^N|\,u^T \qquad (51)$$

Evaluating at N=0 and recognising

$$\lambda_0^0 = 1 \qquad \text{and} \qquad \langle v_0^0 | = u_0$$

independent of the disorder (corresponding to the fact that $\langle 1/t^0 \rangle = 1$) we have

$$\langle \ln t_L^{-1} \rangle = L\dot{\lambda}_0^0 + \langle v_0 | \dot{v}_0 \rangle + \langle \dot{v}_0 | u^T \rangle + \sum_{i=1}^{\infty} (\lambda_i^0)^L \langle v_0 | \dot{v}_i \rangle \langle v_i | u^T \qquad (52)$$

If

$$|\lambda_i| \leq 1$$

the dominant term for large lengths is $L\dot{\lambda}_0^0$ and we identify the localisation length as $(\mathrm{Re}\,\dot{\lambda}_0^0)^{-1}$. The other terms in the equation are assosiated with behaviour for short chains.

4. Limiting Cases

In section 3 we used the zero disorder case to choose the analytic continuation, now we go on to consider small disorder. In the matrix representation the ordered case is diagonalised by choosing $\cos k = \Delta/2$. For weak disorder we use perturbation theory from this limit. First we consider the case where there are no degenerate eigenvalues and first order perturbation theory gives

$$\lambda_0^N = \chi_{00}^N = \langle t^{-N} \rangle \qquad (53)$$

hence

$$\xi_o^{-1} = Re \left\langle \ln \left(\left(1 + \frac{\delta}{2i \sin k} \right) e^{ik} \right) \right\rangle \quad (54)$$

$$\doteq \frac{1}{2} \left\langle \ln \left(1 + \delta^2 / 4 \sin^2 k \right) \right\rangle \quad (55)$$

for small disorder, $\langle \delta^2 \rangle << 1$

$$\xi_o^{-1} = \frac{1}{2} \frac{\langle \delta^2 \rangle}{4 \sin^2 k} \quad (56)$$

in agreement with Thouless (1979) and Pendry (1982). It has been shown by Kappus and Wegner (1981) that there is an anomaly in this result when

$$\langle \Delta \rangle = E = 0$$

In our formalism this is due to degeneracies amongst the zero disorder eigenvalues. The eigenvalues are

$$e^{i(N-2j)k} \qquad j = 0, 1, -\infty \ , \quad k = \pi/2$$

Thus there are two sets of eigenvalues which are degenerate at e^{i2Nk} and $-e^{i2Nk}$. By taking the degenerate subspace which has eigenvalue 1 at N=0 we obtained a perturbation matrix which is tridiagonal and proportional to $\langle \delta^2 \rangle$

$$\chi^N = e^{i2Nk} I + \frac{1}{4} \Delta \chi^N \langle \delta^2 \rangle \quad (57)$$

If $\Delta\chi$ has eigenvalues λ_i', first order pertubation theory gives for the eigenvalues of χ

$$\lambda_i^N = e^{i2Nk} + \frac{1}{4} \lambda_i'^N \langle \delta^2 \rangle \quad (58)$$

hence

$$Re\ \dot{\lambda}_0^0 = \frac{\langle \delta^2 \rangle}{4} Re\ \dot{\lambda}_0^{\prime 0} \qquad (59)$$

We were able to estimate $\dot{\lambda}_0^{\prime 0}$ numerically by truncating Δx^N to a finite matrix and numerically differentiating. We obtained

$$Re\ \dot{\lambda}_0^{\prime 0} = 0.45694$$

and hence

$$\xi_0^{-1} = 0.45694 \langle \delta^2 \rangle / 4$$

Specialising to the case of an Anderson distribution of width W where $\langle \delta^2 \rangle = W^2/12$ we obtain

$$\xi_0 = 105.045 / W^2$$

in exact agreement with Kappus and Wegner.

This result is a dramatic confirmation of the validity of our analytic continuation since it is obtained by an interaction of all the eigenvalues which have been introduced by our procedure and is sensitive to the full structure of χ unlike the non degenerate case which is just sensitive to one element of it.

Degeneracies also occurr at k= π/n but in these cases the degenerate subspaces are diagonal to first order in δ^2. We find, therefore, that each successive degeneracy gives rise to an anomaly in successively higher orders in δ^2 as was found by Lambert (1983)

We now turn to the strong disorder limit. We can find an expression for $\dot{\lambda}_0^0$ provided there is no degeneracy

$$\dot{\lambda}_0^0 = \langle v_0 | \dot{\chi}^0 | v_0 \rangle \qquad (60)$$

where $|v_0\rangle$ and $\langle v_0|$ are the eigenvectors with eigenvalue 1 at N=0. Hence

$$\langle v_0 | = (1, 0, 0 - - -)$$

always and $|v_0\rangle$ is not known in general. Writing

$$|v_0\rangle_j = v_j$$

we have

$$\dot{\lambda}_0^0 = -ik + \ln(1+i\delta') + \sum_{j=1}^{\infty} \left(\frac{i\delta'}{1+i\delta'}\right) \frac{(-1)^{j-1}}{j} v_j \qquad (61)$$

This expression is true for any disorder. However, it is only possible to find v in the limit of weak and strong disorder. In the strong disorder limit $\delta' \gg 1$ most of the time, thus if we put

$$(1+i\delta') \approx i\delta'$$

in χ we have

$$\chi_{m m'} = e^{i2mk} \delta_{m',0} \qquad (62)$$

which gives

$$v_j = (-1)^j e^{i2jk} \qquad (63)$$

Hence

$$\dot{\lambda}_0^0 \approx \left\langle -ik + \ln(1+i\delta') + \ln\left(1 - \frac{i\delta' e^{i2k}}{1+i\delta'}\right) \right\rangle$$

$$\approx \langle \ln \delta \rangle \qquad (64)$$

We see that the result is independent of the choice of k as it should be. The result was obtained by Abrahams and Stephen (1980). We would expect the result to be more valid for distributions with

long tails such as a gaussian for which we have

$$\xi_0^{-1} = \int_{-\infty}^{\infty} \ln \delta \; \exp[-\delta^2/\sigma^2]\, d\delta$$
$$= \sigma \ln \sigma + c \qquad (65)$$

5. Numerical results for ξ_0 for general disorder

We can implement eqn(52) by simply truncating the matrix at some finite size, typically 10 or 20, and evaluating $\dot{\lambda}_0^0$ by numerical differentiation of the numerically determined eigenvalue. We can of course check that convergence is obtained by varying the size of the matrix. We used the simplest possible numerical differentiation which is to evaluate

$$\dot{\lambda}_0^0 = \frac{\lambda_0^{\Delta N} - 1}{\Delta N} \qquad (66)$$

We also checked that the formula is not sensitive to the value of ΔN and 10^{-5} was chosen. The convergence was fastest if we chose $\cos(k) = \langle \Delta \rangle / 2$. We chose two different distributions $P(\Delta)$, two delta functions of equal weight and a gaussian. Forming the matrix χ involves integrating over the distribtion $p(\Delta)$ which is trivial for the two delta function case but for the gaussian we used a numerical procedure of integration over a distribution of 64 delta functions which have the first 128 moments the same as a gaussian.

We also have a simulation procedure, provided by A. MacKinnon (MacKinnon and Kramer 1983) which calculates the localisation length by finding

$$\frac{1}{L} \ln |t_L|^{-1}$$

for one disordered chain for very large lengths. The procedure converges to

$$\frac{1}{L} \langle \ln |t_L|^{-1} \rangle$$

provided self averaging occurs.

The motivation for this section is first to obtain more evidence that our theory is correct, and second to present some actual data for the localisation length. For the first aim we obtained fig 3. which shows ξ_o^{-1} against disorder D for the distribution $P(\Delta)$ which is two delta functions of weight 1/2 at $\Delta = E \pm D$, where E is the energy relative to the average site energy measured in units of V. We chose E=0.0 and 0.5. From observing the convergence of our routine we have concluded that all the results of this section are accurate to 1% although the accuracy is this low only for the most strongly disordered points. The simulation was set to give the same accuracy and run for every other point in the graph. We found complete agreement within the errors mentioned. Naturally we cannot present this information graphically because the two curves would lie on top of each other. We stress that the simulation and analytic work are directly comparable with no fitting or undetermined parameters. For E=0.5 there is an interesting bump in the graph at D=1.5 which we checked to the same accuracy with the sumulation. This is our last piece of evidence that the numerical procedure based on our theory gives the same results as the

simulations and we believe that our analytic continuation is now very strongly supported.

We also present results for E=0.8 and E=1.0 for the two delta function distribution which show several more features (fig 4.). The results for the gaussian distribution with E=0.0 and E=0.5 (fig 5) show none of the structure of the two delta function case.

Thouless (1972) dsicovered the following equation for the localisation length in terms of the DOS,

$$\xi_0^{-1} = \int \ln|E-E'|\, \rho(E')\, dE' \qquad (67)$$

This enables us to account for the features in the localisation length in a general way as follows. Since the system is localised, the energies of the eigenfunctions are determined by local properties. We can imagine that certain orderings of atoms will occur more frequently than others in the chain and the energies of these "clusters" will be more strongly represented in the DOS. The structure in the DOS then manifests itself in the localisation length through (67). For a continuous distribution of site energies the notion of clusters does not apply so we have a relatively featureless localisation length.

The Density of States

The Greens function operator of the Hamiltonian is defined by $G(E)=(EI-H)^{-1}$ where

$$(EI - H) = \begin{bmatrix} \Delta_1 & -1 & & & & \\ -1 & \Delta_2 & -1 & & & \\ & -1 & \Delta_3 & -1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & \Delta_{n-1} & -1 \\ & & & & -1 & \Delta_n \end{bmatrix} \qquad (68)$$

For $1<j<N$ the elements of G satisfy

$$-G_{1j-1} + \Delta_j G_{1j} + G_{1j+1} = 0$$

$$\Rightarrow \begin{pmatrix} G_{1j+1} \\ G_{1j} \end{pmatrix} = \begin{pmatrix} \Delta_j & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} G_{1j} \\ G_{1j-1} \end{pmatrix} \qquad (69)$$

At j=1 and j=N G satisfies the boundary conditions

$$\Delta_1 G_{11} - G_{12} = 1$$

$$-G_{1N} + \Delta_N G_{1N} = 0 \qquad (70)$$

We imagine a system of two ordered sections of length L, $\Delta_i = \Delta_o$, connected by a disordered section and find G_{1N} where 1 and N are at the extreme ends of the system as shown in fig 6. Any disordered section can be described by a transfer matrix, T, of the form (13) which would be diagonal for either of the ordered sections, so we can find G_{1N} in terms of G_{11} and G_{12} and T. Satifying the boundary conditions at both ends fixes G_{1N} in terms of T and L. We can only take the limit $L\to\infty$ if G_{1N} is evaluated at complex energy. Define

$$G^+ = \lim_{\epsilon \to 0} \lim_{L\to\infty} G_{1N}(E + i\epsilon) \qquad (71)$$

We find $G = ct\, e^{-ik2L}$ where $0<k<\pi$, $k=\cos^{-1}\Delta_o/2$ and c is determined by the boundary conditions. This result shows that G^+ is related

to <t> not <1/t> and so it is given by (44) for N=-1. In addition the result is valid if the disordered system is itself infinite.

To obtain the DOS we use another result from Thouless (1972)

$$G_{1N} = \frac{(-1)^{N-1}}{Det(EI-H)} = \frac{(-1)^{N-1}}{\prod_{\alpha=1}^{N}(E-E_\alpha)} \qquad (72)$$

Thus we find

$$\frac{\partial}{\partial E} \ln G_{1N} = \sum_{\alpha} \frac{-1}{E-E_\alpha} \qquad (73)$$

and

$$Im \frac{\partial}{\partial E} \ln G^{+}_{1N} = \frac{\epsilon}{(E-E_\alpha)^2+\epsilon^2} = \pi \rho(E) \qquad (74)$$

where $\rho(E)$ is the DOS for the whole system. Extracting the part of the DOS due to the disordered chain we have

$$\rho(E) = \pi^{-1} \frac{\partial}{\partial E} Im \ln t_+$$

$$= -\pi^{-1} \frac{\partial}{\partial E} Im \ln t_+^{-1} \qquad (75)$$

Applying the results of section 3 we find that the integrated density of states per site for long lengths is

$$-\pi^{-1} \; Im \; \dot{\lambda}_0^0$$

and we have plotted this quantity in fig. 7 for the two delta function distribution (see section 4) with d=0.8 The error bars on the graph are due to lack of convergence of our routine and were estimated by varying k which would not affect a fully converged result. We see

that the DOS goes to zero at E=2.8 as it should according to the Saxon Hutner theorem, and we have confirmed that our theory gives this result analytically.

The limit on the accuracy of the numerical work is that the p summation involved in forming χ (43) has terms of very different sizes for large i and j, which cancel causing loss of precision. This has prevented us from building matrices of size greater than 20 by 20 in a single precision representation. The reason our procedure succeeds is that the largest eigenvalue is very insensitive to the bottom corner of χ.

Conclusions

We have found an analytical method for generating ensemble averages of the transmission coefficient $\langle 1/t_L^N \rangle$ for all N and all lengths, L,including $L=\infty$. From this we have extracted an average Green's function, the localisation length, and the integrated density of states. The equations have been solved in the limits of weak and strong disorder. The agreement with known results and direct simulations provides striking support for our theory.

We believe that the techniques developed here can be extended to tackle the conductivity and variances of all quantities and will ultimately result in a much fuller understanding of the probability distribution of the resistance.

Aknowledgement

We are indebted to A. Mackinnon for many helpful conversations and the provision of the simulation program.

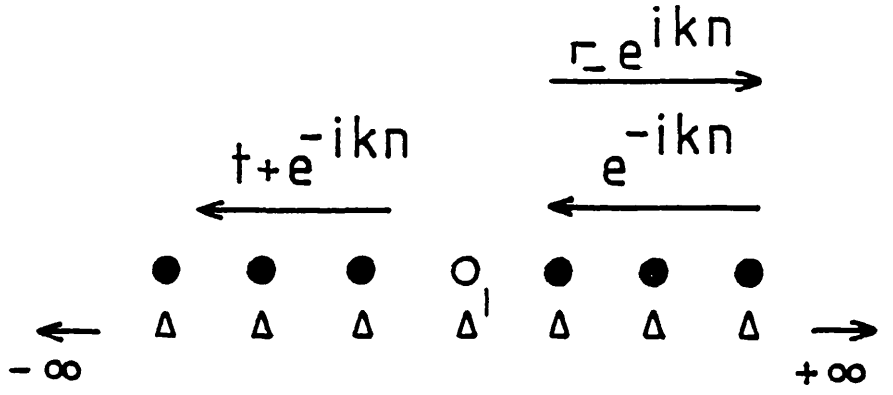


FIG 1

Definition of transmission coefficient for a single scaterrer.

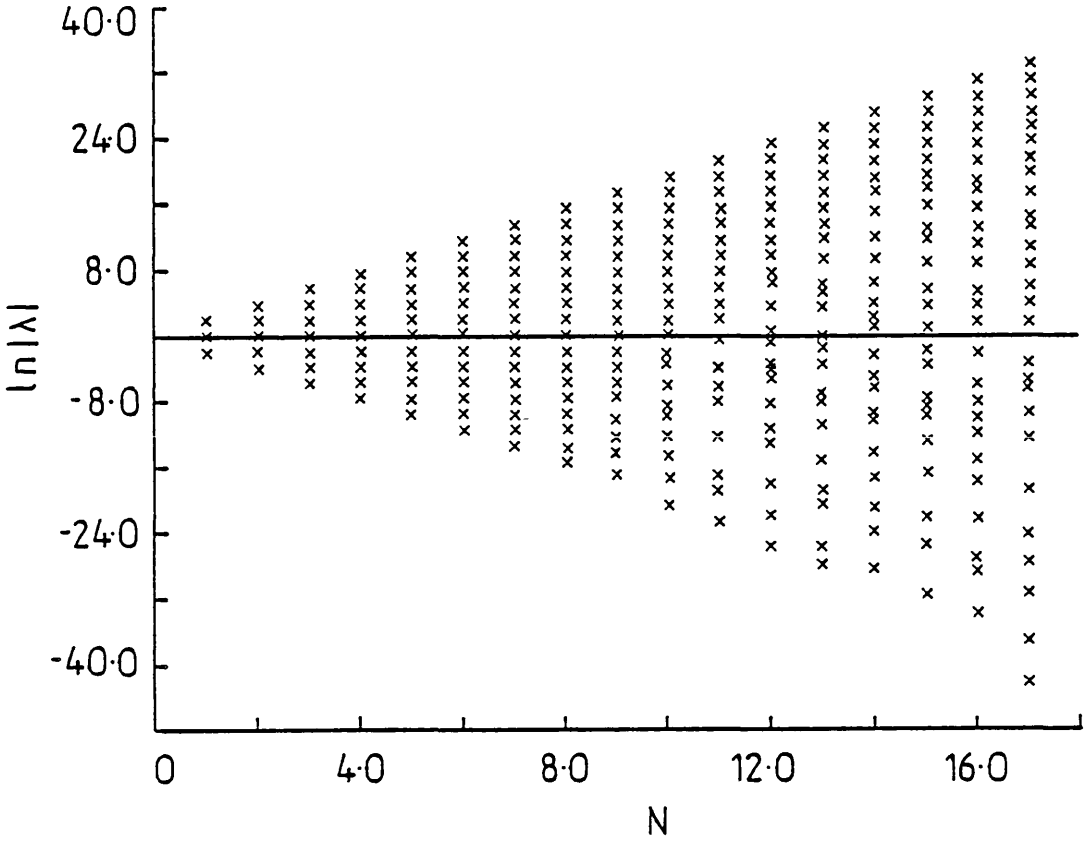


FIG 2

Moduli of the eigenvalue of χ^N against N. The distribution p(Δ) is gaussian with $\langle\Delta\rangle$=E=1.0 and standard deviation 3.0 in units of V, the hopping integral.

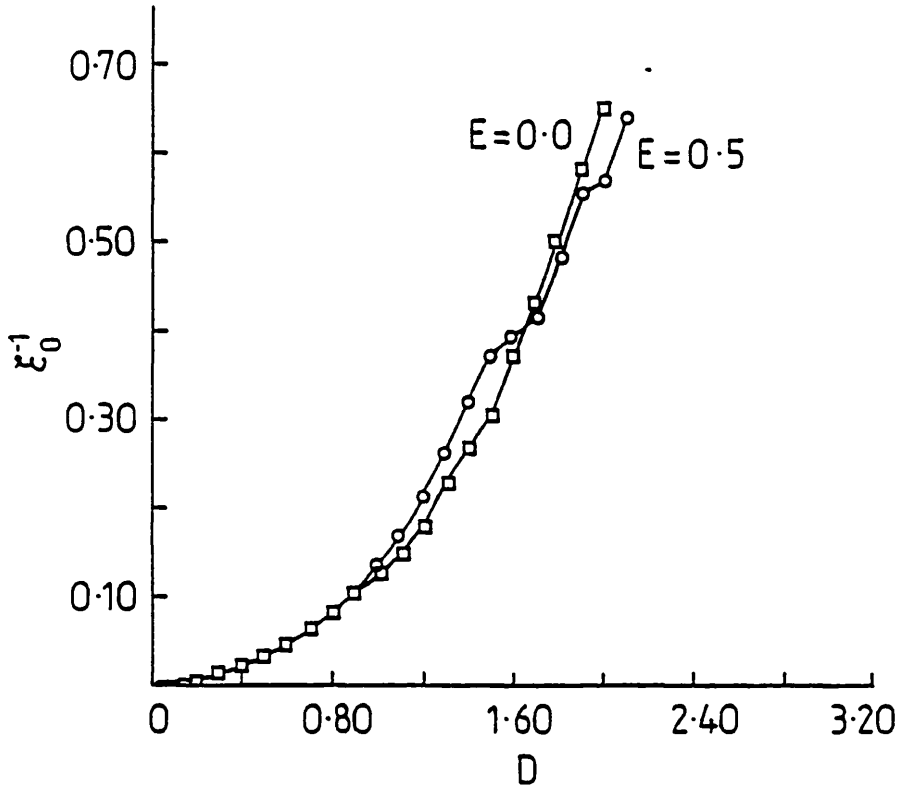


FIG 3

Inverse of the localisation length versus disorder, D, for the two delta function distribution at energies E=0.0 and 0.5. These curves were in exact agreement with the simulations to within the accuracy of the graph.

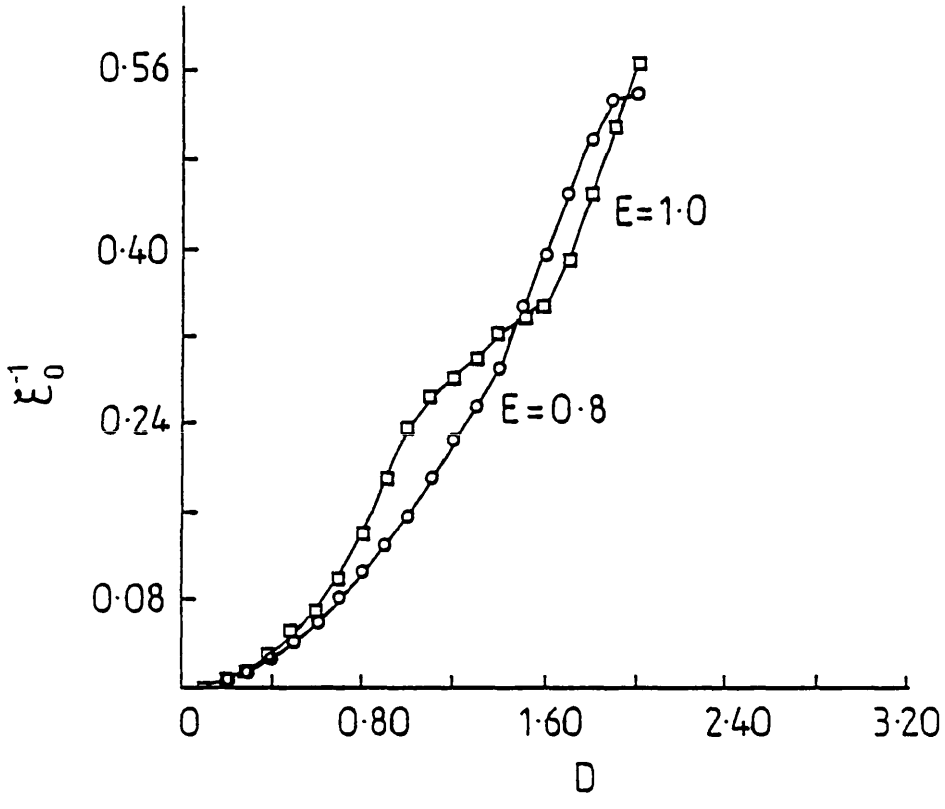


FIG 4

Inverse of the localisation length versus disorder, D, for the two delta function distribution at E=0.8 and 1.0.

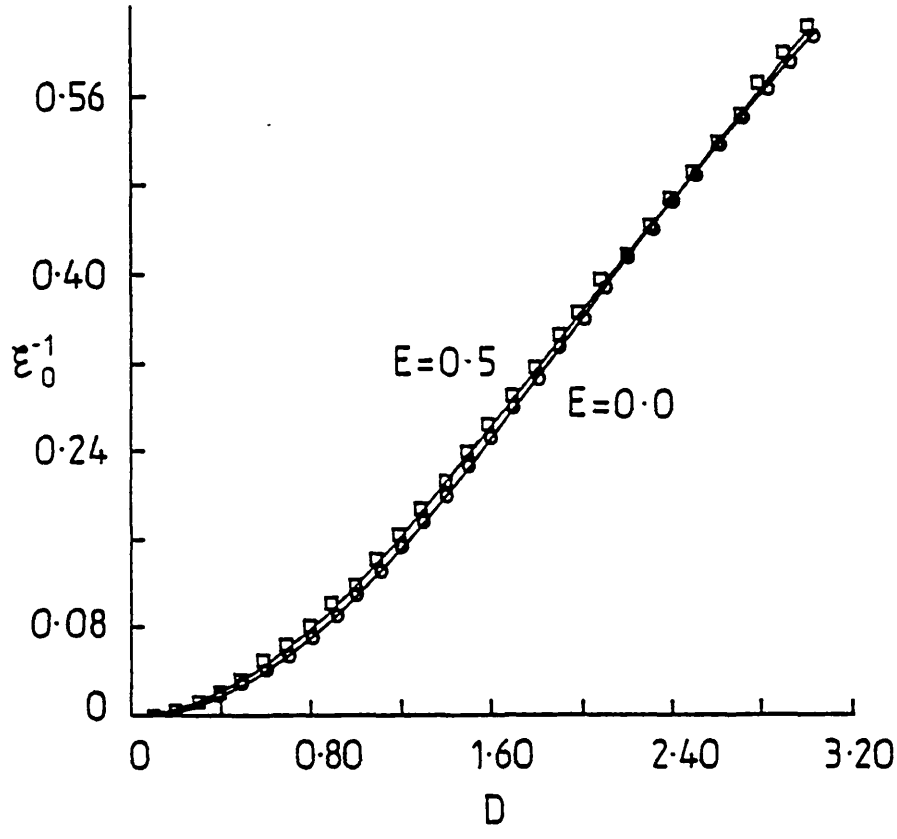


FIG 5

Inverse of the localisation length versus disorder, D, for a gaussian distribution at E=0.0 and 0.5. D is in units of the standard deviation so the scale is comparable with figs. 3 and 4.

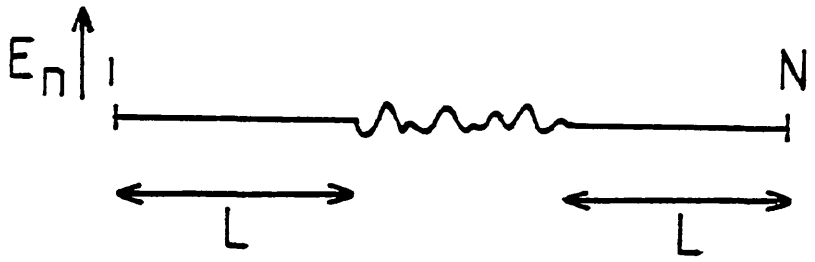


FIG 6

System to be considered for the density of states derivation.

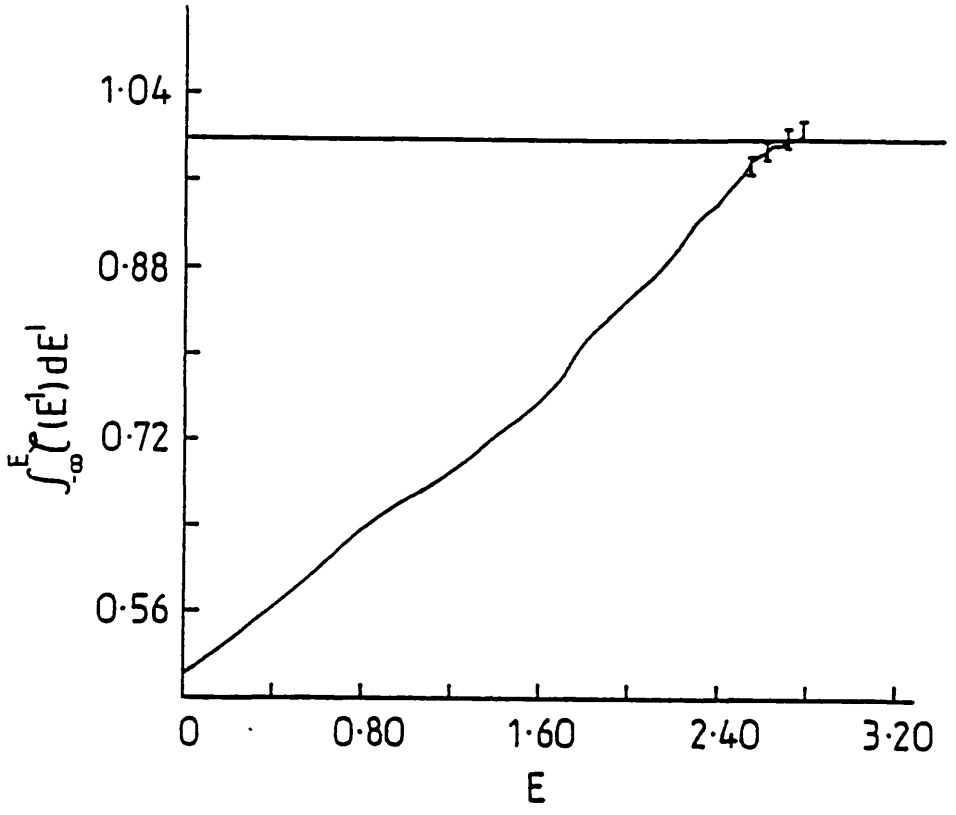


FIG 7

Cumulative density of states versus energy, E, for the two delta function distribution of disorder with D=0.8

V CALCULATION OF AVERAGE POWERS OF CONDUCTANCE BY ANALYTIC CONTINUATION

The method of "generalised transfer matrices" previously used to find the average of any power of the transmission coefficient, $\langle t^x \rangle$ is applied to finding $\langle |t|^y \rangle$ in the cases y=0, -2, -4 --- and Re y>1. These cases include all the integer moments of the conductance, $|t|^2$, and its reciprocal, the resistance. The conductance is the more physically important quantity and is found to have a complicated dependence on chain length. Our formulae are valid for any distribution of disorder and all lengths of sample. Limiting cases and numerical results are presented. An anomaly in the energy dependence of the conductance of a binary alloy is discovered.

1. Introduction

The problem of the propagation of electrons on disordered chains has analogues in many other systems where a wave propagates through a disordered medium in a 1 dimensional manner. The waves may be electromagnetic, acoustic or vibrational. The models proposed for such systems, are often greatly simplified but involve the key ingredient of microscopic variables which are random according to some given distribution. The problem of relating the distribution of macroscopic quantities such as resistance, conductance, density of states, localisation length etc. to the distribution of microscopic variables is a fundamental theoretical

barrier which has hindered the analysis of more complete models and consequently much work has been done to attempt to overcome it. Erdos and Herndon (1982) have written an extensive review of the subject.

Early work (Borland 1963, Casher and Lebowitz 1971, Ishii 1973, Landauer 1970) showed the fundamental localisation effect that for any disorder the average resistance increases exponentially with the length of the chain

$$\langle R \rangle \sim \exp(\alpha L) \qquad (1)$$

Subsequently higher integer powers $\langle R^N \rangle$ were calculated using the simple averaging properties of transfer matrices (Abrahams and Stephen 1980, Stone, Joanopolous and Chadi 1981). The essential ingredient of symmetry was introduced by Pendry (1982) which made these techniques more manageable. It was discovered that the distribution of resistance is extremely broad and gets broader with length and it is this that makes the problem complicated. Furthermore these moments of resistance do not directly enable you to calculate other quantities such as $\langle R^{-1} \rangle$ and $\langle \ln R \rangle$ because the positive integer moments are dominated by the very large R part of the distribution whereas $\langle R^{-1} \rangle$ for example is clearly sensitive to very small R properties. In a previous paper (Kirkman and Pendry 1984) we showed how to analytically continue the transfer matrix expression for the moments of the inverse of the transmission coefficient, $\langle 1/t^N \rangle$, to all N. We found that the expressions now involved "generalised transfer matrices" of infinite dimension. The advantage of the transfer matrix formalism, which is the

simple averaging procedure, was retained at all N. Differentiation w.r.t. N yielded $\langle \ln 1/t \rangle$, which since $\ln 1/t$ is known to obey the central limit theorem for large lengths in this system, is a quantity of fundamental importance.

For the conductance, the subject of this paper, there is no central limit theorem which means that for a single wire it does not self average as the length becomes very great. Thus a numerical simulation procedure or analytical approach based on self averaging will fail and one is forced to make a true ensemble average. Furthermore it is not possible to make the average by taking results for many chains on a computer because for long chains the distribution of conductances is very broad, as we shall see.

Knowledge of the statistics of the conductance is important from two points of view. Firstly, if a measurement is to be made on a single chain, one wants to know the probability of obtaining various results. On the other hand it may be possible, in some man made systems or in some highly anisotropic material, to measure the conductance of a large number of chains in parallel, and depending on the regime, one could measure an averaged conductance. Thus the averaged conductance could be a physical quantity in these systems. The average resistance, which is so easily calculated, is never a physically measurable quantity.

In section 2 we define the model and present the result of our previous work, the expression for $\langle 1/t^N \rangle$. We found that this quantity evolves according to a matrix of infinite dimension χ^N. Following that paper we define resistance as

$$R = \frac{\pi\hbar}{e^2} |t|^{-2} = 12.89 \; |t|^{-2} \; K\Omega$$

It is clear that $\frac{1}{|t|^{2N}}$ evolves according to $\chi^N \otimes \chi^{N*}$ and so at first sight we have achieved our goal. In our numerical work we calculate eigenvalues of the evolution operator by truncating the infinite matrix at a finite dimension and it is found that $\chi^N \otimes \chi^{N*}$ is very weakly convergent from this point of view. We analyse it in the weak disorder limit and obtain the same eigenvalue equation as Abrikosov and Ryzhkin (1978) who analysed the the same limit in a rather different model using a quite different formalism. Their analysis of this equation is quite complicated but we find, in later sections, that it has great relevance for the case of general disorder which their approach could not treat.

In section 3 we examine the symmetry decomposition of $\chi^N \otimes \chi^{N*}$ into subspaces at integer N. There are now two possible approaches. One would be to discover whether $\chi^N \otimes \chi^{N*}$ has subspaces at general N, the other is to take the symmetry reduced expressions at integer N and analytically continue them to all N. We take the latter option since it is simpler and we are now able to rigorously justify our analytic continuation so the procedures are equivalent. The result is an expression for all moments of the conductance which trivially agrees with Abriksov's result for weak disorder and which is sufficiently convergent to permit numerical analysis at general disorder. The result shows that the moments of the conductance are far more complicated than any of the other quantities we have so far calculated and the situation is not the simple sum of exponential decays with length as might be expected.

In section 5 we consider the analytic properties of the solution and extract the typical long length behaviour. Finally, in section 6 we use a numerical procedure to evaluate the most important parameter in the long length behaviour, the exponential decay rate, as a function of energy for two examples of disorder. An anomaly is found in the case of the binary alloy model and accounted for with an analytic theory.

2 Weak disorder result without symmetry reduction. First we outline the approach of a previous paper (Kirkman and Pendry 1984) which lead to an expression for $\langle 1/t^N \rangle$.

We model the wire by a tight binding hamiltonian in which the wave amplitudes on successive sites a_n are related by

$$\underline{E}\ a_n = \underline{E}_n\ a_n + V a_{n+1} + V a_{n-1} \tag{2}$$

$$\text{or}\quad a_{n+1} = \Delta_n\ a_n - a_{n-1} \tag{3}$$

$$\text{where}\ \Delta_n = \frac{E - \underline{E}_n}{V.} \tag{4}$$

E_n is the site energy and is taken to be the random variable. Equation 4 can be written in transfer matrix notation

$$\begin{pmatrix} a_{n+1} \\ a_n \end{pmatrix} = \begin{pmatrix} \Delta_n & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a_n \\ a_{n-1} \end{pmatrix} \tag{5}$$

where the disorder appears in Δ_n . This transfer equation may be transformed to a basis of waves propagating forward and backwards and the transfer matrix becomes

$$T_n = Q \begin{pmatrix} \Delta_n & - & 1 \\ 1 & & 0 \end{pmatrix} \qquad Q^{-1} \tag{6}$$

$$\text{where}\quad Q^{-1} = \begin{pmatrix} 1 & & 1 \\ e^{-ik} & & e^{ik} \end{pmatrix} \tag{7}$$

and k defines the wave basis but is arbitrary. T takes the well known form

$$T_n = \begin{pmatrix} 1/t & r/t \\ r^*/t^* & 1/t^* \end{pmatrix} = \begin{pmatrix} (1-i\delta')\, e^{ik} & -i\delta' e^{ik} \\ i\delta' e^{-ik} & (1+i\delta')\, e^{-ik} \end{pmatrix} \qquad (8)$$

where $\delta = \Delta_n - 2\cos k$,

$\delta' = \delta/2 \sin k$

and t and r are the transmission and reflection coefficients for the scatterer. Denoting the transmission coefficient for the whole chain by t_L we found

$$\langle t_L^{-N} \rangle = (1,0) \otimes (1,0) \otimes \cdots (1,0) \;.\; \langle T \otimes T \otimes \cdots T \rangle^L. \qquad (9)$$

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdots \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

where the --- denotes N cross products of the same object. The simple averaging procedure is a consequence of the statistical independence of the transfer matrix and the vector on which it acts and is the feature of the technique which enables us to obtain results for any length of system with any degree of disorder. It is an exact and completely rigorous step. We reduced the complexity of (9) by finding a subspace of $T \otimes T \cdots T$. The space contains vectors $V_{j_1 j_2 \cdots j_N}$ which are symmetric under interchange of all pairs of subscripts. Since the

projection vectors of (9) lie completely within this subspace there was no need to consider other subspaces. As we shall see in later sections this is not the case for $\frac{1}{|t|^{2N}}$ and is the basic reason why this quantity has a more complicated evolution. We obtained the symmetry reduced from

$$\langle 1/t_L^N \rangle = u^T . \quad \langle \chi^N \rangle^L \, u \tag{10}$$

where $u_j = \delta_{jo}$

and $\chi^N_{ij} = \sum_{p=0}^{\min(i,j)} {}^{i}C_{p}{}^{N-i}C_{j-p} T_{22}^{p} \, T_{21}^{i-p} \, T_{12}^{j-p} \, T_{11}^{N-i-j+p}$ (11)

At integer N the subscripts i,j run from 0 to N. The central achievement of our work was to analytically continue equation (10) in N. We found that equation (10) could be generalised by making the subscripts run from 0 to ∞. At integer N the extra part of the matrix has no projection on to u so it makes no difference, at other N the extra terms are essential. χ^N may be regarded as a generalised transfer matrix which has a form such that for any N we can write

$$\frac{1}{t_L^N} = u^T \prod_{i=1}^{L} \chi^N(T_i) \quad u \tag{12}$$

From the form of this equation the averaging procedure is applicable to give (10). It is clear then that a suitable generalised transfer matrix for $1/|t_L|^{2N}$ is given by $\chi^N(T) \otimes \chi^N(T^*)$ and the equation analogous to (10) is

$$\langle \frac{1}{|t_L|^{2N}} \rangle = (u^T \otimes u^T) \cdot \langle \chi^N(T) \otimes \chi^N(T^*) \rangle^L \cdot (u \otimes u) \tag{13}$$

where we have used the fact that u is real. In the case of no disorder, when $|\Delta| < 2$, the parameter k of (7) can be chosen to make δ of (8) vanish which results in a diagonal form for $\chi^N(T) \otimes \chi^N(T^*)$. The eigenvalues are given by

$$\lambda_{mm'} = e^{ik2(m-m')} \quad m,m' = 0,1, -- \infty \tag{14}$$

From which it will be seen that there is a high degree of degeneracy. This means that to treat the weak disorder case we must use degenerate perturbation theory. Now we choose k so that

$$\langle \delta \rangle \doteq 0 \tag{15}$$

The next term in $\chi(T) \otimes \chi(T^*)$ is proportional to $\langle \delta^2 \rangle$ and is assumed small for the weak disorder limit. Since the projection vectors of (13) only have a projection on to the eigenvalue of unity in zero disorder, at weak disorder, we only have to analyse the subspace of all unperturbed eigenvalues which are unity. Restricting our attention to N = -1 we obtain in the limit of weak disorder

$$|t_L|^2 = V^T \cdot \left[I + \Delta\chi \ \langle \delta'^2 \rangle \right]^L \cdot V \tag{16}$$

$$V_j = \delta_{jo}$$

where $\Delta\chi$ is the part of $\chi^{-1}(T) \otimes \chi^{-1}(T^*)$ which is proportional to $\langle \delta'^2 \rangle$. To solve the problem explicitly we must find the eigenvalues of $\Delta\chi$

and expand the projection operators V in terms of the eigenvectors. $\Delta\chi$ is found to be tridiagonal and its eigenequation is

$$\alpha A_j = j^2 A_{j-1} + (j+1)^2 A_{j+1} - \left[j^2 + (j+1)^2\right] A_j \qquad (17)$$

$$j = 0 \text{ --- } \infty$$

where α is the eigenvalue and A_j the associated eigenvector. The difficult problem posed by (16) and (17) has been solved by Abrikosov and Ryzhkin (1978) c.f. eq 2.51 They obtained equation (17) by a completely different technique which we consider to be rather more complicated and not applicable to general disorders. The model chosen by these authors was one of a weak gaussian random potential uncorrelated in space, which is rather different from our own. It is pleasing that both models give the same equation in the weak disorder limit and it has been argued that this should be the case on physical grounds by Thouless and Kirkpatrick (1981).

The analysis of this equation is required in a different context in a subsequent section and we go through it briefly here to highlight points which are significant from our point of view.

First we define

$$A(x) = \sum_{j=0}^{\infty} A_j x^j \qquad (18)$$

From (17) it can be shown that A(x) satisfies the equation

$$\alpha A = x(1-x)^2 \frac{\partial^2 A}{\partial x^2} + (1-x)(1-3x) \frac{\partial A}{\partial x} - (1-x) A \qquad (19)$$

The solutions to this equation which have power series expansions (18) are

$$A_\lambda(x) = (1-x)^{-\frac{1}{2}+i\lambda}\, F(\tfrac{1}{2}+i\lambda,\ \tfrac{1}{2}+i\lambda,\ 1,\ x) \qquad (20)$$

with $\alpha_\lambda = -\frac{1}{4}-\lambda^2$

where F is the Hypergeometric function of Gauss.

From the differential equation (19), the $A_\lambda(x)$ are found to obey an orthogonality relation

$$\int_0^1 A_\lambda(x)\, A_{\lambda'}(x)\, dx = \frac{\delta(\lambda-\lambda')}{2\lambda \tanh \pi\lambda} \qquad (21)$$

where $\quad \mathrm{Im}\ \lambda = 0, \quad \lambda \geq 0$

By choosing $\lambda \geq 0$ we avoid having to consider A_λ with degenerate eigenvalues, α_λ. λ must be real for the A_λ functions to be normalisable. The factor

$$\frac{1}{2\lambda \tanh \pi\lambda}$$

on the RHS of

(21) is an approximation which is exact for small λ but the orthogonality of the A_λ functions is exact. To solve (16) we expand the function V(x), corresponding to the projection operator in terms of A_λ. Since

$V(x) = 1$

we get

$$\int_0^1 dx\, A_\lambda(x) = \frac{\pi}{\cosh \pi\lambda} \tag{22}$$

by a standard integral.

The eigenvalues of

$$I + \Delta\chi \langle\delta'^2\rangle$$

are given by

$$\gamma_\lambda = 1 - (\tfrac{1}{4} + \lambda^2) \langle\delta'^2\rangle \tag{23}$$

provided the perturbation is small. We see that for sufficiently large λ the perturbation is not small hence this theory is only asymptotically correct. When the perturbation is small the eigenvalues may be written

$$\gamma_\lambda = \exp\left[-(\tfrac{1}{4}+\lambda^2) \langle \delta'^2\rangle\right] \tag{24}$$

After multiplying V in (16) by

$$\left[I + \Delta\chi \langle\delta'\rangle^2\right]^L$$

we obtain the vector V^L at the end of the chain where

$$\sum_{j=0}^{\infty} V_j^L x^j = \int_0^\infty d\lambda \frac{2\pi\lambda \sinh \pi\lambda}{\cosh^2 \pi\lambda} \exp\left[-(\tfrac{1}{4}+\lambda^2) \langle\delta'^2\rangle L \right].$$

$$(1-x)^{-\frac{1}{2}+i\lambda} F(\tfrac{1}{2}+i\lambda, \tfrac{1}{2}+i\lambda, 1, x) \qquad (25)$$

Taking the final projection at the end of the chain corresponds to putting x=0. Thus we obtain

$$|t|^2 = \int_0^\infty d\lambda \frac{2\pi\lambda \sinh\pi\lambda}{\cosh^2 \pi\lambda} \exp\left[- (\tfrac{1}{4}+\lambda^2)\langle\delta'^2\rangle L \right] \qquad (26)$$

We see that in contrast to our expressions for $\langle \frac{1}{t^N} \rangle$, where the spectrum of eigenvalues of χ^N was discrete, the spectrum of the corresponding operator for $\langle |t|^2 \rangle$ is continuous with a spectrum limit of $-\frac{1}{4}\langle\delta'^2\rangle$. The additional complexity makes us wonder how things behave for stronger disorders. How does the spectrum limit change? Does the spectral density change? are there gaps in the spectrum? What effect do the eigenvalues which were not degenerate have? Further direct analysis of equation (13) seems impossible and numerical analysis would be expected to be poorly convergent as a function of the size of the approximating matrix due to there being an infinite number of eigenvalues arbitrarily close to any given eigenvalue. The approach we have taken is to obtain an expression for $\langle |t|^{-2N} \rangle$ at integer N by the same approach as lead to (9). We find that we are able to symmetry reduce this expression to a greater degree than that embodied in equation (13). We then analytically continue our improved symmetry reduced equation for $|t|^{-2N}$ to general N. In principle it should be possible to symmetry reduce equation (13) directly at general N but this seems intractable and our procedure is equivalent.

3. Symmetric decomposition at integer N

The expression for $|t|^{-2N}$ corresponding to (13) for t^{-N} is

$$<|t|^{-2N}> = \left[(1,0) \otimes (0,1)\right]^{\otimes N} \cdot < T^{2N} >^{L} \cdot \left[\begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix}\right]^{\otimes N} \quad (27)$$

We are faced with the problem of finding subspaces of $T^{\otimes 2N}$ which evolve separately due to symmetry differences and which span the projection vectors shown in (27). We shall see that $T^{\otimes 2N}$ has many symmetries and reducing it is a complex task, however the result we obtain by this procedure has a simple interpretation given at the end of this section and it is this simple interpretation which helps us with the eventual analytic continuation to all N.

A vector in the space of $T^{\otimes 2N}$, $V_{j_1 j_2 \cdots j_{2N}}$ has 2N subscripts labelled 1 to 2N, each of which for definiteness we assume to take the values 0 and 1. We will need to consider the symmetry of these vectors under interchange of subscripts and adopt a notation which gives a concise description. If when a pair of subscripts is interchanged in a vector the vector is unchanged it is said to be symmetric in this pair. If the vector is unchanged except that it changes sign it is said to be antisymmetric in this pair. A vector may be symmetric under interchange of any pair from a set e.g. 12 23 13 but can only be antisymmetric in distinct pairs e.g. 12, 34. The notation we use is to enclose antisymmetric pairs in square brakets and sets for which any pair is symmetric in round brakets.

In general a vector in the space of $T^{\otimes 2N}$ has no particular symmetry but the point is that such a vector may be expanded in terms of vectors which do have definite symmetry and whose evolution is simpler.

In the case of $1/t^N$ we found that the subspace of $T^{\otimes N}$ which was totally symmetric in all pairs of subscripts evolved separately. In the present notation this symmetry is (123 -- N). Furthermore the projection vectors of eqn.(9) also have this symmetry and so evolve completely within this space. We chose a set of N+1 orthogonal vectors $V^{J,N}$ labelled by J to span the space

$$V^{J,N}_{j_1,j_2\ --\ j_N} = 1 \qquad \text{if} \quad \sum_{i=1}^{N} j_i = J,\ J = 0,1,2,\ --\ N$$

$$0 \text{ otherwise} \tag{28}$$

where $j_i = 0,1.$

Expanding the symmetric part of $T^{\otimes N}$ in terms of these vectors gives

$$A(I,N)\ \ V^{I,N^T}\ T^{\otimes N}\ V^{J,N} = \chi^N_{I,J} \qquad I,J = 0,\ 1\ --\ N \tag{29}$$

where A(I,N) is chosen to normalise the expansion vectors

$$A(I,N)\ V^{I,N^T}\ V^{I,N} = 1 \tag{30}$$

and $\chi^N_{I,J}$ is given by (11)

The projection vectors of (27) have the symmetry (1,3,5, -- 2N-1) (2,4,6,-- 2N) so they do not lie completely within the subspace of vectors with symmetry (12 -- 2N). This is the reason for the additional complication of $|t|^{-2N}$. We must now find some other subspaces of $T^{\otimes 2N}$.

It is a trivial matter to show that vectors of the type $[1,2]$ $(34 -- 2N)$, for example, also remain of the same type as they are propagated down the chain by $T^{\otimes 2N}$. Such a vector must have the form

$$V_{01\ j_3 -- j_{2N}} = - V_{10\ j_3 j_4 -- j_{2N}}$$
$$V_{11\ j_3 -- j_{2N}} = V_{00\ j_3\ j_4\ -- j_{2N}} = 0 \tag{31}$$

In addition of course the vector must be symmetric under interchange of $j_3\ j_4 -- j_{2N}$. This means that vectors of this type may be written as the cross product of a certain vector in the space of $j_1\ j_2$ and a vector which is symmetric in the remaining subscripts

$$V_{j_1 j_2\ -- j_2 N} = V^{A}_{j_1 j_2} \otimes V^{S}_{j_3 -- j_2 N} \tag{32}$$

$V^{A}_{j_1 j_2}$ is completely specified

j_1	j_2	$V^{A}_{j_1 j_2}$
0	0	0
0	1	1
1	0	-1
1	1	0

(33)

Applying $T \otimes T$ to V^A one finds that V^A is an eigenvector with eigenvalue 1 independent of the disorder provided

$$|r|^2 + |t|^2 = 1 \tag{34}$$

for every member of the ensemble, which corresponds to current conservation. Thus vectors of the space $[12]\ (34\text{-}2N)$ evolve in the same way as vectors of the totally symmetric space with 2N-2 subscripts i.e. $(12\text{--}2N\text{-}2)$. If we choose the basis vectors of $V^S_{j_3 j_4 \cdots j_{2N}}$ as in (28) we obtain a set of orthogonal vectors with symmetry $[12]\ (34\text{-}2N)$ labelled by J. Thus a vector chosen according to this scheme may be labelled by its symmetry and its J, $[12]\ (34\text{--}2N)_J$. Expanding $T^{\otimes 2N}$ in terms of these vectors, as in 26 yields χ^{2N-2} because $V^A_{j_1 j_2}$ evolves in a trivial manner dictated by current conservation leaving only the evolution of the symmetric states to be accounted for.

Basis vectors which are antisymmetric in a different pair of subscripts evolve in the same way e.g. $[13]\ (245\text{-}2N)_J$, $[23]\ (145\text{--}2N)_J$. Let us denote by $P^{2N}_{1\ J}$ the sum of all vectors with just one pair of subscripts antisymmetric where there is always an odd and an even subscript in the pair.

The overall sign of each vector making up $P^{2N}_{1\ J}$ is determined by making the odd antisymmetric subscript play the role of j_1 in equation 29 and 30. In this way we guarantee that $P^{2N}_{1\ J}$ does not vanish. For example

$$P^{4}_{1\ J} = [12]\ (34)_J + [14]\ (23)_J + [3\ 4]\ (12)_J + [32]\ (14)_J \tag{35}$$

The vectors P^{2N}_{1J} have the symmetry (13 -- 2N-1) (24 -- 2N) so we have found that the part of this space spanned by P^{2N}_{1J} can be expressed in terms of vectors which evolve as χ^{2N-2}.

In a similar way, vectors with the pattern [][] ( ) all evolve according to χ^{2N-4} and the vectors P^{2N}_{2J} may be constructed which have the same symmetry as P^{2N}_{1J}. Ultimately, by considering all possible numbers of pairs of subscripts we obtain the set of vectors

$$P^{2N}_{kJ} \qquad \begin{matrix} k=0,\ 1,\ 2 \text{ -- } N \\ J=0 \text{ -- } 2(N-k) \end{matrix} \tag{36}$$

All these vectors are orthogonal, have the symmetry (13 -- 2N-1) (24 -- 2N) and in total there are $(N+1)^2$ of them. This means that they completely span the space. To express any vector of this space in terms of vectors with simpler evolution we first project it onto the set $P^{2N}_{K,J}$. Then we use the fact that P^{2N}_{kJ} can be expressed in terms of vectors which evolve as $\chi^{2(N-k)}$. We obtain the result that for any vectors v, u in the space (1 3--2N-1) (24 --- 2N)

$$u\ (T^{\otimes 2N})^{L}\ v = \sum_{k} u^{k}\ (\chi^{2N-2k})^{L}\ v^{k} \tag{37}$$

where u^k and v^k are the parts of u and v obtained by the above procedure. For the projection vectors of eqn.24 we find the projection onto P^{2N}_{kJ} is zero unless J = N-k so we obtain

$$\langle |t|^{-2N} \rangle = \sum_{k} a^{N}_{k}\ S^{N,k\,T}\ \langle \chi^{2N-2k} \rangle^{L}\ S^{N,k} \tag{38}$$

where $S^{N,k}_{j} = \delta_{j,N-k}$

and a detailed working of the above argument gives

$$a^N_k = ({}^NC_k)^2 / \left[\sum_{j=0}^{N} \left(\sum_{p=0}^{k} (-1)^p \, {}^{N-k}\zeta_{j-p} \; {}^jC_p \; {}^{N-j}\zeta_{k-p} \right)^2 \right] \quad (39)$$

From the point of view of reducing the complexity of our expression for $|t|^{-2N}$ we have reduced the dimension of the transfer matrix from $(N+1)^2$ to a sum of matrices whose dimension is $2(N-k) + 1$. We are fortunate that the expression only involves the χ matrices that we have used before and whose properties were extensively considered in Pendry (82). In that paper a definition of resistance was chosen whose moments evolved as just χ^{2N}. In the large length limit that definition becomes equivalent to ours because χ^{2N} dominates in this limit. Notice that the term which dominates the positive moments of resistance will not, when analytically continued dominate the inverse moments. This is a key difficulty in the theory of our system and for example means that a technique based on numerical calculation of the positive moments, reconstruction of the distribution function, and extraction of the negative moments is extremely unstable and gets more unstable with length.

Equation (38) and (39) are the main result of this section and a simple interpretation of them has been promised.

Define the quantity Z(N) for any scatterer by

$$Z(N) = \sum_{p=0}^{N} ({}^N C_p)^2 \; \frac{|r|^{2p}}{|t|^{2N}} \quad (40)$$

From the definition of the χ matrix (11) and the T matrix (8) we find

$$Z(N) = S^{N,0^T} \chi^{2N}(T)\, S^{N,0} \tag{41}$$

where $S^{N,k}$ is given in (38)

If T_L is the effective T matrix for a chain of length L

$$T_L = \prod_{i=1}^{L} T_i \tag{42}$$

we have

$$Z_L(N) = S^{N,\,0^T} \chi^{2N}\left(\prod_{i=1}^{L} T_i\right) S^{N,\,0} \tag{43}$$

χ is readily shown to have the property

$$\chi^{2N}(T) \cdot \chi^{2N}(T') = \chi^{2N}(T.T') \tag{44}$$

hence

$$Z_L(N) = S^{N,0^T} \left(\prod_{i=1}^{L} \chi^{2N}(T_i)\right) S^{N,0} \tag{45}$$

Using the averaging properties of χ matrices we have

$$\langle Z_L(N)\rangle = S^{N,0^T} \langle\chi^{2N}\rangle^L S^{N,0} \tag{46}$$

We see that (38) can be written

$$\langle |t_L|^{-2N} \rangle = \sum_{k=0}^{N} a_k^N \langle Z_L(N-k) \rangle \tag{47}$$

From equation (33) we see that the definition of Z(N) given in (40) that it is a polynomial in $\frac{1}{|t|^2}$ of order N. The a_k^N are completely determined by the condition that powers of $\frac{1}{|t|^2}$ in (47) cancel leaving just the $\frac{1}{|t|^{2N}}$ term. The argument we have given in equation (40) to (47) is an alternative proof of equations (38) (39).

The disadvantage of this method is that you have to essentially guess equation (38) and then prove that the guess is correct. The symmetric reduction procedure on the other hand provides an algorithmic method of generating equation (38) although it is somewhat cumbersome.

Apart from the moments of $\frac{1}{|t|^2}$, the moments of $|\frac{r}{t}|^2$ are also physically interesting and are simply found to be given by

$$\langle |\frac{r}{t}|^{2N} \rangle = \sum_{k=0}^{N} b_k^N \langle Z_L(N-k) \rangle \tag{48}$$

where the b_k^N can be derived by expanding both sides in terms of powers of $\frac{1}{|t_L|^2}$ and solving the resulting equations, just as was done for eqn.(47)

The aim of this work is to discover the statistics of the conductance, $|t|^2$. To do this we must analytically continue equation (38) to N=-1 and this is the key new ingredient of this paper. The reason for obtaining such a concise expression for $|t|^{-2N}$ in this section was that since the conductance is a much more complicated quantity we must start from the simplest possible expression before we analytically continue.

4. Analytic continuation

In the previous section we found the quantities $\langle |t_L|^{-2N} \rangle$ for integer N in terms of the quantity $Z_L(N-k)$, k=0 1 -- N. $Z_L(N)$ is only defined for integer values of the argument, N, and evolves according to χ^{2N}. In this section we show that $Z_L(N)$ can be generalised to all values of the argument, N, and evolves according to a generalised χ^{2N} matrix. We use the same argument to prove this as was used in eqn. 40-47 at integer N but we go through it in more detail since some of the statements we made about χ^{2N} are not so clearly true for the generalised form. Having obtained $Z_L(N)$ for all N we express $|t|^{2N}$, i.e. the conductance and its moments, in terms of this quantity.

First we choose a generalised definition of $Z_L(N)$ which reduces to (40) at positive integer N.

$$Z_L(N) = \sum_{P=0}^{\infty} ({}^{N}C_p)^2 \quad \frac{|r|^{2p}}{|t|^{2N}} \tag{49}$$

Next we guess a generalised evolution operator $\tilde{\chi}^{2N}$ which we construct to be the same as χ^{2N} at integer N. At integer N we define

$$\tilde{\chi}^{2N}_{ij} = \chi^{2N}_{i+N,j+N} \qquad i,j = -N \text{ -- } 0 \text{ --- } N \tag{50}$$

where χ^{2N} is given by (11). Clearly putting N into the subscripts introduces a new dependence on N into equation (11). Substituting for χ^{2N} we have

$$\tilde{\chi}^{2N}_{ij} = \sum_{p}^{N+i} C_p \; {}^{N-i}C_{N+j-p} \; T_{22}{}^{p} \; T_{21}{}^{N+i-p} \; T_{12}{}^{N+j-p} \; T_{11}{}^{-i-j+p} \tag{51}$$

and the p summation runs over all terms where the lower argument of the binomial coefficients are non negative. Redefining p by putting

$$p = N+j-p' \tag{52}$$

and then dropping the prime we have

$$\overset{\sim}{\chi}{}^{2N}_{ij} = \sum_{p}^{N+i} C_{i-j+p}\, {}^{N-i}C_{p}\; T_{22}^{N+j-p}\; T_{21}^{i-j+p}\; T_{12}^{p}\; T_{11}^{N-i-p} \tag{53}$$

At integer N $\overset{\sim}{\chi}{}^{2N}$ is still the same as χ^{2N} except that the subscripts have been shifted by N as expressed by (50). Defining the vector u

$$u_j = \delta_{jo} \qquad j = -N \text{ -- } 0 \text{ -- } N \tag{54}$$

we have

$$Z(N) = u^{T}\; \overset{\sim}{\chi}{}^{2N}\; u \tag{55}$$

The advantage of these manipulations is that u is independent of N apart from its dimensionality, in contrast to the $s^{N,k}$ of (41) which were defined to depend on N in (38).

Our proposed analytic continuation is to take the subscripts i,j of (53) to run between $-\infty$ to $+\infty$. In the light of our work on $\langle t^{x} \rangle$ this seems natural but we will prove its correctness. The expression for the elements of $\overset{\sim}{\chi}_{ij}$ in (53) is unchanged: all the functions used in it have well defined continuations. The p summation in 53 has a lower bound determined by the condition that the lower argument of the binomial coefficients be non negative, but at non positive integer N it has no upper bound. The first thing to show is that all

elements of $\tilde{\chi}^{2N}$ are finite. Substituting the form (8) for the elements of T we find that in the limit of large p the ratio between one term in the p summation and the previous one is $|r|^2$ which being less than 1 for any scatterer in our model means the sum is uniformly convergent.

Simple substitution of (53) into (55) shows that (55) is consistent with our definition of the analytically continued Z(N) given in (49) In an analogous way to equation (43) but for all N we have

$$Z_L(N) = u^T \tilde{\chi}^{2N} \left(\prod_{i=1}^{L} T_i\right) u \qquad (56)$$

To separate this into a product of χ matrices we need to use the relation

$$\tilde{\chi}^{2N}(T) \,.\, \tilde{\chi}^{2N}(T') = \tilde{\chi}^{2N}(T.T') \qquad (57)$$

at all N. This is the only non trivial property that a generalised transfer matrix must have. It is particularly non trivial because, since the dimension of the $\tilde{\chi}$ matrices is infinite, it is not clear that the product of two $\tilde{\chi}$ matrices is even defined. However we now show explicitly that (57) holds. We wish to calculate

$$\sum_{k=-\infty}^{\infty} \tilde{\chi}^{2N}_{jk}(T) \quad \tilde{\chi}^{2N}_{kl}(T') \qquad (58)$$

To handle the complicated sum we use the relation

$$\tilde{\chi}^{2N}_{kl}(T') = \frac{1}{2\pi} \int_0^{2\pi} dy (T'_{11} + T'_{12} e^{iy})^{N-k} (T'_{22} + T'_{21} e^{-iy})^{N+k} \qquad (59)$$

$$e^{i(k-l)y}$$

as may be verified by using the binomial expansion to expand in powers of e^{iy}. This use of the binomial theorem is valid for any N since

$$\left|\frac{T_{12}}{T_{11}}\right| < 1 \text{ and } \left|\frac{T_{21}}{T_{22}}\right| < 1 \qquad (60)$$

Substituting (53) for $\tilde{\chi}(T)$ in (58) we obtain

$$\tilde{\chi}^{2N}(T) \cdot \chi^{2N}(T') = \sum_{k=-\infty}^{\infty} \sum_{p=o}^{\infty} {}^{N-j}C_{p}\, {}^{N+j}C_{p-k+j} \qquad (61)$$

$$\frac{1}{2\pi}\int_{0}^{2\pi}\left[T_{11}(T'_{11}+T'_{12}e^{iy})\right]^{N-j-p}\left[T_{21}(T'_{11}+T'_{12}e^{iy})\right]^{j+p-k}$$

$$\left[T_{22}(T'_{22}+T'_{21}e^{-iy})\right]^{N+k-p}\left[T_{12}(T'_{22}+T'_{21}e^{-iy})\right]^{p} e^{i(k-l)y}dy$$

Now we can change the summation on k which is restricted such that p-k+j is non negative to a sum on p-k+j which goes from o to ∞, we obtain

$$\tilde{\chi}^{2N}(T).\tilde{\chi}^{2N}(T') = \frac{1}{2\pi}\int_{o}^{2\pi}\left[T_{11}T'_{11}+T_{12}T'_{21}+(T_{11}T'_{12}+T_{12}T'_{22})e^{iy}\right]^{N-j}$$

$$x\left[T_{22}T'_{22}+T_{21}T'_{12}+(T_{22}T'_{21}+T_{21}T'_{12})e^{-iy}\right]^{N+j} e^{i(j-l)y} \qquad (62)$$

Here too the reverse use of the binomial expansion is always justified by eqn (60). By direct calculation of $T.T'$ we form $\tilde{\chi}^{2N}_{jl}(T.T')$ using eqn. (59) and it is found to agree with (62). This completes the proof of eqn. (57).

Now developing equation (56) we have

$$Z_L(N) = u^T \prod_{i=1}^{L} \tilde{\chi}^{2N}(T_i) \quad u \tag{63}$$

and using the statistical independence of $\tilde{\chi}^{2N}$ and the vector on which it acts we average to obtain

$$\langle Z_L(N)\rangle = u^T \langle \tilde{\chi}^{2N}\rangle^L \quad u \tag{64}$$

Now that we have $\langle Z_L(N)\rangle$ for any N we must tackle the problem of expanding $|t|^2$ in terms of it. We first notice that the definition of Z given in (49) can be rewritten in terms of the hypergeometric function F. The function F may be defined in terms of a power series and identifying the terms gives

$$Z_L(N) = |t|^2 (1-|r|^2)^{-(N+1)} F(-N,-N,1,|r|^2) \tag{65}$$

The problem of expanding $|t|^2$ in terms of Z(N) is the same as the problem of expanding 1 in terms of the functions g given by

$$g(N,|r|^2) = (1-|r|^2)^{-(N+1)} F(-N,-N,1,|r|^2) \tag{66}$$

If we put $N = -\frac{1}{2} - i\lambda$ the function of becomes the $A_\lambda(|r|^2)$ of eqn. (20) and the problem of expanding 1 in terms of A_λ was solved in that section using the orthogonality relation for the A_λ functions.

We find

$$1 = \int_0^\infty g(-\tfrac{1}{2}-i\lambda,\ |r|^2)\ 2\pi\ \frac{\lambda \sinh \pi\lambda}{\cosh^2 \pi\lambda}\ d\lambda \tag{67}$$

and hence, using equation (62) and averaging

$$\langle |t_L|^2 \rangle = \int_0^\infty \langle Z_L(-\tfrac{1}{2}-i\lambda) \rangle \frac{2\pi\lambda \sinh \pi\lambda\ d\lambda}{\cosh^2 \pi\lambda} \tag{68}$$

This in conjunction with the expression for Z_L in (64) is our final solution for $|t_L|^2$.

To find an expression for $|t_L|^{2N}$ we must expand

$$(1 - |r|^2)^{N-1}$$

in terms of $g(N,|r|^2)$. This can be simply done using the orthogonality relation (21) we find

$$\langle |t_L|^{2N} \rangle = \int_0^\infty \langle Z_L(-\tfrac{1}{2}-i\lambda) \rangle 2\pi\lambda \tanh \pi\lambda\ \not{g}(N,\lambda)\ d\lambda \tag{69}$$

where

$$\not{g}(N,\lambda) = \int_0^1 (1 - |r|^2)^{N-1}\ g(-\tfrac{1}{2}-i\lambda,\ |r|^2)\ \ d(|r|^2) \tag{70}$$

the integral (70) is a standard one.

$$\phi(N,\lambda) = \frac{\Gamma\left(N-\frac{1}{2}+i\lambda\right)\,\Gamma\left(N-\frac{1}{2}-i\lambda\right)}{\Gamma^2(N)} \qquad (71)$$

$\mathrm{Re}\ N > \frac{1}{2}$

This achieves the goal of this paper since we have found the conductance and its moments. The solution is expressed in (64), (69) and (71). It is natural to ask whether the $N > \frac{1}{2}$ restriction in (71) can be overcome and we find that it can but defer the discussion of this to a later paper since it involves some complications. One might expect that it would be possible to find the moments of $|t|^2\ |r|^{-2}$ by the approach since in the previous section we found moments of $|r|^2\ |t|^{-2}$ by a simple extension to the theory for the moments of $|t|^{-2}$. In fact this question too requires rather involved consideration since the singularity of $|t|^2\ |r|^{-2}$ at $|r|=0$ cannot be expanded in terms of $Z(N)$.

5. Analytic properties and limiting cases

The first property we show is

$$Z(N) = Z(-N-1) \tag{73}$$

First we write

$$Z(N) = (1 - |r|^2)^{-N} F(-N,-N, 1, |r|^2) \tag{74}$$

Now using a standard relation for the hypergeometric function we have

$$Z(N) = (1-|r|^2)^{N+1} F(N+1, N+1, 1, |r|^2) \tag{75}$$

$$= Z(-N-1)$$

The same symmetry of the evolution operator was found by Kappus and Wegner (1981) although their formulation was quite different. By expressing the elements of $\overset{\sim}{\chi}^{2N}$ in terms of hypergeometric functions the symmetry in this operator may be extracted. We find

$$\overset{\sim}{\chi}^{2N}_{ij} = \overset{\sim}{\chi}^{-2(N+1)}_{ij} \frac{(N+i)!\ (-N-1+j)!}{(-N-1+i)!\ (N+j)!} \tag{76}$$

which is a similarity transformation.

Putting $N = -\frac{1}{2}-i\lambda$ in (73) we have

$$Z(-\tfrac{1}{2}-i\lambda) = Z(-\tfrac{1}{2}+i\lambda) \tag{77}$$

but we also have

$$Z(-\tfrac{1}{2}+i\lambda) = Z(-\tfrac{1}{2}-i\lambda)^* \tag{78}$$

hence $Z(-\frac{1}{2}+i\lambda)$ is real for any λ

The next property is to find the maximum of $Z_L(-\frac{1}{2}-i\lambda)$ as a function of λ. It is convenient to write

$$Z(-\tfrac{1}{2}-i\lambda) = \frac{1}{2\pi}\int_0^{2\pi} dy\ (T_{11} + T_{12}e^{iy})^{-\frac{1}{2}-i\lambda}(T_{22}+T_{21}e^{-iy})^{-\frac{1}{2}-i\lambda}$$

$$= \frac{1}{2\pi}\int_0^{2\pi} (T_{11}T_{22} + T_{12}T_{21} + T_{11}T_{21}e^{-iy} + T_{12}T_{22}e^{iy})^{-\frac{1}{2}-i\lambda} \tag{79}$$

Note that the quantity in the braket of (79) is real and non negative. Now we use the Cauchy Schwarz inequality

$$\left| \int f(Z)\, dZ \right| \leq \int |f(Z)|\, dZ \tag{80}$$

Hence

$$|Z(-\tfrac{1}{2}-i\lambda)| \leq \frac{1}{2\pi}\int_0^{2\pi} (T_{11}T_{22}+T_{12}T_{21}+T_{11}T_{21}^{-iy}+T_{22}T_{12}e^{iy})^{-\frac{1}{2}}dy \quad (81)$$

$$\Rightarrow \quad |Z(-\tfrac{1}{2}-i\lambda)| \leq |Z(-\tfrac{1}{2})| \quad (82).$$

This statement is true for any value of r and t. So we can be sure that it holds for the ensemble average.

$$\langle|Z(-\tfrac{1}{2}-i\lambda)|\rangle \leq \langle Z(-\tfrac{1}{2})\rangle \quad (83)$$

Using (74) again

$$|\langle Z(-\tfrac{1}{2}-i\lambda)\rangle| \leq \langle Z(-\tfrac{1}{2})\rangle \quad (84)$$

Calculations to be presented in this section show that the spectrum of eigenvalues of $\tilde{\chi}^{2N}$ at $N=-\frac{1}{2}-i\lambda$ is discrete for weak disorder and we assume this is always true. The reality condition means that the eigenvalues are either real or occur in complex conjugate pairs. The requirement that $Z(-\frac{1}{2})$ be non negative means that the possibility of its two largest eigenvalues being a complex pair is excluded. The eigenvalue with largest modulus in the evolution of $Z(-\frac{1}{2})$ must be real and non negative and since this will dominate for large lengths we see from (84) that this must be the largest eigenvalue at any λ. In general, however, when $\lambda\neq 0$ the possibility of the largest eigenvalue being a complex conjugate pair cannot be excluded.

Let us call the largest eigenvalue of χ^{2N} at $N=-\frac{1}{2}-i\lambda$, $\exp\left[\alpha_o(\lambda)\right]$ If $\alpha_o(\lambda)$ is an analytic function of λ at $\lambda=0$, as we expect is "usually" the case, then the symmetry (77) shows that for small λ

$$\alpha_o(\lambda) = \alpha^{(o)} - \alpha^{(2)}\lambda^2 \tag{85}$$

where $\alpha^{(2)}$ is positive. If we assume that for other λ the eigenvalue does not come close to $\alpha^{(0)}$ we can extract a long length limit for $\langle|t_L|^{2N}\rangle$ from (69). $\langle Z(-\frac{1}{2}-i\lambda)\rangle$ will have the form

$$Z_L(-\tfrac{1}{2}-i\lambda)=\left[C^{(o)} + C^{(2)}\lambda^2\right]\exp\left[(\alpha^{(o)}-\alpha^{(2)}\lambda^2)L\right] \tag{86}$$

$$\lambda << 1$$

The function multiplying Z in (66) may be expanded to give

$$2\pi\lambda \tanh \pi\lambda f(N,\lambda) = B(N)\lambda^2 \qquad \lambda << 1 \tag{87}$$

For very large lengths small values of λ are significant in the integral and we find

$$|t_L|^{2N} \simeq \int_0^\infty B(N)C^{(o)}\lambda^2 \exp\left[(\alpha^{(o)} - \alpha^{(2)}\lambda^2)L\right] d\lambda \tag{88}$$

$$= \frac{\pi}{4}^{\frac{1}{2}}B(N)\, C^{(o)} \quad \frac{1}{(\alpha^{(2)}L)^{3/2}} \quad \exp \alpha^{(o)}L \tag{89}$$

Physically α^o must be negative in a disordered system so the moments of the conductance decay exponentially to zero with the length of the chain but the exponential is multiplied by $L^{-3/2}$. This pre-multiplier originates from the integral over λ and although it is

quite natural within the development of our theory it is perhaps not what one would naively have expected a transfer matrix approach to give. Transfer matrices would normally be expected to give the decay with length as a sum of exponentials. We see that the spectrum limit, $\alpha^{(o)}$ plays a dominant role in (89).

Evaluating B(N) we have

$$B(0) = 2\pi^2 \quad , B(1)=\pi^2/2 \tag{90}$$

and we find the relative fluctuation of the conductivity is

$$\frac{(\langle|t|^4\rangle - \langle|t|^2\rangle^2)^{\frac{1}{2}}}{\langle|t|^2\rangle} \tag{91}$$

$$= \pi^{-5/4} \left[2C^{(o)}\right]^{-\frac{1}{2}} (\alpha^{(2)}_L)^{-\frac{3}{4}} \exp\left[-\tfrac{1}{4}\alpha(o)L\right]$$

$$-\alpha(o)L \gg 1$$

This is exponentially divergent for large lengths so we see that the distribution of conductances, like the distribution of resistances gets broader as the length increases i.e. there is no thermodynamic limit.

To make contact with the theory of section 2 we turn to the weak disorder limit which is now very greatly simplified. For no disorder the eigenvalues γ_j of $\underset{\sim}{\chi}^{2N}$ at $N=-\frac{1}{2}-i\lambda$ are found by choosing k to diagonalise as before for eqn.(14) and (15) and

$$\gamma_j = e^{-i2kj} \qquad j=-\infty \text{ -- } o \text{ -- } \infty \tag{92}$$

The projection vectors u of (64) are eigenvectors corresponding to the eigenvalue with j=0. If $k \neq p\pi/n$ non degenerate perturbation theory may be used. We obtain

$$\gamma_0 = 1 - \langle \delta'^2 \rangle \, . \, (\tfrac{1}{4} + \lambda^2)$$

$$= \exp\left[-(\tfrac{1}{4}+\lambda^2) \langle \delta'^2 \rangle \right] \qquad (93)$$

where δ is given in (15). In this case we have

$$Z_L(-\tfrac{1}{2}-i\lambda) = \exp\left[-(\tfrac{1}{4}+\lambda^2) \langle \delta'^2 \rangle \; L \right] \qquad (94)$$

which when substituted into the general form (68) or (69) gives eqn.(24) which we found by more specialised arguments in the first section and was originally found by Abriksov and Ryhzkin. Abriksov (1981) also took the long length limit for this case and it takes precisely the form of our previous argument when the parameters $c^{(o)}$, $\alpha^{(o)}$ and $\alpha^{(2)}$ are obtained from the weak disorder limit. In other words we have shown that the long length behaviour for general disorder is qualitatively the same as for weak disorder but involves parameters which cannot be found analytically in general. In the next section we use a numerical technique to evaluate some of these parameters.

In the case where $k = p\pi/n$, non degenerate perturbation theory cannot be used. This effect was discovered by Kappus and Wegner (1981) and further work on it for the localisation length was done

by Lambert (1983) and ourselves. The only anomaly to order $<\delta^2>$ is at $k=\pi/2$ corresponding to the band centre and causes the largest eigenvalue of $\chi^{2(-\frac{1}{2})}$, which dominates the long length behaviour (94), to be altered. We analysed this by finding the perturbation matrix and diagonalising the degenerate subspace. We found

$$Z_L(-\tfrac{1}{2}) = \exp\left[-0.225<\delta'^2>L\right] \tag{95}$$

which agrees with Kappus and Wegner's value.

To gain further insight into the behaviour of our symmetry reduced equations for $|t|^{2N}$ we examine the strong disorder limit although this limit can be obtained from the un-reduced form (13). To find the form of $\tilde{\chi}^{2N}_{ij}$ in the strong disorder limit we write it in terms of hypergeometric functions, (53) becomes

$$\tilde{\chi}^{2N}_{ij} = T_{22}^{N+j}\, T_{21}^{i-j}\, T_{11}^{N-i}\, F(i-N,-N-j,1+i-j,|r|^2)^{N+i}\, C_{j-j'} \tag{96}$$

$$i,j = -\infty \text{ -- } -1\ 0\ 1 \text{ --- } \infty \quad , \quad i-j > 0$$

$$\chi^{2N}_{ij}(T) = \chi^{2N}_{-i,-j}(T^*)$$

Substituting the form (8) for T and taking the strong disorder limit we have

$$\tilde{\chi}^{2N}_{m\,m'} = {}^{N+m}C_{m-m'}(-1)^m\, e^{-ik2m}\, \delta'^{2N}$$

$$\lim_{\delta\to\infty} F\left(m-N,\ -N-m',\ 1+m-m',\ \frac{\delta'^2}{1+\delta'^2}\right) \tag{97}$$

$$m - m' \geq 0$$

The behaviour of the hypergeometric function as the argument tends to 1 is found from a standard relation. We find

$$\overset{\sim}{\chi}{}^{2(-\frac{1}{2}-i\lambda)}_{m\,m'} = (-1)^m\, e^{-i2km}\left[\frac{\Gamma(-2i\lambda)\quad \delta'^{-1-2i\lambda}}{\Gamma(\frac{1}{2}-i\lambda-m')\,\Gamma(\frac{1}{2}-i\lambda+m')}\right. \tag{98}$$

$$\left. + \quad \frac{\Gamma(2i\lambda)\quad \delta'^{-1+2i\lambda}}{\Gamma(\frac{1}{2}+i\lambda+m)\;\Gamma(\frac{1}{2}+i\lambda-m)}\right]$$

Expression (98) is the same for both $m - m' \geqslant 0$ or $m - m' \leqslant 0$. We see that $\chi^{2(-\frac{1}{2}-i\lambda)}$ has two separable parts which we interpret as a spectral representation of the matrix

$$\chi^{2(-\frac{1}{2}-i\lambda)} = \sum_{m=1}^{2} \gamma_m\, |v_m\rangle\langle v_m| \tag{99}$$

Unfortunately the eigenvectors we can identify from (98) are not normalisable although we know from (57) that all eigenvectors must be normalisable. Clearly by taking the strong disorder limit the normalisation of the eigenvectors has been lost. This can be circumvented by calculating the square of (99) by forming

$$\chi\ (T(\delta'_1)\ .\ T(\delta'_2))$$

and then taking the strong disorder limit of this quantity. Comparison with (98) then enables us to identify the eigenvalues as

$$\gamma_{\pm} = \langle \delta^{-1 \pm 2i\lambda} \rangle \tag{100}$$

As we would expect the eigenvalues are not functions of k. For a distribution consisting of a single value of Δ well outside the band the eigenvalues have the same modulus for all values of λ. For other distributions of Δ where the strong disorder limit holds the eigenvalues at λ are in general a complex conjugate pair except at $\lambda=0$. This seems to be a rather pathological result which one might expect to give rise to some odd behaviour for $|t|^{2N}$. In fact we will show that this is not the case and hence we learn what could be an important lesson for numerical work on these eigenvalues, that this type of behaviour (100) does not necessarily give anomalous behaviour for $|t|^{2N}$. Evaluating the projections (64) we have

$$Z_L(-\tfrac{1}{2}-i\lambda) = \frac{\Gamma(-2i\lambda)}{\Gamma^2(\frac{1}{2}-i\lambda)} \langle \delta^{-1-2i\lambda} \rangle^L (2 \sin k)^{1+2i\lambda}$$

$$+ \frac{\Gamma(2i\lambda)}{\Gamma^2(\frac{1}{2}+i\lambda)} \langle \delta^{-1+2i\lambda} \rangle^L (2 \sin k)^{1-2i\lambda} \tag{101}$$

The 2 sin k factors are an uninteresting complication so let us set them to 1. Now write

$$\langle \delta^{-1 \pm 2i\lambda} \rangle^L = \int P(\delta_1) P(\delta_2) \cdots P(\delta_L) (\delta_1 \delta_2 \cdots \delta_L)^{-1 \pm 2i\lambda} \, d\delta_1 d\delta_2 \cdots d\delta_L \tag{102}$$

we obtain

$$Z_L(-\tfrac{1}{2}-i\lambda) = \int P(\delta_1)\, P(\delta_2) \cdots P(\delta_L)\, d\delta_1 d\delta_2 \cdots d\delta_L$$

$$\left(1 - \frac{d^2}{1+d^2}\right)^{-\frac{1}{2}+i\lambda} F\left(\tfrac{1}{2}+i\lambda,\ \tfrac{1}{2}+i\lambda,\ 1,\ \frac{d^2}{1+d^2}\right)$$

$$\text{where } d = \delta_1 \delta_2 \cdots \delta_L \quad >> 1 \tag{103}$$

substituting into (69) gives

$$|t_L|^{2N} = \langle (\delta_1 \delta_2 \cdots \delta_L)^{2N} \rangle \qquad N \gg \tfrac{1}{2}$$

$$\Rightarrow |t_L|^{2N} = \langle \delta^{2N} \rangle^L \tag{104}$$

The same result holds for the moments of $\frac{1}{|t|^N}$ as shown originally by Abrahams and Stephen (1980) and may be considered as being due to the dominance of Δ_n in (5) making the matrix behave as a scalar.

The preceding analysis may be used in reverse to find the eigenvalues of $\overset{\sim}{\chi}$ in the ordered case outside the band. Elementary band theory gives

$$|t|^{2N} \sim e^{-2kLN} \qquad \cosh k = \Delta/_2 \tag{105}$$

hence the largest eigenvalues of $\overset{\sim}{\chi}^{2(-\frac{1}{2}-i\lambda)}$ are

$$\gamma_\pm = e^{k(-1\pm 2i\lambda)} \tag{106}$$

6. Numerical investigation - Anomaly for binary alloys

The complicated nature of the solution (65) means that we cannot calculate the moments of $|t|^2$ exactly for any length. However in the long length limit the situation is simpler and it is possible to evaluate the parameters in (83) for general disorder. The most interesting parameter is $\exp[\alpha^{(o)}]$ which dominates the decay of all the moments. This quantity is just the largest eigenvalue of $\tilde{\chi}^{2N}|_{N=-\frac{1}{2}}$. Equation (83) is applicable when all other eigenvalues of $\tilde{\chi}^{2N}|_{N=-\frac{1}{2}-i\lambda}$ are less than this one which is the usual case. However the case where other eigenvalues have modulus equal to this is very interesting.

The largest eigenvalue of $\tilde{\chi}^{2N}$ may be calculated by truncating the matrix which should be infinite to one of finite dimension by taking subscripts to range from -M --- 0 --- +M. The convergence of this procedure can be checked numerically by altering M. The transformation to propagating waves (6) involves an arbitrary parameter k. The eigenvalues of the full $\tilde{\chi}^{2N}$ matrix are independent of the choice of k but this is only the case for the truncated form if the approximation is well converged. Changing the choice of k changes the elements of the matrix quite drastically but the degree to which the eigenvalues are unchanged provides a check on convergence.

It is clear that in the limit of weak disorder the truncation approx will be a good one however we find it is adequate in many regimes.

Forming the matrix $\tilde{\chi}^{2N}$ poses a few minor problems. Firstly the definition (50) involves an infinite sum on p. Since this sum is uniformly convergent this is easily approximated by a finite sum. We found 20 terms to be sufficient. The average of $\tilde{\chi}$ over a distribution of disorder must be calculated numerically. We chose two distributions $P(\Delta)$. One comprises two delta functions of weight $\frac{1}{2}$ at $\Delta = E \pm D$, the other is a gaussian centred on E with standard deviation D. Integration over the two delta function distribution is of course trivial but for the gaussian we use a numerical procedure of integration over a distribution of 64 delta functions which have the first 128 moments the same as a gaussian. Fig. 1 and 2 show the moduli of the largest and second largest eigenvalue against energy with D=1.0 for the two delta function and gaussian distribution respectively. We find that the smaller the eigenvalue the worse the convergence. For the two delta function graph we find a worst case error of $2\frac{1}{2}\%$ in the largest eigenvalue and 10% for the second largest on changing the choice of k and reducing the dimension of the approximating matrix from 21 to 11, which indicates that all features of the largest eigenvalue are significant, but only the large features of the second largest eigenvalue are significant. For the gaussian the error in the largest eigenvalue was only 0.1% and for the second largest 3%, estimated by the same procedure.

The graph for the two delta function distribution shows many features which are completely absent for the gaussian. This was also found in our work on the average of ln t and is attributable

to residual band structure effects. There is a very marked feature in the largest eigenvalue of the two delta function curve at E=1.0. Further investigation of the nearby disorders, D=0.9, 1.1, 1.3, shows that for D=0.9 the feature is almost entirely absent. At D=1.1 (Fig. 3) it is even broader and deeper and infact the largest and second largest eigenvalues collide and become complex. D=1.3 is similar to D=1.1. The feature seems to be associated with one of the delta functions being at $\Delta=0$ while the other is $\Delta > 2$ i.e. outside the band edge for the pure system. Infact we know that the largest eigenvalue at $\lambda=0$ cannot be complex so our numerical procedure is evidently failing to represent this feature correctly. The feature is clearly one of great importance since it may give a qualitative departure from the weak disorder perturbation theory result and it appears the feature can only be obtained within a theory capable of dealing with rather general types of disorder which is the essential advance of this work.

In section 5 we used perturbation theory to handle the weak disorder case when the distribution of disorder is very narrow. It is intriguing and surprising that when one of the δ functions is within the band and the other is far outside the band another perturbation theory may be used.

For the two delta function distribution of disorder the averaged $\tilde{\chi}$ is given by

$$\tilde{\chi}=\tfrac{1}{2}\{\tilde{\chi}(\Delta_1)+\tilde{\chi}(\Delta_2)\} \qquad (107)$$

where the $\tilde{\chi}$ on the RHS are the ordered $\tilde{\chi}$ at the given Δ. Suppose that Δ_1 is within the band then $\tilde{\chi}(\Delta_1)$ may be diagonalised such that

$$\tilde{\chi}_{m\,m'}(\Delta_1) = e^{-i2mk}\,\delta_{m\,m'} \quad m,m' = -\infty \cdots 0 \cdots \infty \tag{108}$$

$$\cos k = \frac{\Delta_1}{2.}$$

If $|\Delta_1 - \Delta_2| \gg 1$, $\tilde{\chi}(\Delta_2)$ can be approximated by the strong disorder limit(98). We see that $\tilde{\chi}(\Delta_2)$ is a small perturbation when $|\Delta_1 - \Delta_2|$ is sufficiently large. Non degenerate perturbation theory for the m=0 eigenvalue gives

$$\gamma = \tfrac{1}{2}\left[1 + \delta'^{-1}\left(\frac{\Gamma(-2i\lambda)}{\Gamma^2(\frac{1}{2}-i\lambda)}\,\delta'^{-2i\lambda} + \delta'^{2i\lambda}\,\frac{\Gamma(2i\lambda)}{\Gamma^2(\frac{1}{2}+i\lambda)}\right)\right]$$

In the case where $\Delta_1 = 0$, $k = \pi/2$, and the eigenvalues of even m are degenerate with value 1. Degenerate perturbation theory requires us to find the eigenvalues of the perturbation matrix in the degenerate subspace. We use (99) to expand $\tilde{\chi}(\Delta_2)$ in the strong disorder limit and taking the subspace of m, m' even gives a separable matrix just as for the strong disorder case. The difficulty we found in the strong disorder limit, that the eigenvectors are not normalisable, recurs here. The perturbation we must diagonalise is $\Delta\chi$ given by

$$\Delta\chi_{m\,m'} = \tfrac{1}{2}\left[1 + (-1)^{m+m'}\right]\,\tilde{\chi}_{m\,m'}^{\,2}(\Delta_2) \tag{109}$$

which has zero elements when one subscript is even and the other odd. We are only really interested in the subspace of both subscripts even but it is convenient to diagonalise both subspaces together. We notice that when $k = \pi/2$ we have

$$\Delta\chi = \frac{1}{2}\left[\tilde{\chi}(\Delta_2) + \tilde{\chi}(0)\,\tilde{\chi}(\Delta_2)\,\tilde{\chi}(0)\right] \tag{110}$$

Now we can easily form $\Delta\chi^2$ as a sum of products of $\tilde{\chi}$ matrices. Each product of $\tilde{\chi}$ matrices may be written as a single $\tilde{\chi}$ matrix formed by the resultant T matrix using (57). We can then take the strong disorder limit and compare with the strong disorder limit of (109) We find that to leading order in $1/S$ the eigenvalues of $\Delta\chi$ are

$$\lambda_{\pm} = \frac{1}{4}\, 2^{1\pm i2\lambda} \tag{111}$$

It is very surprising that this result is independent of Δ_2 and can be traced to the fact that for large Δ_2

$$T(0)\,T(\Delta_2)\,T(0)\,T(\Delta_2) \;\alpha\; \Delta_2 \tag{112}$$

where $T(\Delta)$ is the T matrix (8) for that value of Δ. One would expect the product (112) to scale as Δ_2^2 for large Δ but a special cancellation gives the linear result. Thus we find that the perturbation doesn't vanish as $\Delta_2 \to \infty$ so the perturbation theory is never exact. However we proceed with our approximate perturbation theory and find that the eigenvalues of (107) are

$$\gamma_{\pm} = (1 + \frac{1}{4}\; 2^{\pm 2i\lambda}) \tag{113}$$

consequently

$$Z_L = \gamma_+^L + \gamma_-^L$$

For large lengths the dominant contribution to $|t|^{2N}$ will come from λs for which γ is largest i.e. in the neighbourhood of

$$\lambda = \frac{\pi n}{\ln 2} \qquad n = 0, 1, \text{---} \tag{114}$$

Thus

$$Z_L(-\tfrac{1}{2}-i\,(\frac{\pi n}{\ln 2} + \Delta\lambda\,))$$

$$= 2\left(\frac{1}{2}\right)^L \exp\left[-(\ln 2)^2 \Delta\lambda^2 \; L\right] \cos \frac{\ln 2\, \Delta\lambda L}{2}$$

$$n=0,\ 1,\ 2\ \text{---} \tag{115}$$

Substituting this form into (69) and expanding the factor which multiplies Z about each point (114)

$$2\pi\lambda \quad \tanh \pi\lambda f(N,\lambda) = \sum_{i=o}^{\infty} a_{ni}\, \Delta\lambda^i \tag{116}$$

we can approximate $|t|^{2N}$ by an integral for every n of (116) over $\Delta\lambda$ from $-\infty$ to ∞. The terms in odd powers of $\Delta\lambda$ vanish and the even ones give contributions which scale as

$$L^{-\frac{1}{2}} \exp\left(-\frac{L}{4}\right)\left(\frac{1}{2}\right)^L \tag{117}$$

for large lengths which differs from our general form (89) in the prefactor of the exponential decay. We have found that not only does the exponential decay rate change dramatically as one of the delta functions goes through the band centre but also that the general form is slightly modified.

Conclusion

We have developed the transfer matrix approach by applying improved symmetry reduction to give expressions for $\langle|t|^{-2N}\rangle$ at integer N. The generalised transfer matrix approach of our previous work has been made more rigorous and extended in the light of the symmetry reduction to give expressions for $\langle|t|^{2N}\rangle$, $N > \frac{1}{2}$ which we use to find the average conductance and its moments. The theory is valid for any distribution of disorder and any length of chain. We have presented limiting behaviour for weak and strong disorder and long length behaviour for "typical" disorders. A simple numerical procedure has been developed to evaluate the important parameters in the long length behaviour for any disorder and results were presented. A new anomaly was found in the conductance of the binary alloy model as a function of energy and was interpreted as being due to one type of atom being at the band centre while the other is well outside the band.

Acknowledgements

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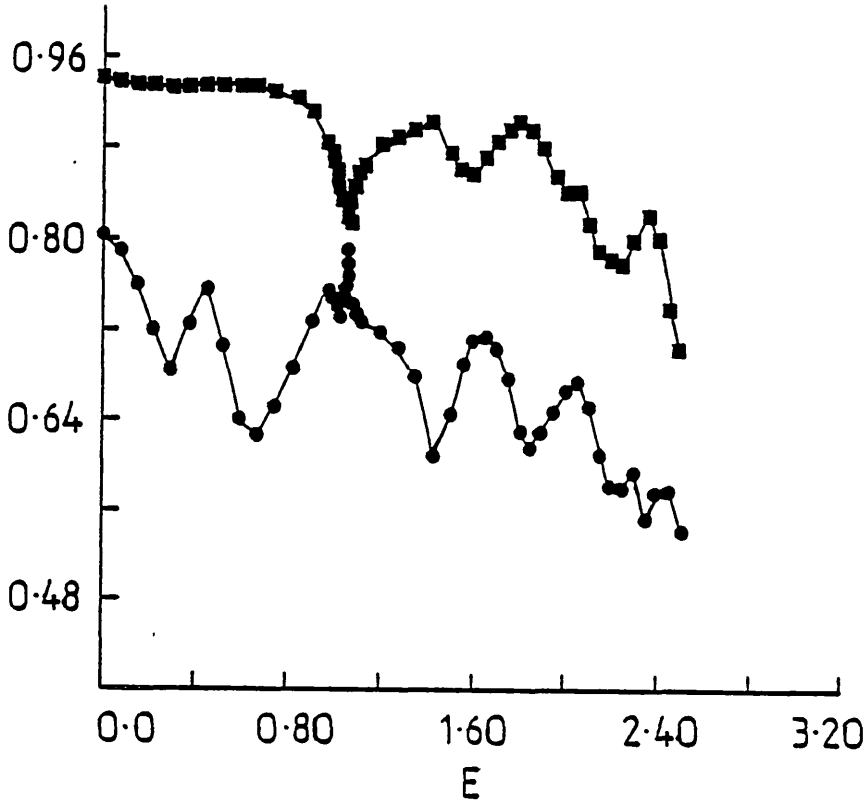

FIGURE 1

Moduli of the largest and second largest eigenvalues of $\tilde{\chi}^{2(-\frac{1}{2})}$ for the binary alloy model of disorder plotted against energy in units of V. The separation of the site energies of the two types of atom is 2 i.e. variance is 1.

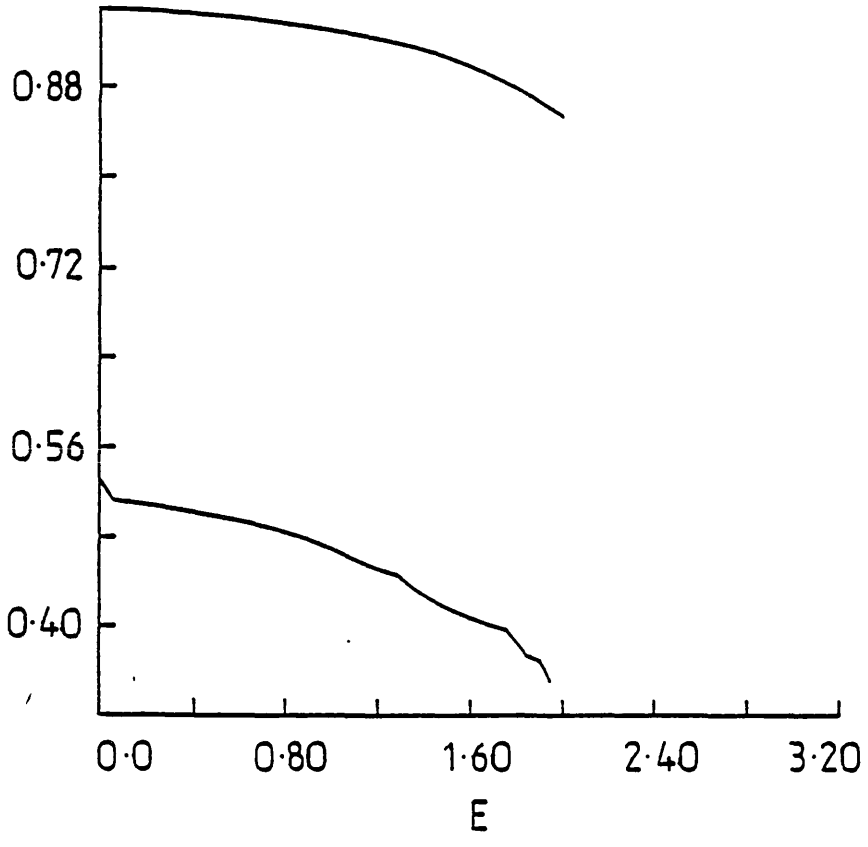

FIGURE 2

Moduli of the largest and second largest eigenvalues of $\overset{\sim}{\chi}^{2(-\frac{1}{2})}$ for a gaussian distribution of disorder plotted against energy in units of V. The variance of the gaussian is 1.

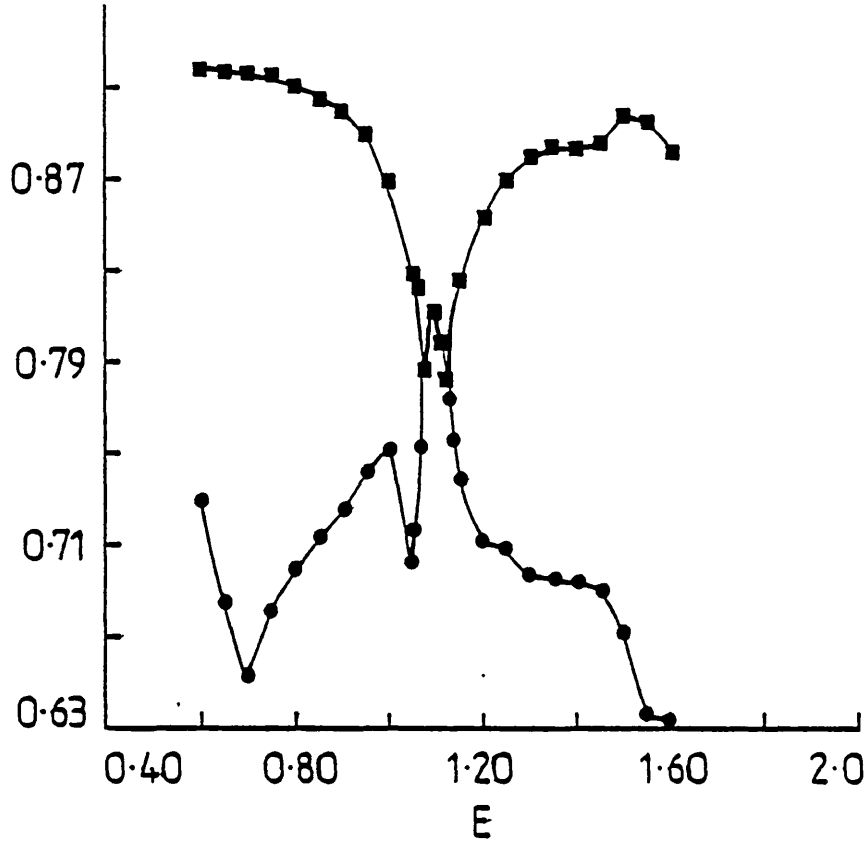

FIGURE 3

As for fig. 1 but here the separation of the site energies of the atoms is 2.2. The collision of the eigenvalues cannot be correct (see text) but shows that the anomaly is larger than in Fig. 1.

VI FUTURE WORK

The techniques of Chapter V make it possible to average almost any function of $|t|^2$. In that chapter some restrictions were imposed on the powers of $|t|^2$ which can be averaged but extension to all powers is straight forward. Although a few mathematical points remain to be cleared up it should be possible to average all powers of $|r||t|^{-1}$ and even $\delta(x - |t|^2)$. The average of this last function is of course just P(x) which would be a complete solution to the problem. Extensions of the theory to include off diagonal disorder are probably straightforward.

It should be possible by straightforward application of the principles established in the work to find averages of correlation functions, as mentioned in Section I.9, which would lead to better understanding of the conductive properties of a single chain as a function of energy and to an understanding of the frequency dependence of ballistic transport.

More theoretically challenging are the possibilities of extension of the model, either by inclusion of inelastic scattering effects or extension to higher dimensions. The techniques developed in this work are not intrinsically limitted to 1D and extension to higher dimension has been achieved to some extent by Pendry (1984).

"No man but a blockhead ever wrote except

for money"

Samuel Johnson

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