

Reflection of Waves from Disordered Media

by
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Thesis submitted for the degree of
Doctor of Philosophy of the University of London
and the
Diploma of Imperial College

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August 7, 1990

Abstract

For one-dimensional (1-D) disordered systems, we establish a new formalism, involving an infinite transfer matrix, to calculate the moments of the reflection coefficient. We use this formalism, together with perturbation theory, to find analytical expressions for these moments and for the Fourier components of the distribution of the phase of the reflection coefficient $P(\theta)$, for weak disorder. These solutions allow us to examine analytically properties of these quantities, including anomalies which occur at weak disorder. Also in 1-D, we use a formalism involving an integral Dyson equation to find $P(\theta)$ for two different types of disorder, the binary alloy and the symmetric exponential. In particular, for the binary alloy, we find that $P(\theta)$ contains an infinity of power-law singularities under generic circumstances. For the symmetric alloy, we find an exact solution for $P(\theta)$ which we also use to find analytical properties. In 3-D, we use a simple perturbation theory to calculate the moments of the reflected intensity and the distribution of each element of the reflection matrix for a single scattering model.

We extend the formalism used for reflection to include moments of the transmitted intensity in 1-D and use it together with an approximate technique to find analytic forms for these moments. Finally, we give a new simplified derivation of the generalised transfer matrices of Kirkman and Pendry [1,2] and Pendry and Castaño [3] which does not require analytic continuation.

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Acknowledgements

I would like to thank John Pendry, my supervisor; Jean–Marc Luck, an academic visitor to Imperial College in 1989; and Jean Heinrichs, a distant acquaintance; for their great contribution to my work and for helping me form the ideas for this thesis over the past three years.

I would also like to thank all members of the Imperial College Solid State Theory Group past and present, for help I have received with academic problems and for making my stay so enjoyable. In particular I would like to thank Pavel Pinkava, Karl Hugill, John Taylor and John Roberts.

Finally, I would like to thank Nina, my family and my friends for their love and support during the writing of this thesis.

Chapter 1

Introduction

In 1987, on the suggestion of J B Pendry, we began to look at a new formalism for calculating reflection from disordered surfaces. This research has led to an in-depth study of reflection, both from disordered one dimensional (1-D) wires and, for weak scattering, from three dimensional (3-D) wires. We have used both the new formalism as well as other methods, through collaborative work. The study of the new formalism has also led to a greater understanding of the generalised transfer matrices [4] used in calculating transport properties of disordered systems. This thesis is a part of the considerable effort which has gone into understanding the properties of disordered systems.

For an in-depth review of the field the reader is referred to the many books reviews and conference proceedings e.g [5,6,7,8,9,10]. The following sections of the introduction will concentrate on defining the problem of disorder and setting the context for this thesis.

1.1 Survey

‘Insofar as a collection of things is not in conformity with an ordering rule the collection is disordered’ *Cusack* 1987.

Within this definition, a disordered system can simply be one which is finite or one which possesses even a single defect. However, we will be considering more

drastic forms of disorder. Three main types exist: topological, vibrational and substitutional. Topological (or geometric) disorder is a form of randomness in which there is no translational periodicity. It can occur to different degrees, some amorphous materials have considerable short range order while others do not, however, none have any long range order. Examples are, liquids and glasses where bond lengths and numbers of nearest neighbours can be quite different from site to site. Vibrational disorder occurs at finite temperatures because the atoms in a crystalline lattice vibrate about their lattice sites, breaking perfect periodicity. This type of disorder is not the same as topological disorder since the atoms vibrate about their equilibrium positions which lie on a crystal lattice. Substitutional disorder occurs when one type of atom randomly substitutes for another in an otherwise crystalline lattice. An example is the random binary alloy Cu–Au. In the following chapters of this thesis we will concentrate on this type of disorder.

The observable properties of any system, disordered or otherwise are, in principle, well described by the solutions to the full many body Schrödinger equation. However, in practice, the exact solution of this equation for any real system is impossible to find due to the large number of interacting particles involved.

In the crystalline case a very good characterisation of a system may be gained by working within one-electron theory [11,12] in which the Schrödinger equation simplifies to:

$$\left[-\nabla^2 + V(\underline{r}) \right] \psi_i(\underline{r}) = E_i \psi_i(\underline{r}) \quad (1.1)$$

This approximation is justified within Fermi liquid theory in which the motion of strongly interacting electrons, such as in a metal, is rewritten in terms of weakly interacting quasi-particles.

The solution to equation 1.1 for crystalline systems is considerably simplified by two facts. First, the electronic states are restricted to the periodic form:

$$\psi(\underline{k}, \underline{r}) = u(\underline{k}, \underline{r}) \exp(i\underline{k} \cdot \underline{r}) \quad (1.2)$$

where the function $u(\underline{k}, \underline{r})$ has the periodicity of the crystal lattice (in which a

lattice translation vector connects all points $\underline{R}_i$):

$$u(\underline{k}, \underline{r} + \underline{R}_i) = u(\underline{k}, \underline{r}) \quad (1.3)$$

and $\underline{k}$ is the crystal momentum. This result, Bloch's theorem, is extremely powerful, reducing the problem to one of finding solutions within the unit cell, since the wave function outside this region may be constructed from 1.2. Second, the aim is always to find the properties of a *specific* crystalline structure for which the translation vectors are known.

1.1.1 The loss of Bloch States.

As disorder is introduced into a system translational invariance is lost and therefore so is the simplification which Bloch's theorem brings. However, the Bloch states still form a complete basis and new electronic states can be written as linear superpositions of them. This allows us to think in terms of a picture of a disordered system in which we consider electrons (or quasi-electrons) propagating in Bloch states and scattering from impurities. The scattering may be split into two main categories elastic and inelastic.

For elastic scattering, the electron propagates in a Bloch state, with a mean free path ℓ_e , then scatters without losing phase coherence or energy. If the size of the system L is much smaller than ℓ_e then electrons will pass through the system ballistically, scattering from boundaries. As ℓ_e is decreased, by increasing the amount of disorder, weak scattering begins to occur. First, single scattering events dominate, as in the Born approximation [12], then higher order scattering events. Systems in which scattering is a complex interplay between diffusive behaviour and interference effects are often referred to as *weakly localised*. As the disorder is increased still further ℓ_e begins to compete with the wavelength of the electrons λ and the fundamental nature of the wave functions changes, leading to an absence of diffusion [13]. The electronic states are no longer well described by a superposition of Bloch states. They become physically *localised* to within the sample. An example of this is the wave function of a electron in a hydrogen like state centered on a single donor impurity in an otherwise perfectly crystalline system. The wave function decays away expo-

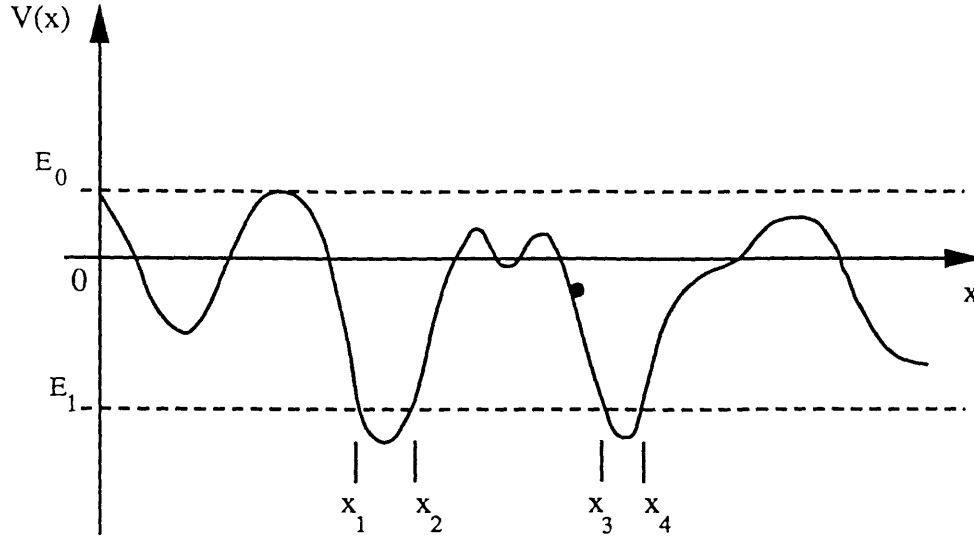


Figure 1.1: A classical particle in a random potential.

nentially, over a characteristic distance L_c referred to as the *localisation length*, leaving it isolated and localised about the impurity site. Localisation by more general types of disorder may be envisaged by considering the case of a classical particle in a random potential [14] figure 1.1. If the particle has energy greater than E_0 , the classical mobility edge, then it is free to move through the whole random system but if it has energy less than E_0 then it will become caught in one of the many minima and hence be localised. For instance, at energy E_1 the particle will be localised to the finite regions $(x_1, x_2), (x_3, x_4) \dots$. The quantum mechanical situation is similar but has two major differences. Firstly, the particle may tunnel from one well to another, due to uncertainty in its energy over short periods of time, tending to de-localise the particle. Secondly, coherent interference between partial waves taking different multiple scattering paths through the system enhances the localisation and can cause localised states to appear above the classical mobility edge. The regime in which all the states of a system are localised, well within the system, so that there is little interaction with boundaries is known as the *strongly localised* regime.

Inelastic scattering is complicated by the many different mechanisms by which it may occur. These principally come from interaction with collective modes or other electrons. Each different scattering process will have a different

mean free path associated with it. As far as looking at localisation is concerned, it is the shortest inelastic mean free path ℓ_i which is the most important. It is this length which determines whether partial waves retain their phases sufficient to cause localisation. In general as this length is reduced, perhaps due to an increase in temperature, the scattering in a localised system tends to become more diffusive.

1.1.2 The Introduction of Equiprobable Configurations.

As disorder is introduced into a system the number of equiprobable configurations which it may take quickly becomes enormous. A knowledge of the configuration of the impurities in any particular sample is impossible to gain and even if it were, it is uncertain what information this would give about any other configuration. Hence, we are interested in the statistical behaviour of ensembles of disordered systems, and in particular, the way in which observable properties are distributed. This information gives an idea of what a measurement is likely to yield and an insight into the fundamental processes which are occurring.

In general, these distributions will depend on the microscopic distributions of disorder, but there are powerful simplifications which arise for large systems. For instance as the size of systems in an ensemble increases, the distributions of certain properties can become more peaked about a mean value which is independent of system size: this phenomenon is referred to as self-averaging and forms the basis of statistical mechanics. An example is the instantaneous pressure of a dilute gas, at constant density and temperature. This pressure becomes increasingly independent of microscopic details and equal to its mean value as the volume of the gas is increased.

In the study of electronic properties of disordered systems many quantities of interest do not self-average. An example is the conductance $G = e^2 g / h \pi$ of a disordered wire, which fluctuates wildly between different members of an ensemble, regardless of system size e.g refs [15,16,17,18]. In order to find the generic behaviour of quantities which do not self average, we need to look at

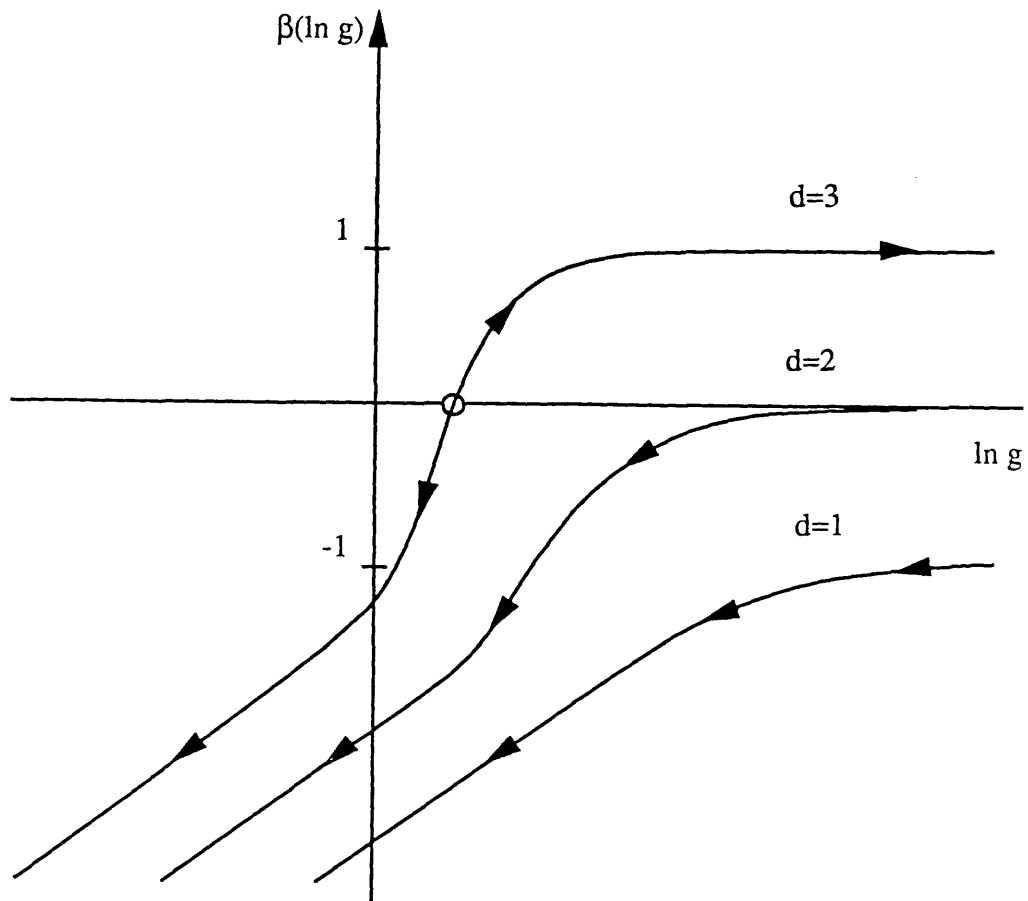
the more generalised statistical concept of how they *scale* with system size. It is thought that the properties of certain ensembles scale with system size such that a knowledge of their properties for one size is sufficient to determine them for any other size [8.9]. This concept may be expressed by the differential equation:

$$\frac{d\underline{a}}{d \ln L} = \mathbf{f}(\underline{a}) \quad (1.4)$$

where the vector $\underline{a}_L$ contains the properties of an ensemble of size L^d . This vector will be infinite for most ensembles. The equation 1.4 may also be written in discrete form for systems in which the presence of an underlying lattice is important. The properties of this type of first order differential equation have been studied in great depth and it is known that as L increases certain sub-spaces of $\underline{a}_L$ evolve in an increasingly independent manner. Some of these sub-spaces can even contain single parameters. Often quoted is the single parameter scaling behaviour of $\ln \langle g \rangle$ [19.20] (the notation $\langle \dots \rangle$ represents an ensemble average)

$$\frac{d \ln \langle g \rangle}{d \ln L} = \beta(\ln \langle g \rangle) \quad (1.5)$$

which is thought to apply for systems in which interactions between electrons, temperature effects and the effect of external fields may be neglected. The general form of the β function is shown in figure 1.2 for one, two and three dimensions $d = 1, 2, 3$ and its form is essentially an extrapolation of the asymptotic behaviour at large and small conductance [9]. The arrows indicate the direction in which $\ln \langle g \rangle$ flows with increasing system size. If $\beta > 0$ then the average conductance increases with increasing system size indicating metallic behaviour, characterized by $\beta = d - 2$. On the other hand, if $\beta < 0$, $\langle g \rangle$ decreases with increasing L , eventually terminating in the localised regime where $\beta = \ln \langle g \rangle$. In 3-D the existence of a fixed point indicates that as disorder is increased a system may make a transition from being metallic to being insulating for any size system. In 1-D and 2-D β is always negative indicating that these systems become increasingly insulating with increasing system size.

Figure 1.2: The β function.

1.1.3 Models of disorder.

In order to ascertain the form of a particular distribution function, check whether some property self averages or find a simple scaling relation, a specific model of a disordered systems must be used. The exact solution of the one-electron Schrödinger equation 1.1 for the statistical properties of disordered systems is in practice not possible. Instead workers have considered simplified models of disorder the best known of which is the Anderson Hamiltonian [13]:

$$\mathbf{H} = \sum_{n\underline{r}} \epsilon_{n\underline{r}} |n\underline{r}\rangle \langle n\underline{r}| + \sum_{n\underline{r}, n'\underline{r}'} V_{n\underline{r}, n'\underline{r}'} |n\underline{r}\rangle \langle n'\underline{r}'| \quad (1.6)$$

Here, the diagonal element $\epsilon_{n\underline{r}}$ is the energy associated with the n^{th} state at the site $\underline{r}$, and off-diagonal element $V_{n\underline{r}, n'\underline{r}'}$ represents the hopping amplitude between $n, \underline{r}$ and $n', \underline{r}'$. The diagonal part of the Hamiltonian represents potential energy and the off-diagonal part represents kinetic energy and disorder is introduced into this model through these elements. This model is thought to contain the essence of the problem of disorder and has presented a major challenge to theorists for over thirty years. In this thesis we will mainly consider its simplest form which consists of taking a single energy $\epsilon_{\underline{r}}$ at each site and assumes that the hopping term is constant between nearest neighbours and zero elsewhere. An ensemble is defined by assuming that the site energies are statistically independent and identically distributed according to some density $\rho(\epsilon)$. This is essentially a model for a substitutionally disordered system in which inelastic effects are negligible and there is no external field.

1.2 Review on Reflection.

For crystalline systems, reflection of waves, such as electrons and electromagnetic radiation, has proved to be a very effective probe of surface structure [21]. Theory has advanced from interpretation of data from simple surfaces to high Miller index surfaces and even to surfaces with a single disordered overlayer. The study of reflection from general types of disordered system has been left (by comparison) relatively untouched.

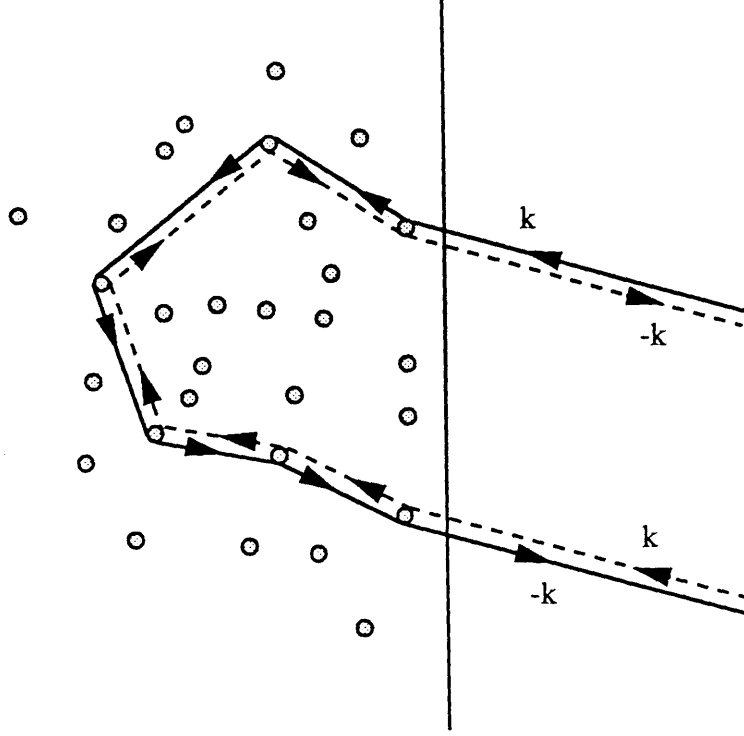


Figure 1.3: Two partial waves interfering coherently.

In optics, interest has been shown in reflection of electromagnetic waves from disordered random media e.g [22,23,24] and rough surfaces e.g [25]. Initially this interest stemmed from its practical application to remote sensing, but a strong motivation for further research lies in the possibility of localising light [26]. Scattering from disordered optical systems appears mostly diffusive. However, by increasing the ratio of the wavelength of the incident light to its elastic mean free path $\kappa = \lambda/\ell_e$, the effects of weak localisation may be seen. The most striking effect is a peak appearing in the back-scattered direction, so called *coherent back-scattering*. This effect is a direct consequence of the fact that two partial waves taking the same scattering path, one in the forward direction and one in the time reversed direction interfere coherently, figure 1.3. The sum over all such paths gives a doubling of intensity into the back scattered direction and an increased intensity over a small angular width proportional to κ . Figure 1.4 gives an example of coherent backscattering from a gaussian rough surface $\sigma_h = 1\mu m$ using light from a He-Ne laser $\lambda = 0.633\mu m$ [25]. It shows a diffusive back ground with a clear peak in the back scattered direction $\theta = 20^\circ$.

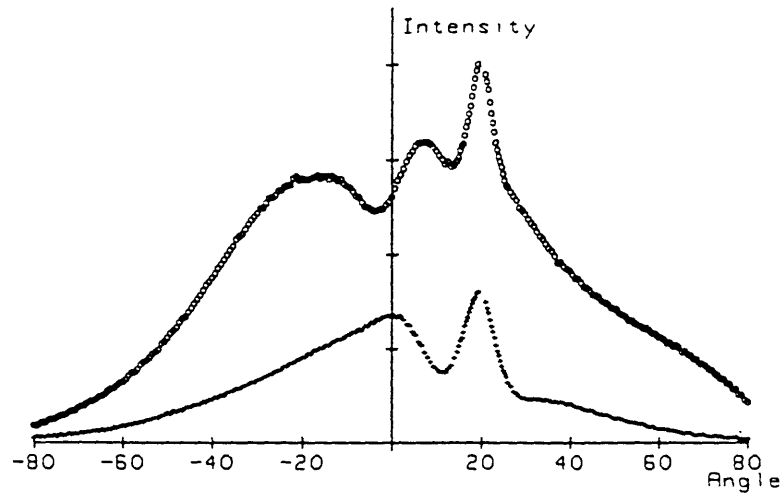


Figure 1.4: Back scattered peak appearing in diffusive scattering from a disordered surface. Incident angle $\theta = 20^\circ$.

The polarisation for the incident wave was vertical and for the detected beam it was vertical for the upper curve and horizontal for the lower curve. As yet the effects of strong localisation have not been seen.

The electronic case is similar to the optical case for weak disorder. We expect to find a transfer from diffusive scattering to weak localisation as disorder is increased. However, in this case, strongly localised systems are more easily realisable experimentally than in the optical one. To our knowledge, this problem has not been investigated further than the examination of reflection from 1-D disordered chains and has not concentrated specifically on the reflection coefficient. One set of investigations has looked at the transmitted intensity e.g [27.28.29.30.31] related to the reflected intensity through conservation of probability $|R|^2 + |T|^2 = 1$. Another set has concentrated on the phase ϵ , related to that of the reflection coefficient, which appears in a recursion relation for the Landauer resistance [32]. This research occurred as a result of a controversy over whether it is possible to assume that ϵ becomes random with increasing system size [33.34.35.36]. A number of authors had made this assumption in deriving scaling relationships for the conductance e.g [37.38.39.40.41.42]. Since the determination of the distribution of reflection phase plays a major part in this thesis we review more closely the work carried out on ϵ and show its relation

to the reflection phase.

The phase ϵ appears in a model in which a disordered system is considered as consisting of connected disordered units, each unit, or collection of units, being defined by a reflection and a transmission coefficient, R and T . In this model the Landauer resistance Z_L , for L connected units, obeys the recursion relation:

$$Z_{L+1} = Z_L + z_{L+1} + 2Z_L z_{L+1} - 2\sqrt{Z_L z_{L+1}(1 + Z_L)(1 + z_{L+1})} \cos(\epsilon_{L+1}) \quad (1.7)$$

where $Z_L = |R_L|^2/|T_L|^2$ and z_L is the Landauer resistance of a single unit. The phase ϵ_{L+1} is related to the reflection phase θ_L , of L units, and ϕ_{L+1} , the reflection phase of a single unit, through

$$\epsilon_{L+1} = \theta_L + \phi_{L+1} \quad (1.8)$$

giving rise to a simple convolution relation between the distributions of these three phases

$$Q_{L+1}(\epsilon) = \int P_L(\theta) p(\epsilon - \theta) d\theta \quad (1.9)$$

The first authors who deal specifically with ϵ , Lambert and Thorpe [36], look at a model which consists of a set of randomly spaced delta functions of equal strength. They find that in general that Q_L has no reason to be random unless $p(\phi)$ is random, a simple consequence of the convolution relation 1.9. They also find that as L increases Q_L reaches a stationary limit.

The second authors, Stone *et al* [35], look at Q_L using the tight-binding model with diagonal binary disorder mostly through numerical work. They find that for weak disorder Q_L becomes smooth and nearly random when L is greater than some independent length scale. An exception to this is found at the band center where it remains peaked however weak the disorder. For strong disorder they find that Q_L is never random.

Finally, two papers by Heinrichs [33,34] look directly at the reflection coefficient R_L for weak disorder using a continuum model with diagonal disorder. In the first, he finds the exact distribution of the R_L in the complex plane for a gaussian white noise distribution of site energies in the weak scattering regime

$L \ll \ell_c$. The distribution is an elliptical gaussian but is only significantly non-cylindrical if $k_F L \ll 10^2$. k_F is the Fermi wave vector. In his second paper he concentrates on the strongly localised regime and finds that the stationary distribution of reflection phases is nearly random if $L_c \gg k_F$.

1.3 Summary of Thesis.

This thesis is composed of four chapters which are principally concerned with reflection from disordered systems and two which are concerned with showing how the formalism we have used to study reflection may be adapted to look at transport properties.

In chapter 2, we derive a formalism for calculating the reflection coefficient of disordered chains for the tight binding model with diagonal disorder. We then use this formalism to calculate numerically, statistical properties of the reflection coefficient in 1-D. We look at the, length, disorder, type of disorder and wave-vector dependence of the distribution of reflection coefficients showing features which we look at in depth in later chapters.

In chapter 3, we derive a novel formalism for the reflection coefficient involving a generalised transfer matrix by using multiple scattering theory. We use this formalism with perturbation theory to calculate the statistical moments of the distribution of reflection coefficients showing their characteristic spiral dependance on wave-vector. In the strongly localised regime we use these moments to find the distribution of reflection phases $P(\theta)$ and give an account of the appearance of anomalies.

In chapter 4, we calculate $P(\theta)$ using an exact Dyson-equation formalism for two different types of disorder, discrete and continuous. For discrete disorder, we deal with the binary alloy and find that under generic circumstances that $P(\theta)$ contains an infinity of power law singularities. For continuous disorder, we look at the symmetric exponential alloy and find that we can solve exactly for $P(\theta)$.

In chapter 5, we derive an exact perturbation expansion for the reflection

matrix of a disordered 3-D wire in the weakly scattering regime. We use the first term, which constitutes single scattering, to calculate the distribution of each element of the reflection matrix for a gaussian ensemble and also calculate some of the moments of this distribution.

In chapter 6, we show how a simple adaptation of the formalism used in chapter 3 may be used to calculate moments of the distribution of transmitted intensities.

In chapter 7, we extend the transfer matrix formalism of chapter 3 to include the transmission coefficient and discuss the relation between these new transfer matrices and the generalised transfer matrices of Kirkman and Pendry [1,2] and Pendry and Castaño [3].

Chapter 2

Numerical Simulation in 1-D

2.1 Introduction

With access to fast computers many workers in the field of ‘localisation’ have gained insight into their particular aspect through numerical techniques. For instance, the one parameter scaling theory has been numerically tested quite extensively [43,44]. Simulation is one such technique and in its simplest form consists of calculating a quantity of interest for as many members of an ensemble as possible—chosen randomly if it is not possible to look at all members of the ensemble—then either placing them in a histogram or calculating average quantities such as the moments. In this chapter we use the numerical simulation technique to find statistical properties of the reflection coefficient for an ensemble of 1-D tight-binding chains with diagonal disorder.

In section 2.2, we use the tight-binding formalism to derive a recursion relation which allows us to calculate numerically the reflection coefficient of a disordered chain of atoms. We then use a numerical simulation technique to calculate the generic properties of the distribution of reflection coefficients. In section 2.3 we use an adaptation of the recursion relation for the reflection coefficient to calculate the generic properties of the distribution of reflection phases in the strongly localised regime.

2.2 Finite Chains

In this section, we derive a recursion relation for the reflection coefficient using the tight-binding formalism and discuss some of the direct consequences of its functional form. We then describe two different approaches to the numerical problem: the exact enumeration technique and the random sampling technique. We describe where these techniques are applicable and use them to show some generic behaviour of the distribution of reflection coefficients as the various parameters of the tight-binding model are changed.

We will be considering ensembles of disordered systems described by the tight-binding Schrödinger equation

$$\phi_{n+1} + \phi_{n-1} + \epsilon_n \phi_n = E \phi_n \quad (2.1)$$

Each system, consisting of a central disordered region of L atoms, ($1 \leq n \leq L$), connected to two semi-infinite perfect leads ($n > L$ and $n < 1$). In the disordered region, the site energies ϵ_n are independent random variables, with a common probability density $\rho(\epsilon)$, symmetrically distributed about $\epsilon = 0$. In the leads the site energies vanish $\epsilon_n = 0$ so that the eigenstates there are superpositions of traveling waves

$$\phi_n = a^+ e^{ikn} + a^- e^{-ikn} \quad (2.2)$$

where the wavevector k is related to the energy E by

$$E = 2 \cos k, \quad 0 < k < \pi \quad (2.3)$$

The generic properties of these ensembles are determined by four parameters: the length L ; the strength of disorder $\sigma^2 = \langle \delta^2 \rangle$, where $\delta = \epsilon/2 \sin k$ and the notation $\langle \dots \rangle$ represents an ensemble average; the type of disorder ρ and the wave vector k .

The reflection and transmission coefficients R_L and T_L for a wave incident from the right with wave vector $-k$ are defined such that the wave function in the leads takes the following form:

$$\phi_n = e^{-ik(n-L)} + R_L e^{ik(n-L)} \quad \text{for } n \geq L$$

$$= T_L \epsilon^{-ikn} \quad \text{for } n \leq 1 \quad (2.4)$$

Adding impurities to a disordered chain causes the reflection coefficient to evolve in a simple manner, so that R_L is related only to R_{L-1} and a disorder parameter δ_L characterizing the L^{th} site. The derivation of this recursion relation is as follows: Defining the Riccati Variable Y_n by

$$Y_n = \frac{\phi_{n+1}}{\phi_n} \quad (2.5)$$

and in terms of this variable the tight-binding equation 2.1 takes the form

$$Y_n = E - \epsilon_n - \frac{1}{Y_{n-1}} \quad (2.6)$$

For any chain of atoms equation 2.4 implies $Y_0 = \epsilon^{-ik}$. Hence, adding an L^{th} impurity to a chain of length $L-1$ does not change Y_0 and therefore through equation 2.6 does not change $Y_1 \cdots Y_{L-1}$, it only changes Y_L . Hence, equation 2.6 expresses the evolution of the Y_L at the surface of a disordered chain, as L increases. The reflection coefficient R_L and Y_L are related through equation 2.4 by

$$Y_L = \frac{\epsilon^{-ik} + R_L \epsilon^{ik}}{1 + R_L} \quad (2.7)$$

so that substituting this relation 2.7 into equation 2.6 and rearranging yields a recursion relation for the evolution of their reflection coefficient.

$$R_L = \frac{\epsilon^{2ik} R_{L-1} + i\delta_L (1 + \epsilon^{2ik} R_{L-1})}{1 - i\delta_L (1 + \epsilon^{2ik} R_{L-1})} \quad (2.8)$$

with the notation

$$\delta_L = \frac{\epsilon_L}{2 \sin k} \quad (2.9)$$

We will refer to 2.8 as the ‘reflection recursion relation’ (RRR). The initial condition to this recursion is clearly $R_0 = 0$, since no random region is present in this case. A derivation of 2.8 for a continuum model using the invariant embedding method [45] is given in [46].

Looking at the modulus of the RRR we not only see that the unitarity condition $|R_L| \leq 1$ holds but also see an interesting effect: adding new atoms

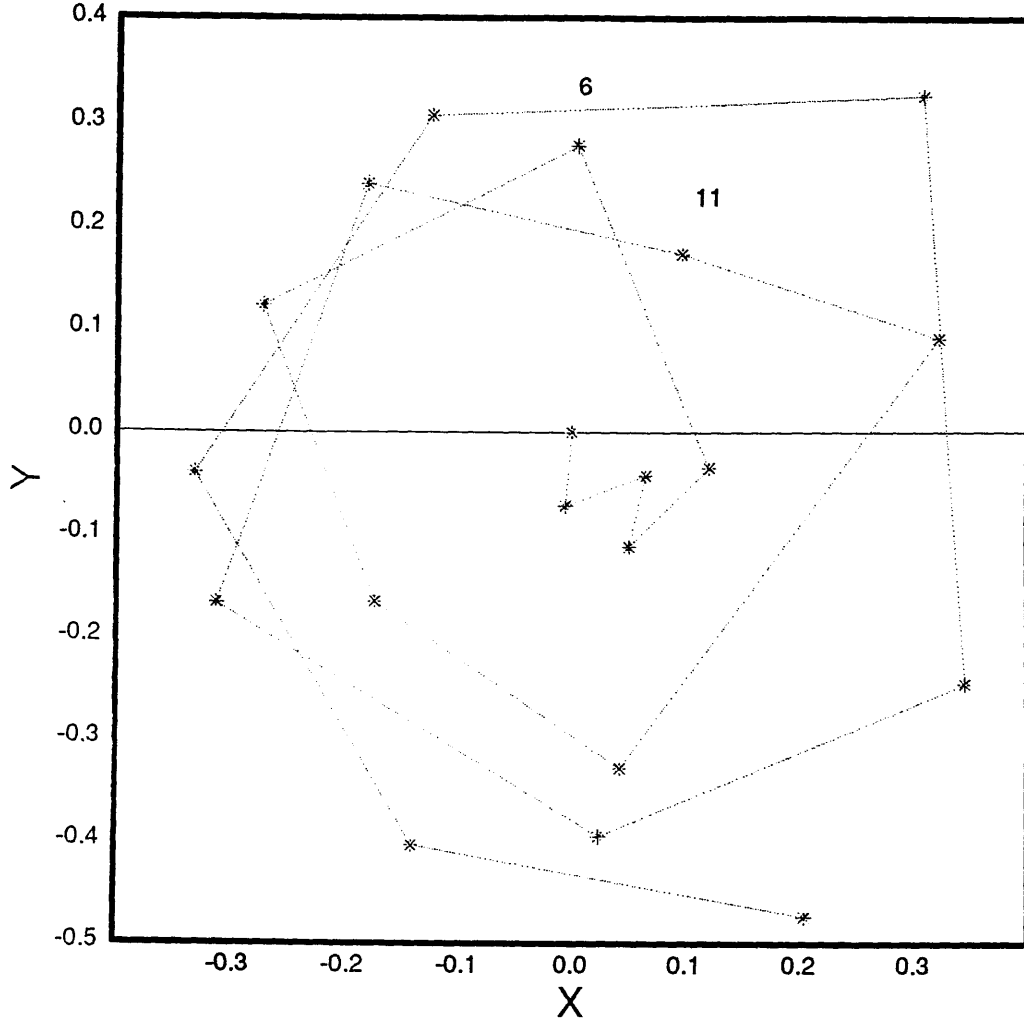


Figure 2.1: Evolution of the reflection coefficient with length.

to a disordered chain does not necessarily increase its reflectivity, it only has a higher probability of doing so if the site energies of the added atoms are chosen randomly. This effect is analogous to ‘blooming’ in optics. Figure 2.1 shows a typical evolution of the reflection coefficient of a disordered chain with increasing length $L = 0 \rightarrow 20$, $\sigma = 0.1$ and $k = 0.4\pi$. It has been plotted in the complex plane, with $X = \text{Re}R_L$ and $Y = \text{Im}R_L$. Comparing the modulus of point 6 with that of point 11 we see that between these two points the chain has become less reflective but over all for the first twenty points the chain has become more reflective. This plot was achieved by simply iterating the RRR 20 times taking the site energies from a random number generator.

The form of the RRR also implies a simple symmetry in the wave-vector dependence of the distribution of reflection coefficients $P(X, Y)$. Comparing the RRR for the two wavevectors $k^\pm = \pi/2 \pm k'$ we see that one is the complex conjugate of the other, except for the sign of the disorder parameter δ , which does not affect the form of $P(X, Y)$ because δ is symmetrically distributed. Hence, since both RRR's have the same initial conditions $R_0 = 0$ $P(X, Y)$ has the symmetry

$$P(X, Y : k^+) = P(X, -Y : k^-) \quad (2.10)$$

The RRR represents an excellent basis for carrying out numerical work since all the parameters involved are, and remain, finite as it is iterated. Figure 2.2 shows a general algorithm, using the RRR, which calculates the probability distribution or the moments of any function of the reflection coefficient. The inner loop iterates the RRR over n, L times, choosing the disorder parameters according to a given sequence (exact enumeration), or randomly from a specific distribution (random sampling), in order to find the reflection coefficient R_L of a particular chain in the ensemble. The outer loop, iterating over i, N times, then calculates the required function of R_L and contributes it to a sample histogram or a sample moment. The algorithm is designed to allow N to be as large as possible without filling the computer memory with unwanted data. In the next two sub-sections we will discuss the algorithm's use in looking at $P(X, Y)$ and its moments for different ensembles.

2.2.1 Exact Enumeration

If the site energies in an ensemble take only certain discrete values, ϵ_i with probability p_i then any finite length ensemble will contain a finite number of members. Hence in principle it is possible to find $P(X, Y)$ exactly by 'exact enumeration' if N is chosen to be the size of the ensemble and the disorder parameters are chosen so that each reflection coefficient in the ensemble is found. In practice this exact enumeration method is quite limited since the number of chains in these ensembles increases exponentially with the length of the chain.

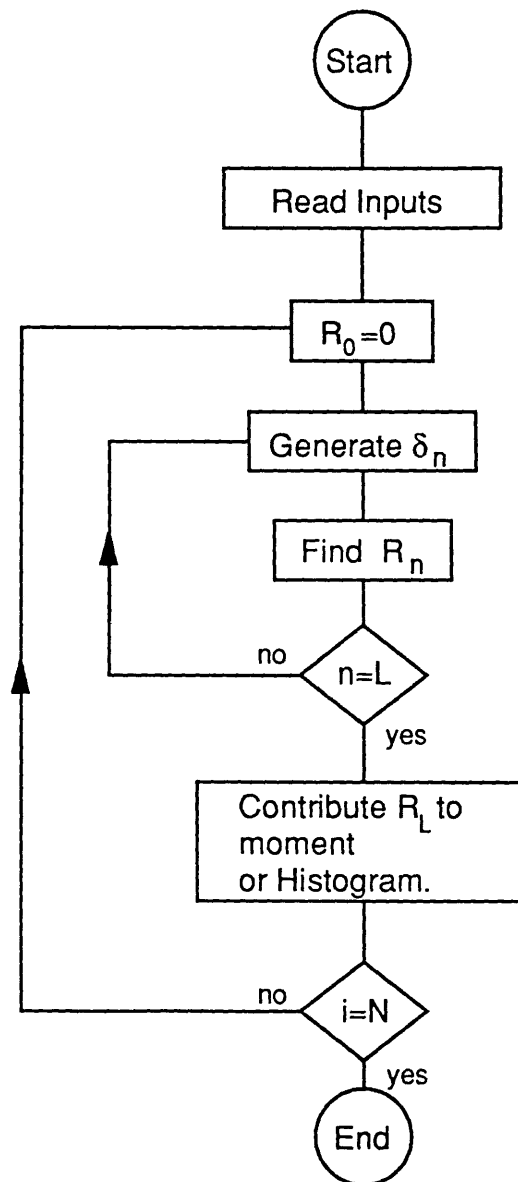


Figure 2.2: Algorithm for reflection coefficient.

For discrete distributions of disorder, $P(X, Y)$ is composed of delta functions, due to the finiteness of the ensemble, and therefore a histogram of it can appear very rough. However, the generic form of these histograms and their dependence on the ensemble parameters L, σ and k is not affected by this roughness and hence we will defer their discussion to the next sub-section where we describe a faster more versatile technique. The exact technique is however very good for calculating the moments of the reflection coefficient as they do not appear to be affected by the discreteness of $P(X, Y)$, for weak disorder, and are quite hard to find accurately by any other numerical method. The binary symmetric ensemble in which the site energies are $\epsilon_n = \pm\epsilon$ with equal probability $1/2$ proves quite amenable to the exact technique for lengths up to $L = 20 - 22$. Figure 2.3 shows a locus in the complex plane of the first moment of the distribution of reflection coefficients with wave vector $k = [0, \pi/2]$ at fixed disorder $\sigma = 0.1$ and length $L = 10$. The locus has been shown for only half the band because equation 2.10 predicts that the line $Y = 0$ is as a line of mirror symmetry giving the other half of the band. The figure illustrates nicely why it is so difficult to evaluate this curve, in any way other than exactly, with its minute foray into the complex plane $\sim 10^{-2}$ and intricate spiral shape. The left hand side of the figure corresponds to $k = 0$. We will come back to the moments of the reflection coefficient in chapter 3 where we give an analytic theory for them.

2.2.2 Random Sampling

If we wish to look at ensembles which are too large to make exact enumeration practicable we can use ‘random sampling’. In this technique the inner loop in figure 2.2, takes random numbers from the machine generator and transforms them to give δ from a chosen distribution. This produces sample moments and sample histograms. The statistical error on the average diminishes as $(1/N)^{1/2}$ and on the histogram of the distribution functions as $(B/N)^{1/2}$, where B is the number of bins in the histogram.

Random sampling proves to be extremely efficient for calculating the generic dependence of $P(X, Y)$ on the ensemble parameters L, σ and k . We look

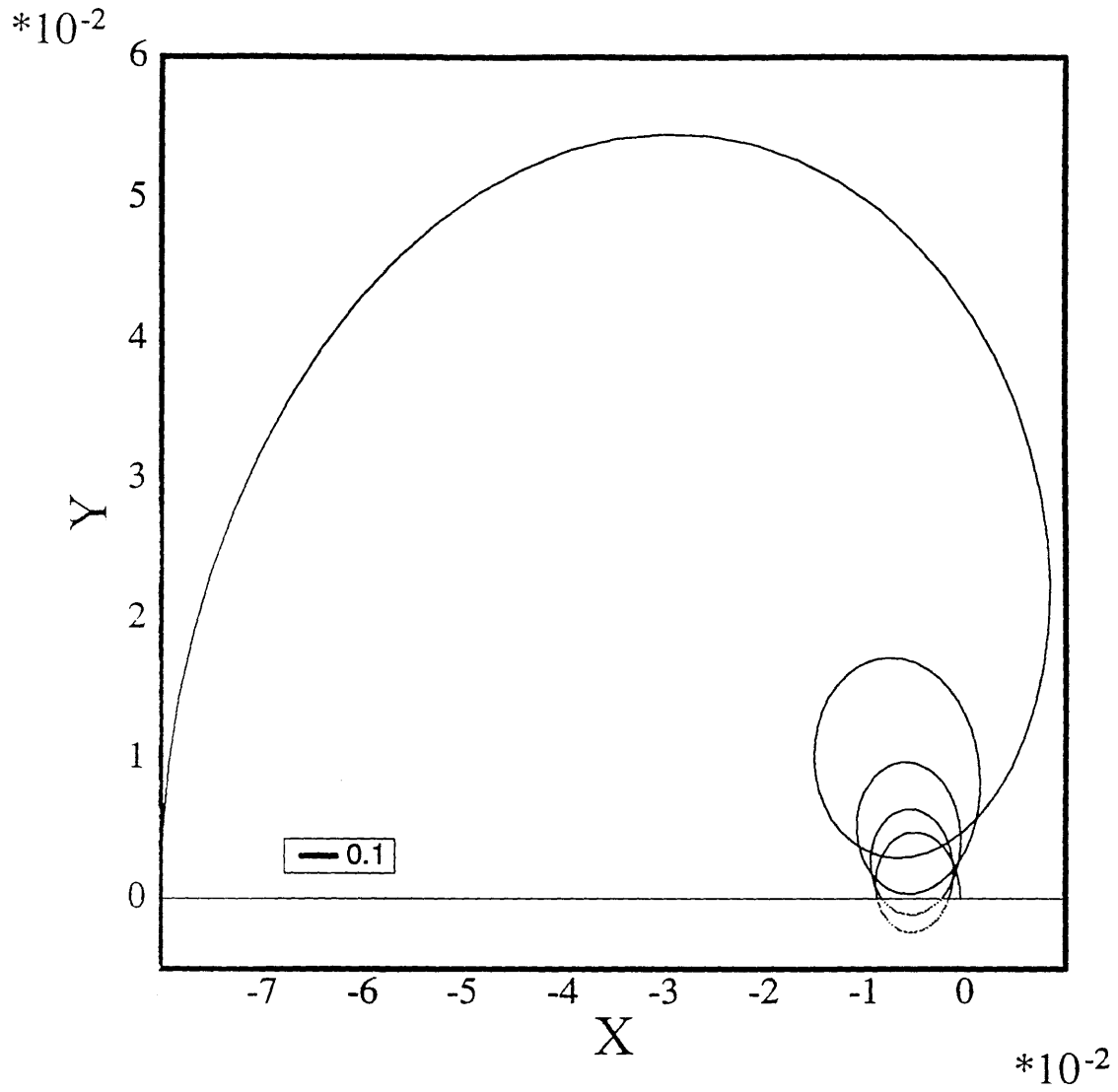


Figure 2.3: Locus in the complex plain of $\langle R_L \rangle$ with $k = [0, \pi/2]$ and $\sigma = 0.1$.

at a top hat distribution of disorder which we do not expect to give any ‘special’ behaviour in $P(X, Y)$ because it is continuous and bounded. The probability density for delta therefore has the form:

$$\begin{aligned}\rho(\delta) &= \frac{1}{W} && \text{for } |\delta| < \frac{W}{2} \\ &= 0 && \text{otherwise}\end{aligned}\tag{2.11}$$

where $\sigma^2 = 12W$. In using the random sampling method we have taken $N = 10^7$ for each plot, described below, to give an idea of how readily each distribution converges with N .

Figures 2.4 show the evolution of $P(X, Y)$ at weak disorder $\sigma = 0.1$ and generic wavevector $k = 0.4\pi$ with increasing length: (a) $L = 10$, (b) $L = 40$, (c) $L = 100$ (d) $L = 200$. The effect of this increase in length is to increase the localisation of the wave function $L/L_c \propto \sigma^2 L = 0.1 \rightarrow 2.0$. This causes the distribution of the modulus of the reflection coefficient $F_L(|R|^2)$ to change from being peaked around zero reflection [28,29] to being peaked around total reflection [30,31]. However, it has little effect on the distribution of the phase of the reflection coefficient $P_L(\theta)$.

Figures 2.5 show the development of $P(X, Y)$ at fixed length $L = 40$ and wave vector $k = 0.4\pi$ with increasing disorder: (a) $\sigma = 0.05$, (b) $\sigma = 0.1$, (c) $\sigma = 0.2$ and (d) $\sigma = 0.7$; $\sigma^2 L = 0.1 \rightarrow 20.0$. The increase in strength of disorder has a dual effect: it causes an increase in localisation, therefore having the same effect on $F(|R|^2)$ as an increase in L , but also causes an increasing distortion in $P_L(\theta)$. This is because electrons are increasingly prevented from penetrating the wires too deeply where they can randomise their phase. From the similarity between figures 2.4(a) and 2.5(a) we can see that the parameter $\sigma^2 L$ is acting as a single parameter scaling $P(X, Y)$. We shall investigate this further in chapter 5. The spiky appearance of $P(X, Y)$ for strong localisation is an artifact, as we shall see, and comes from a combination of the non-convergence in N and a graphics interpolator which works on a square grid.

The general effect of a change in wave vector k is to produce a small shift in the distribution of the phase of the reflection coefficient $P_L(\theta)$. However, for

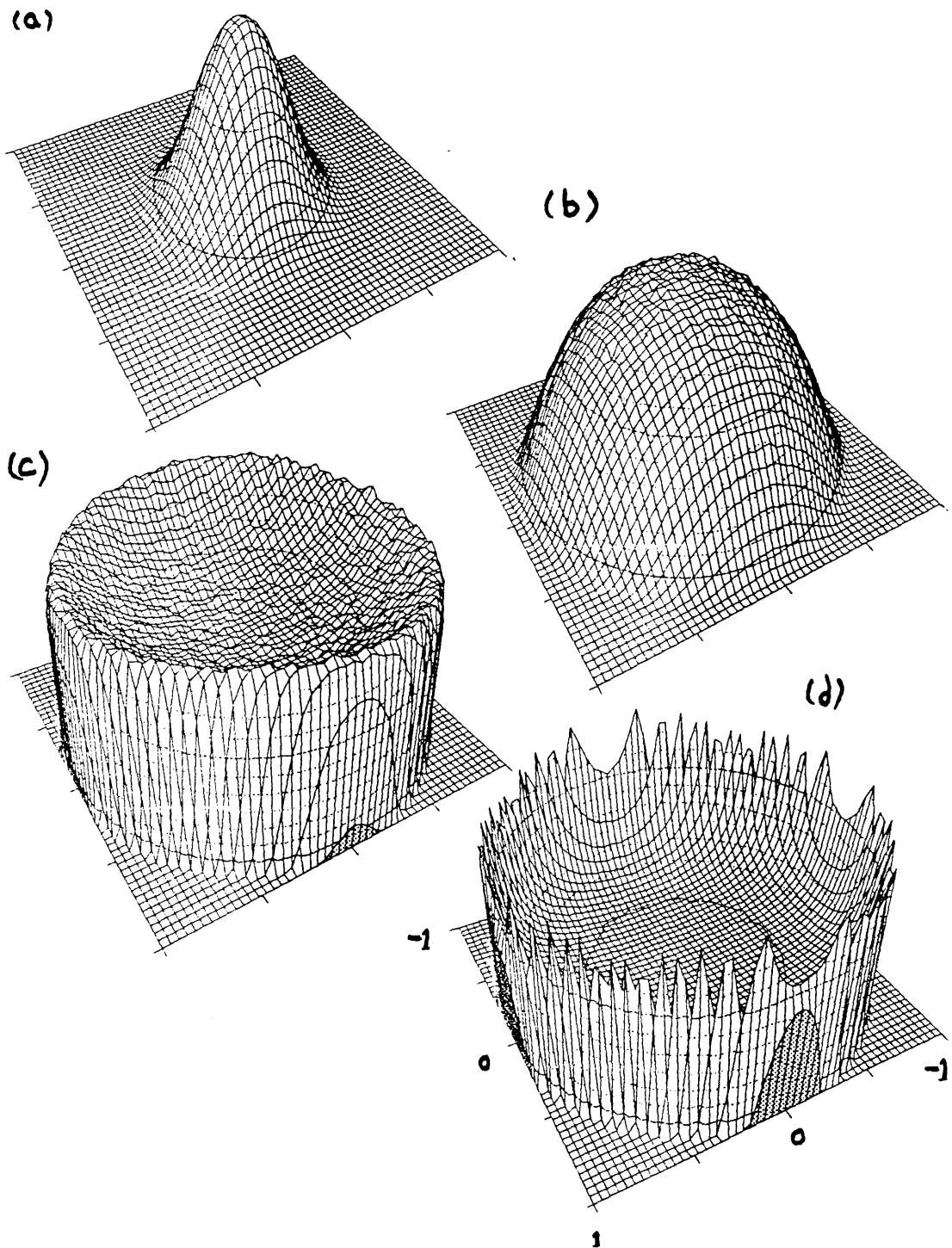


Figure 2.4: Histograms of $P(X, Y)$ for $\sigma = 0.1$, $k = 0.4\pi$ and (a) $L = 10$ (b) $L = 40$ (c) $L = 100$ (d) $L = 200$.

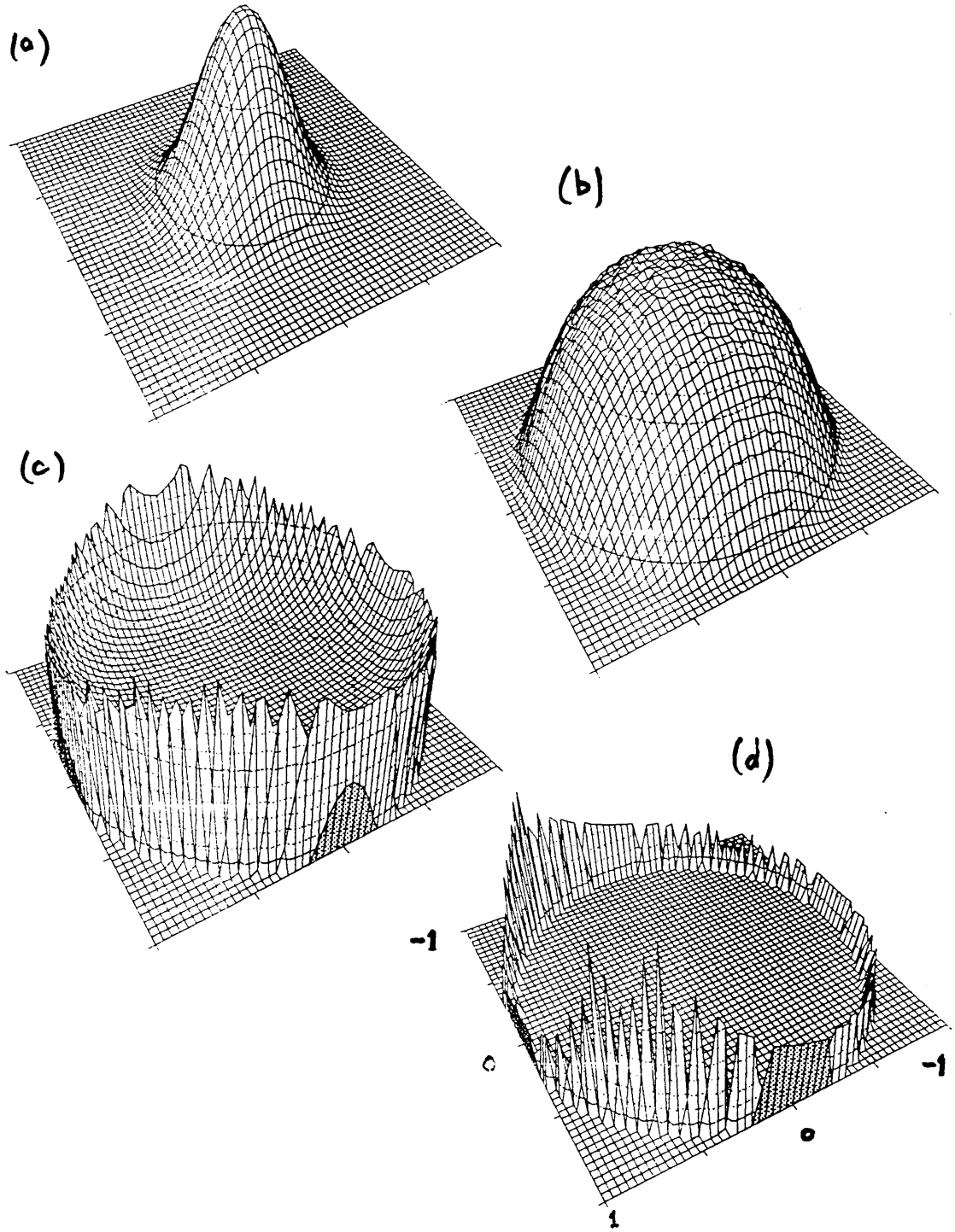


Figure 2.5: Histograms of $P(X, Y)$ for $L = 40$, $k = 0.4\pi$ (a) $\sigma = 0.05$ (b) $\sigma = 0.1$ (c) $\sigma = 0.2$ (d) $\sigma = 0.7$.

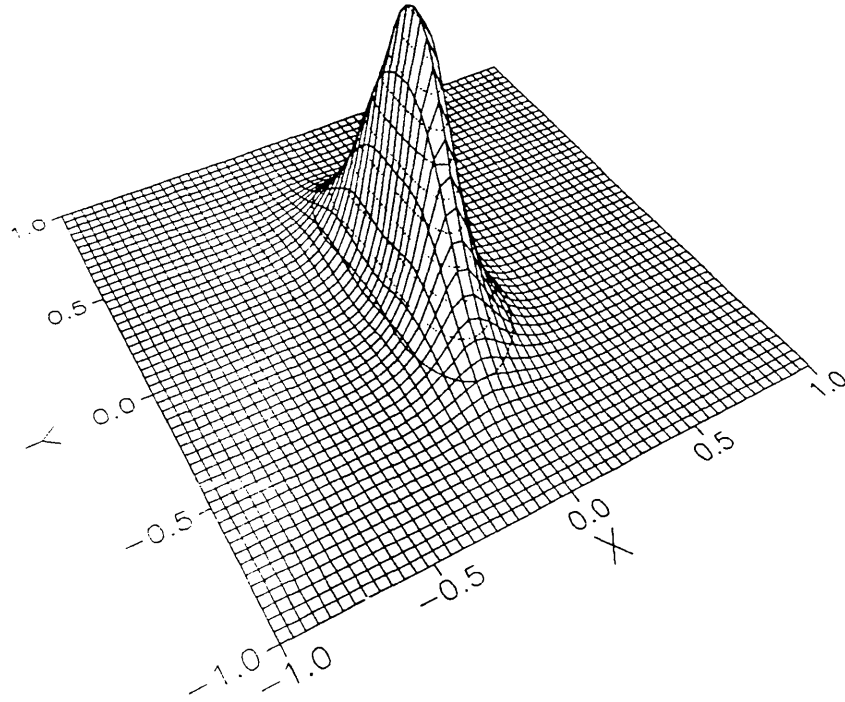


Figure 2.6: Histogram of $P(X, Y)$ at $k = \pi/2$ and $\sigma^2 L = 0.1$

weak disorder where $P_L(\theta)$ is almost entirely random, a striking effect is seen close to the band center $(k - \pi/2)L < 1$. As k approaches $\pi/2$, $P(X, Y)$ changes from being almost cylindrical to being almost flattened onto the imaginary axis. Figure 2.6 shows a histogram of $P(X, Y)$ at the band center $k = \pi/2$ for $\sigma^2 L = 0.1$.

We now concentrate on the distribution of the phase of the reflection coefficient, and since this appears to be broadly unaffected by the length of the system we will concentrate on the strongly localised regime where $P(X, Y)$ has converged onto the unit circle.

2.3 Strong Localisation

Two facts simplify the calculation of the reflection coefficient in the strongly localised regime, characterised by $\sigma L \gg 1$. First, the statistical weight of

chains in $P(X, Y)$ which allow any transmission can be ignored, as figure 2.5 d indicates, allowing us to write the reflection coefficient as a pure phase:

$$R_L = e^{i\theta_L}, \quad -\pi < \theta_L \leq \pi \quad (2.12)$$

where θ_L is the reflection phase. Second, the phase distribution reaches a stationary limit

$$\lim_{L \rightarrow \infty} P_L(\theta) = P(\theta) \quad (2.13)$$

This occurs because the decay of the wave function into a disordered wire causes the reflection phase to be affected only by impurities as far in as the localisation length.

The first simplification allows us to re-arrange the RRR to give us a recursion relation purely for the reflection phase. Defining the parameter t_L by

$$t_L = \tan \frac{\theta_L}{2} = -i \frac{R_L - 1}{R_L + 1} \quad (2.14)$$

we can re-write the RRR in the form

$$t_L = 2\delta_L + \frac{t_{L-1} + \tau}{1 - t_{L-1}\tau} \quad (2.15)$$

where

$$\tau = \tan k \quad (2.16)$$

We will refer to equation 2.15 as the ‘tangent recursion relation’ (TRR). The second simplification, allows us to make an arbitrary choice of the initial boundary condition t_0 since the stationary $P(\theta)$ should not depend upon it. However, in using the algorithm in figure 2.2 the finiteness of L will always lead to a systematic shift in $P(\theta)$ coming from the boundary exponentially decreasing with increasing length.

2.3.1 Exact Enumeration

For discrete distributions of disorder, under generic conditions, $P(\theta)$ contains an infinity of power law singularities with log-periodic modulation [47]. The exact technique proves ideal for looking in detail at this fine structure. Though, due to the systematic shift in $P(\theta)$ produced by having finite L the extent to which

we ‘see’ it depends on how much computer time we are prepared to invest in making L as large as possible. In chapter 4, we will use this exact technique to look in detail at $P(\theta)$ for a binary alloy. However, here we are only interested in generic behaviour and will leave this method for a faster one.

2.3.2 Random Sampling

The random sampling technique may be used to calculate $P(\theta)$, for ^{large} L , if we wish to remove the systematic errors, or for continuous distributions of disorder. However, in looking at generic behaviour it is not the most efficient algorithm. A more efficient algorithm is based on the assumption that in iterating the TTR successive reflection phases are uncorrelated so that each iteration gives a value of θ with probability $P(\theta)$. Using this assumption, we can build up a histogram of $P(\theta)$ very quickly simply by iterating the TRR and placing each calculated value of θ into a histogram. Comparisons between the previous random sampling method and this one show that the form of $P(\theta)$ is broadly unaffected by any correlations and in fact, to the extent to which they are present, they act to converge the random statistical fluctuations much faster.

Figures 2.7 and 2.8 show the evolution of $P(\theta)$ with increasing disorder at a generic position in the band $k = 0.3\pi$ for two different types of disorder, the top-hat distribution and the binary alloy. Both types have the same generic behaviour, they become more peaked towards $\theta = \pm\pi$, but the binary alloy begins to exhibit singularities in its phase distribution as the disorder increases whereas the tophat alloy appears to remain quite smooth. This interesting effect is discussed in more detail in chapter 4.

Finally, figure 2.9 shows a band center effect for the strongly localised regime. At a generic position in the band the distribution of reflection phases becomes completely random in the zero disorder limit, $P(\theta) \sim 1/2\pi$, except at the band center where it tends to a well defined symmetric function with amplitude $\sim 3 * 10^{-2}$. This anomaly and others will be discussed in chapters 3 and 4.

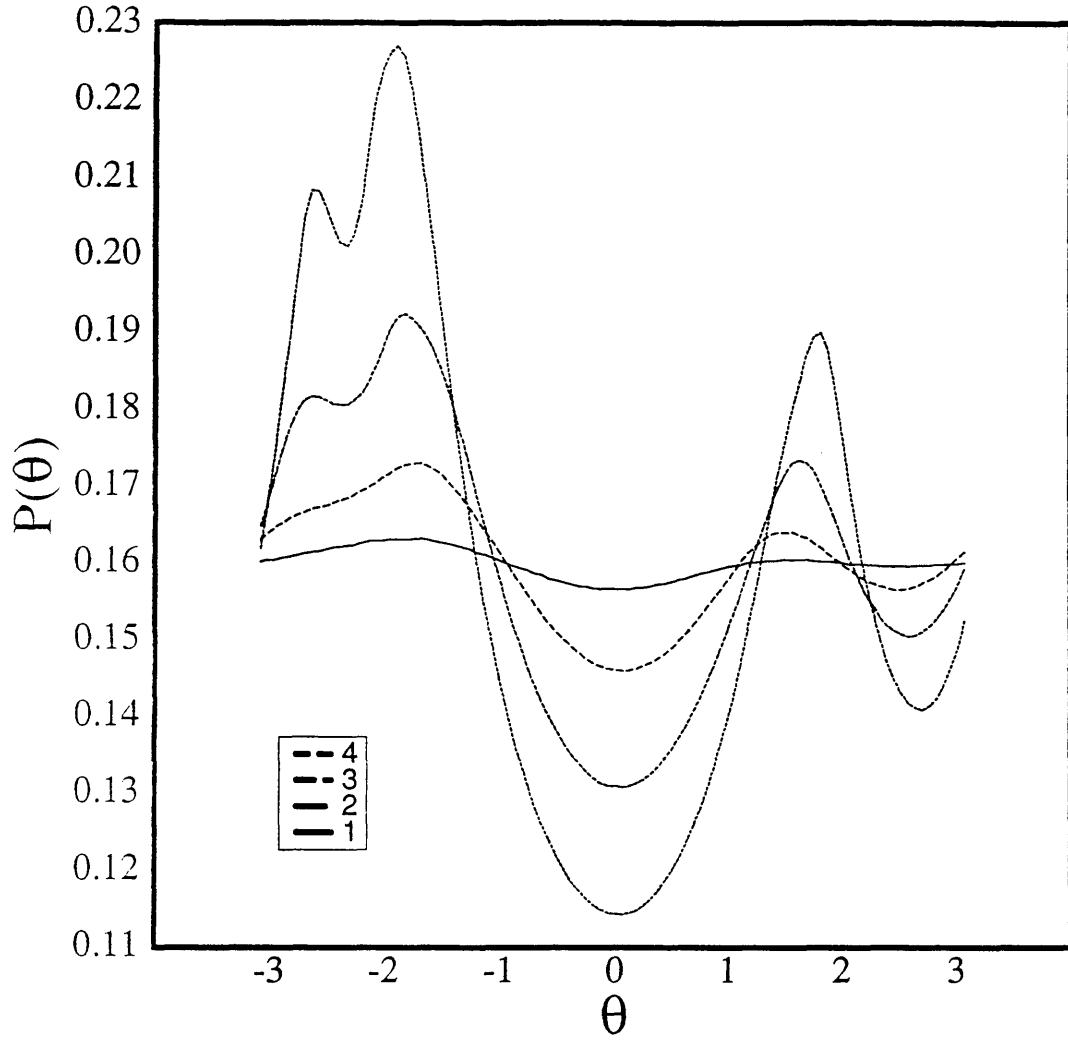


Figure 2.7: $P(\theta)$ for top hat disorder for $k = 0.3\pi$ (1) $\sigma = 0.1$ (2) $\sigma = 0.2$ (3) $\sigma = 0.3$ (4) $\sigma = 0.4$.

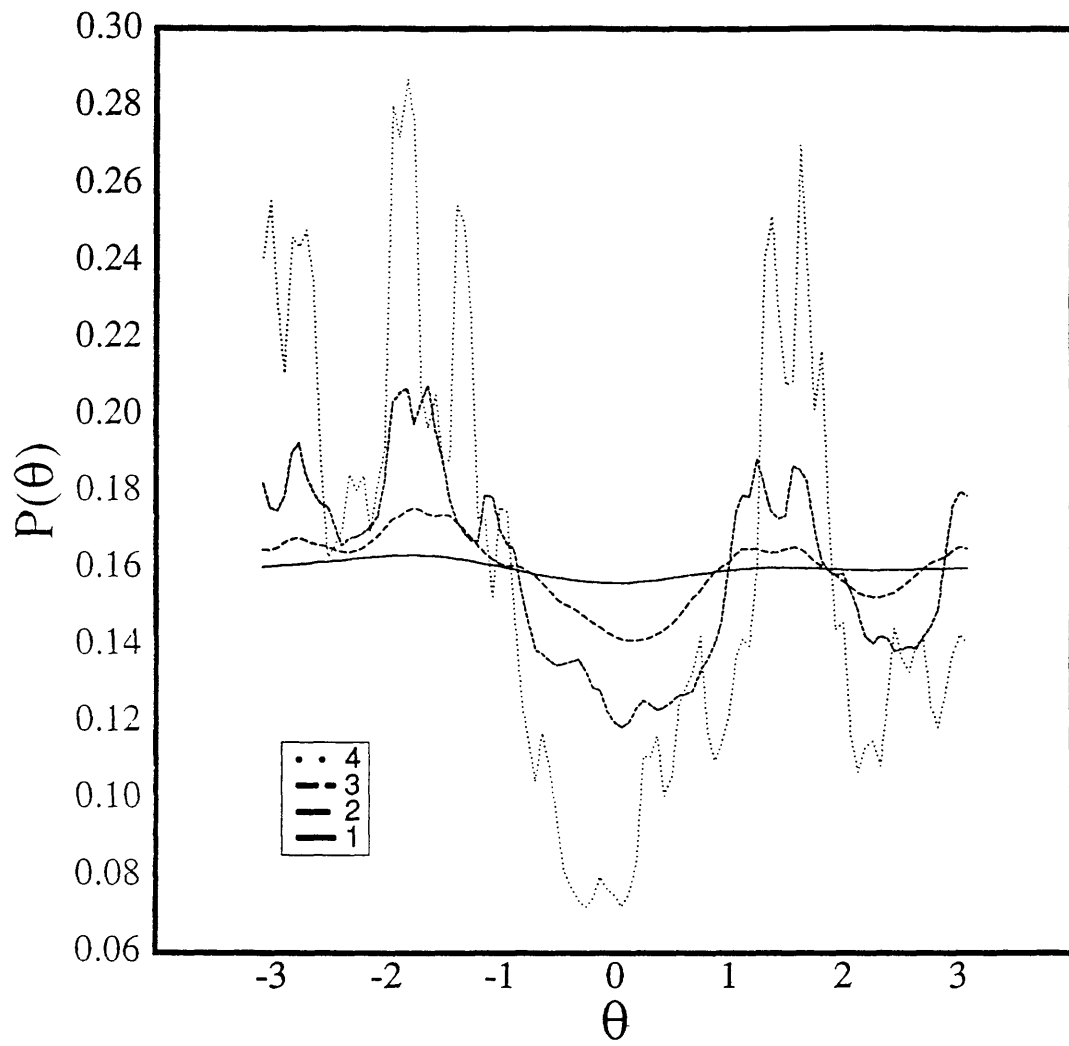


Figure 2.8: Same as figure 2.7 but for binary disorder.

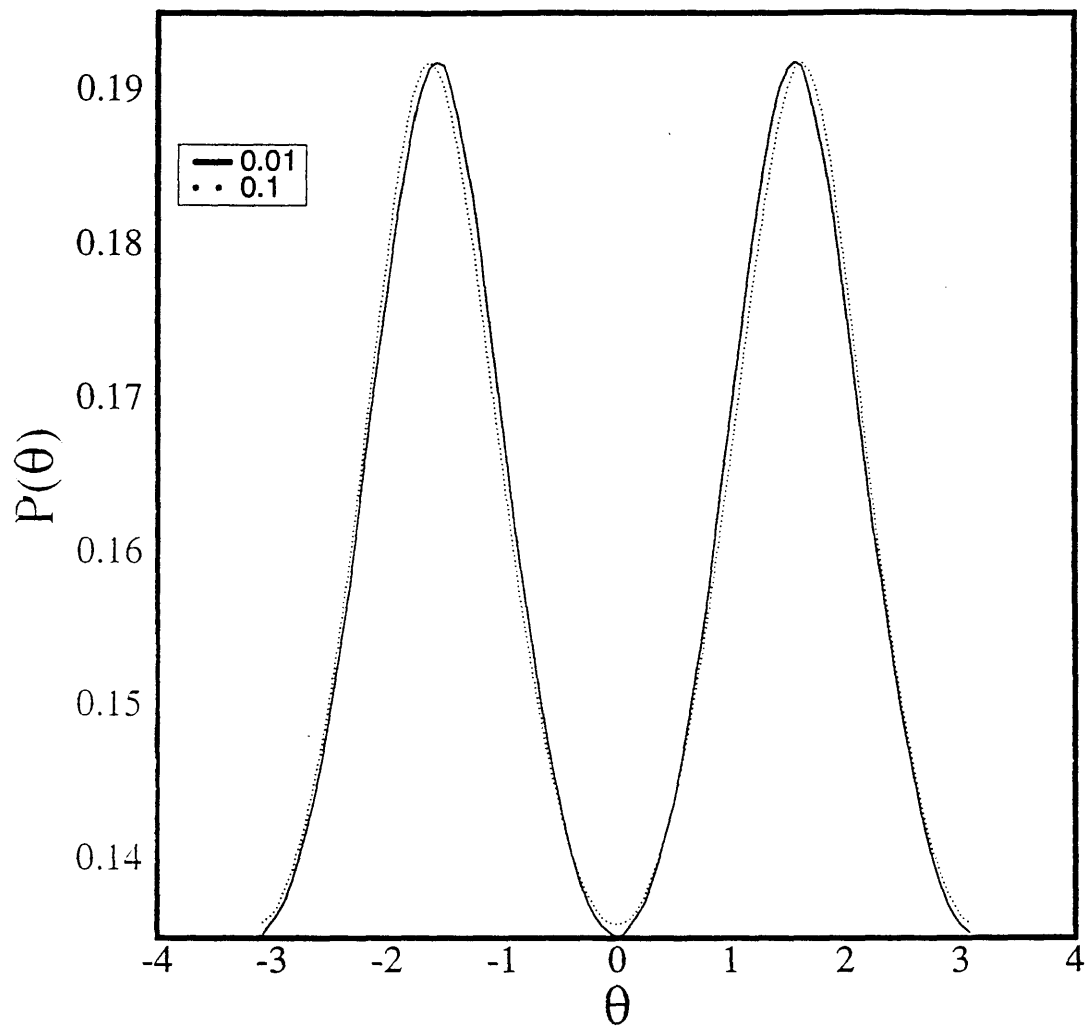


Figure 2.9: The band center anomaly, $k = \pi/2$ for $\sigma = 0.1$ and $\sigma = 0.01$

2.4 Conclusion

In this chapter, we have reported on the study of the distribution of the reflection coefficient for ensembles of disordered systems, described by the tight-binding model. We have considered chains which are made from a central region, with arbitrary diagonal disorder, connected to two semi-infinite perfect leads.

We derived a recursive numerical procedure to calculate the distribution of reflection coefficients $P(X, Y)$ and its moments and have used it to find the generic behaviour of $P(X, Y)$ as a function of the length of the system L , the incident wave vector k , the strength of disorder σ and the type of disorder ρ . The results of our investigation are shown in a series of figures 2.1 to 2.9 and set the basis for the analytical investigations of further chapters.

Chapter 3

The Reflection Transfer Matrix in 1-D

3.1 Introduction

This chapter examines reflection from disordered chains using a transfer matrix for the reflection coefficient. In earlier studies of waves in disordered media transfer matrices have played an important role [27,18,48,4]. These transfer matrices are functions of the reflection and transmission coefficients (R and T) of the system and have the property that they are ordered products of the individual transfer matrices for the component units:

$$M_L = \prod_{n=1}^L m_n \quad (3.1)$$

This linear relationship offers a tremendous advantage in that, for a system of statistically independent units, M_L can be averaged over an ensemble of chains exactly, simply by averaging the individual components. The problem is that, in their elementary form, these transfer matrices contain functions of R and T that are not closely related to observables.

In this work we have succeeded in finding a generalised transfer matrix for the reflection coefficient of a disordered medium which we call, the reflection transfer matrix or RTM. This matrix allows us to evaluate the moments of the distribution of reflection coefficients, for any ensemble of disordered

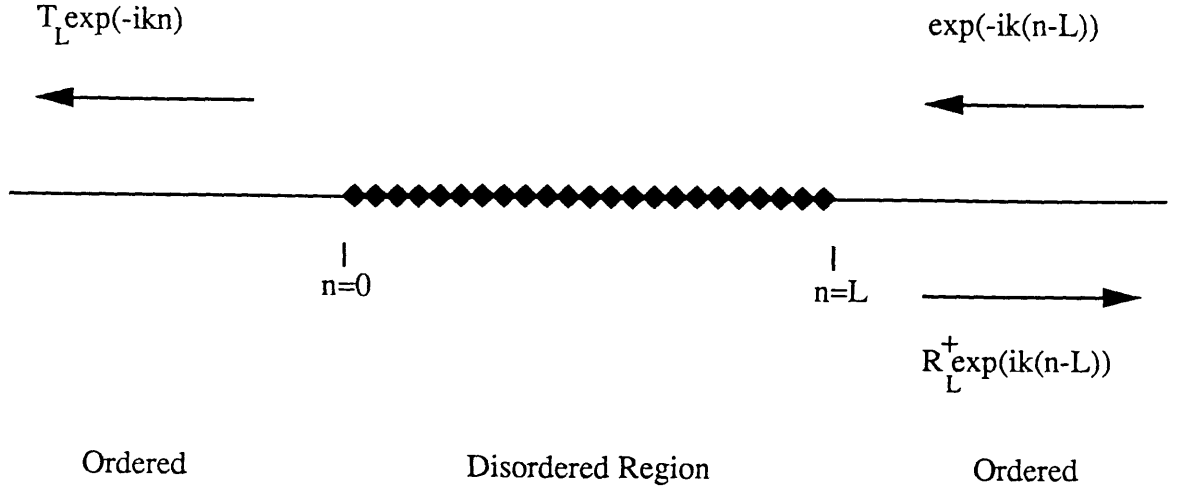


Figure 3.1: A region of disordered material partially reflects an incident wave.

chains composed of statistically independent units. It is infinite but can be approximated by a finite truncation, and is amenable to both perturbative and numerical treatments.

In section 3.2, we show how to derive the RTM using a multiple scattering approach and give an exact form for its elements. In section 3.3, we use the tight-binding model to find a weak disorder perturbation expansion for the RTM. Finally, in section 3.4, we discuss how to calculate the moments of the reflection coefficient, first numerically then using perturbation theory.

3.2 Generalities

We consider a one-dimensional system which consists of two ordered regions sandwiching a region of disorder, figure 3.1 shows what we have in mind. We suppose that we can further decompose the disordered region into statistically independent units. For example in the electron case these units might be atoms in a substitutionally disordered alloy. In the case of sound waves in a rod they might be randomly placed imperfections in the rod. Each of these units is in turn characterised by reflection and transmission coefficients, as shown in figure 3.2. The $\pm$ superscripts indicate the direction $\pm k$ in which the wave is

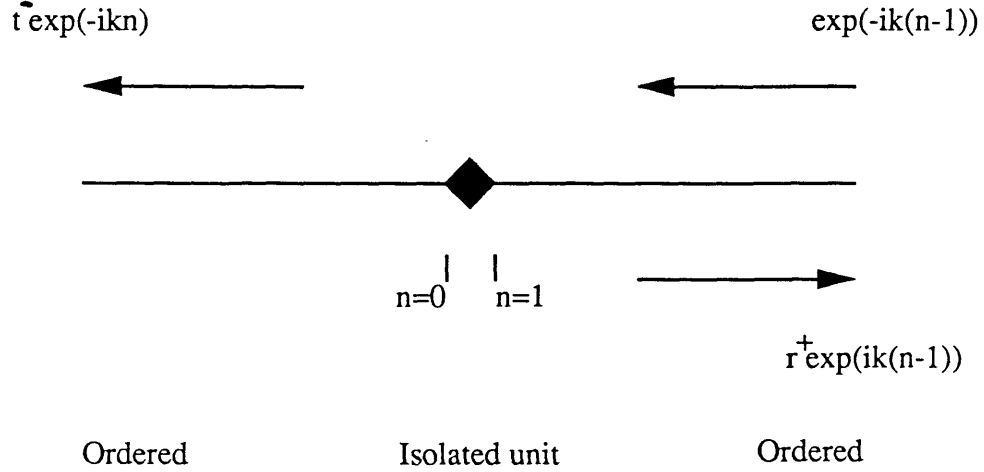


Figure 3.2: A single unit of impurity partly reflects an incident wave.

scattered. This is the simplest formulation of the problem we can make. All manner of embellishments may be imagined, but the model already contains the essence of the problem and presents a major challenge to theorists.

Suppose we have a system of L connected random units with reflection coefficient R_L^+ . If we now add an $(L+1)^{th}$ random unit the new reflection coefficient, R_{L+1}^+ , will be a sum of all reflected multiple scattering paths between the new unit and the rest of the system as in figure 3.3. This gives

$$\begin{aligned}
 R_{L+1}^+ &= r_{L+1}^+ + t_{L+1} R_L^+ t_{L+1} + t_{L+1} R_L^+ (r_{L+1}^- R_L^+) t_{L+1} \dots \\
 &\quad + t_{L+1} R_L^+ (r_{L+1}^- R_L^+)^n t_{L+1} + \dots \\
 &= r_{L+1}^+ + t_{L+1} R_L^+ (1 - r_{L+1}^- R_L^+)^{-1} t_{L+1}
 \end{aligned} \tag{3.2}$$

where we have assumed for simplicity that the transmission coefficient of the unit is symmetrical. This relation is a recursion relation for the reflection coefficient of successive length chains, it is a more generalised version of the RRR in chapter 2.

In our quest for a transfer matrix it is the series that interests us not the closed expression for the sum. It is essentially a series in powers of R_L^+ :

$$R_{L+1}^+ = r_{L+1}^+ R_L^{+0} + t_{L+1}^2 R_L^{+1} + t_{L+1}^2 r_{L+1}^{-1} R_L^{+2} + t_{L+1}^2 r_{L+1}^{-2} R_L^{+3} \dots$$

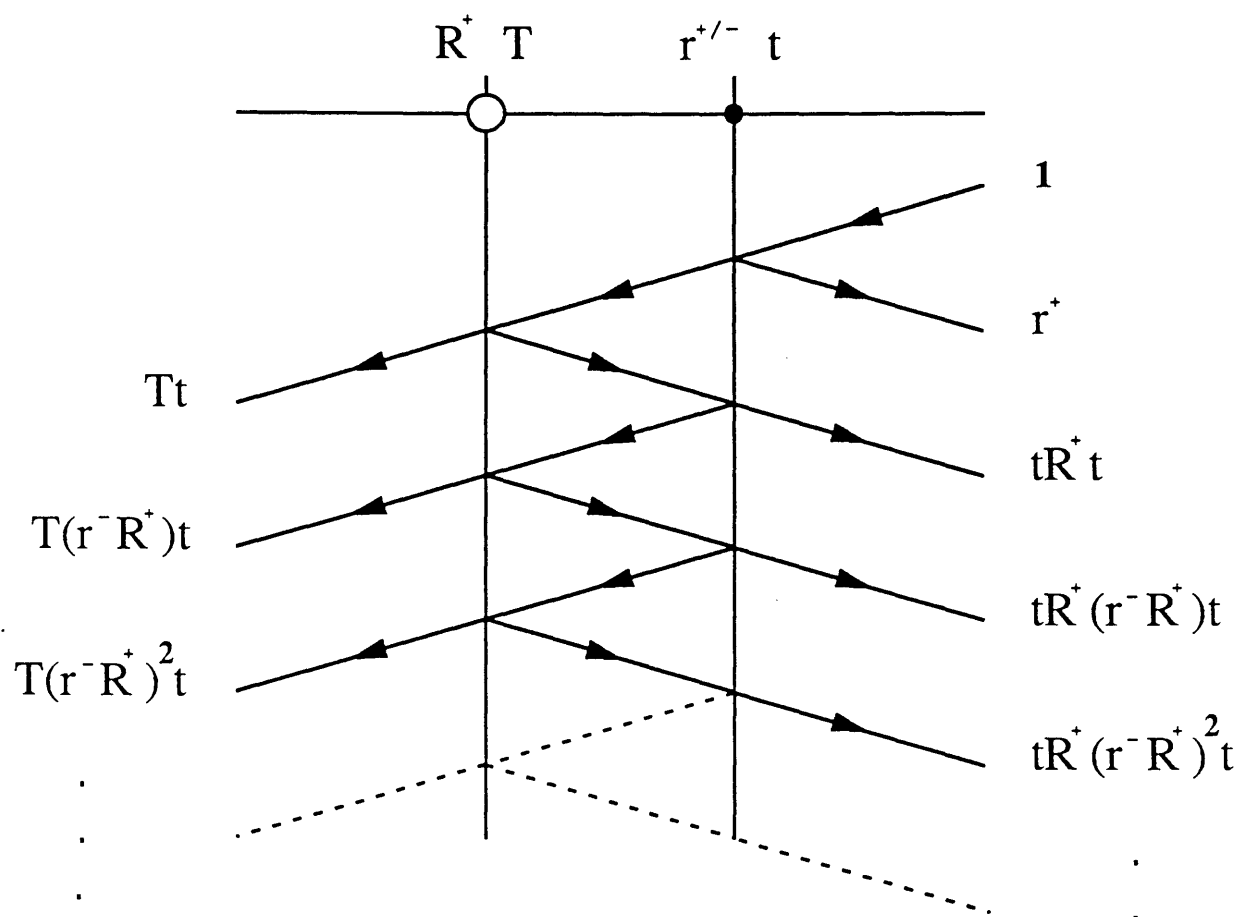


Figure 3.3: Multiple scattering picture of reflection.

$$+t_{L+1}^2 r_{L+1}^- {}^n R_L^{+n-1} + \dots \quad (3.3)$$

Any power of this series will also be a power series in R_L^+ so that if we define a vector whose elements comprise all the powers of R_L^+ :

$$\underline{R}_L = \begin{bmatrix} 1 \\ R_L^{+1} \\ R_L^{+2} \\ R_L^{+3} \\ \vdots \end{bmatrix} \quad (3.4)$$

Then we can write a matrix relation of the form,

$$\underline{R}_{L+1} = \underline{m}_{L+1} \underline{R}_L \quad (3.5)$$

where $\underline{m}_L$ is our new transfer matrix.

$$\underline{m}_L = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \dots \\ r_L^{+1} & t_L^2 & t_L^2 r_L^{-1} & t_L^2 r_L^{-2} & \dots \\ r_L^{+2} & \dots & & & \\ r_L^{+3} & \dots & & & \\ r_L^{+4} & \dots & & & \\ \dots & \dots & & & \\ \dots & \dots & & & \end{bmatrix} \quad (3.6)$$

It has the fundamental property of the old transfer matrix.

$$M_L = \prod_{n=1}^L \underline{m}_n \quad (3.7)$$

and,

$$M_L = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \dots \\ R_L^{+1} & T_L^2 & T_L^2 R_L^{-1} & T_L^2 R_L^{-2} & \dots \\ R_L^{+2} & \dots & & & \\ R_L^{+3} & \dots & & & \\ R_L^{+4} & \dots & & & \\ \dots & \dots & & & \\ \dots & \dots & & & \end{bmatrix} \quad (3.8)$$

Thus we can average any power of R_L^+ using the result:

$$\langle M_L \rangle = \prod_{n=1}^L \langle \underline{m}_n \rangle = \langle \underline{m}_1 \rangle^L. \quad (3.9)$$

provided that all the units are identically distributed and statistically independent giving

$$\langle (R_L^+)^n \rangle = \left(\langle \mathbf{m}_1 \rangle^L \right)_{n0} \quad (3.10)$$

In general these quantities are found by diagonalising $\langle \mathbf{m}_1 \rangle$ and summing the eigenvalue expansion

$$\langle (R_L^+)^n \rangle = \sum_{i=0}^{\infty} (\underline{L}_i^{(r)})_n (E_i)^L (\underline{L}_i^{(l)})_0 \quad (3.11)$$

where $(\underline{L}_i^{(r/l)})_n$ is the i^{th} right/left eigenvector corresponding to the eigenvalue E_i . This series has a particularly simple form in the infinite length limit due to the spectrum of eigenvalues of $\langle \mathbf{m}_1 \rangle$. Every eigenvalue has modulus less than unity except for one which is ejected from the rest of the spectrum and is exactly equal to unity. This gives rise to:

$$\lim_{L \rightarrow \infty} \langle (R_L^+)^n \rangle = \left(\underline{L}_0^{(r)} \right)_n \quad (3.12)$$

since $(\underline{L}_0^{(l)})_i = \delta_{i,0}$. In the infinite length limit any chain in the ensemble which is not completely reflective has zero statistical weight so that the moments of the reflection coefficient have a particular significance

$$\lim_{L \rightarrow \infty} \langle (R_L^+)^n \rangle = \langle \epsilon^{in\theta} \rangle \quad (3.13)$$

They are simply the fourier components of the stationary distribution of reflection phases

$$P(\theta) = \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} \langle \epsilon^{in\theta} \rangle \epsilon^{-in\theta} \quad (3.14)$$

The n^{th} negative moment is simply the complex conjugate of the n^{th} positive moment. Hence, if we can find the moments of the distribution of reflection coefficients in the infinite length limit we can quite simply find the distribution of their phases.

3.2.1 The Transfer Matrix

The exact form of each element in the reflection transfer matrix may be found quite easily. If we write the reflection recursion relation 3.2 in the form

$$R_{L+1}^+ = (T_{21} + T_{22}R_L^+)(T_{11} + T_{12}R_L^+)^{-1} \quad (3.15)$$

with

$$T_{21} = r_{L+1}^+ \quad T_{22} = t_{L+1}^2 - r_{L+1}^+ r_{L+1}^- \quad T_{11} = 1 \quad T_{12} = r_{L+1}^- \quad (3.16)$$

then we can expand its i^{th} power out binomially giving

$$(R_{L+1}^+)^m = \sum_{n=0}^m \binom{m}{n} T_{21}^{m-n} T_{22}^n (R_L^+)^n \sum_{n=0}^{\infty} \binom{-m}{n} T_{11}^{-m-n} T_{12}^n (R_L^+)^n \quad (3.17)$$

The both sums are absolutely convergent. The first, because it is a finite sum and the second, because conservation of probability requires

$$|r_{L+1}^- R_{L+1}^+| \leq 1 \quad (3.18)$$

so we can use the Cauchy sum rule to give

$$R_{L+1}^m = \sum_{n=0}^{\infty} (\mathbf{m}_L)_{mn} (R_L^+)^n \quad (3.19)$$

where

$$(\mathbf{m}_L)_{mn} = \sum_{k=0}^{\min(mn)} \binom{m}{k} \binom{-m}{n-k} T_{11}^{-m-n+k} T_{12}^{n-k} T_{21}^{m-k} T_{22}^k \quad (3.20)$$

which is also absolutely convergent.

3.3 Tight-Binding Model

We now consider the RTM formalism for the tight-binding model with diagonal disorder described in chapter 2. A disordered unit in this model consists of a single disordered site and a single bond. The reflection and transmission coefficients of a particular unit may be found by substituting the boundary conditions shown in figure 3.2 into the Schrödinger equation which gives

$$r^+ = r \quad r^- = \epsilon^{2ik} r \quad t^{\pm} = \epsilon^{ik} t \quad (3.21)$$

where r and t are the reflection and transmission coefficients of individual sites

$$r = \frac{i\delta}{1-i\delta} \quad \text{and} \quad t = \frac{1}{1-i\delta} \quad (3.22)$$

and

$$\delta = \frac{\epsilon}{2 \sin(k)} \quad (3.23)$$

With these expressions for the reflection and transmission coefficients, we are now in a position to re-write the RRR and hence the RTM in terms of a single parameter. Weak disorder proves the most amenable to analytic treatment and we will weigh up two different parameters which could be used for a perturbation expansion in this limit.

3.3.1 The Reflection Coefficient Expansion

Re-expressing the RRR purely in terms of the site reflection coefficient r_{L+1} using equations 3.21 we find

$$R_{L+1} = r_{L+1} + \frac{(1 + r_{L+1})^2 \epsilon^{2ik} R_L}{1 - r_{L+1} \epsilon^{2ik} R_L} \quad (3.24)$$

where for simplicity we have written $R_L^+ = R_L$. Expanding out the m^{th} power of 3.24 binomially as a power series in both r_{L+1} and R_L we can derive the RTM as an expansion in the moments of the reflection coefficient:

$$\langle \mathbf{m}_L \rangle = \sum_{n=0}^{\infty} \langle r_L^n \rangle \mathbf{d}^{r(n)} \quad (3.25)$$

with

$$\begin{aligned} (\mathbf{d}^{r(n)})_{m,m'} &= (-1)^m \epsilon^{2ikm'} \sum_{i=a}^b 2^{2i-n} \binom{m}{i} \binom{-m}{n-i} \binom{i}{m+n-(m'+i)} \\ &\quad \text{for } |m-n| \leq m' \leq m+n \\ &= 0 \text{ otherwise} \end{aligned} \quad (3.26)$$

where

$$\begin{aligned} a &= \text{int}\left(\frac{m'+1}{2}\right) \\ b &= \min(m, n, m') \end{aligned} \quad (3.27)$$

The coefficient of the n^{th} order term is therefore a matrix with $2n+1$ diagonals. This type of expansion has the advantage that equation 3.25 is convergent for

any strength or type of disorder for the same reasons that equation 3.20 converged. However, it has the disadvantage that for weak disorder the moments $\langle r^n \rangle$ do not converge *smoothly* to zero since

$$\langle r^{2n-1} \rangle \sim \langle r^{2n} \rangle \sim \mathcal{O}(\langle \epsilon^{2n} \rangle) \quad (3.28)$$

This arises from the fact that disorder is defined in terms of the site energies and not the reflection coefficients themselves. Thus simply truncating the series, in order to carry out analytic work, does not yield a faithful perturbation.

3.3.2 The Disorder Parameter Expansion

Re-expressing the RRR in terms of the disorder parameter δ we re-derive the RRR of chapter 2:

$$R_{L+1} = \frac{\epsilon^{2ik} R_L + i\delta_{L+1}(1 + \epsilon^{2ik} R_L)}{(1 - i\delta_{L+1}(1 + \epsilon^{2ik} R_L))} \quad (3.29)$$

This expression leads to an expansion for the ensemble average RTM in terms of the moments of the disorder parameter:

$$\langle \mathbf{m}_L \rangle = \sum_{n=0}^{\infty} \sigma^{(n)} \mathbf{D}^{(n)} \quad (3.30)$$

where

$$\begin{aligned} (\mathbf{D}^{(n)})_{m,m'} &= (\mathbf{d}^{(2n)})_{m,m'} = (-1)^m \epsilon^{2ikm'} \sum_{i=a}^b \binom{m}{i} \binom{-m}{2n-i} \binom{2n}{m'-m+i} \\ &\text{for } \min(0, m-2n) \leq m' \leq m+2n \\ &= 0 \text{ otherwise} \end{aligned} \quad (3.31)$$

with $a = \min(0, m-m')$, $b = \min(2n+m-m', \min(m, 2n))$ and

$$\sigma^{(n)} = \langle (i\delta)^{2n} \rangle \quad (3.32)$$

Odd moments in the expansion are zero because we have chosen to look at a symmetric distribution of disorder and the even moments converge smoothly

to zero with increasing order provided the moments of ϵ converge. Thus, equation 3.30 is a faithful perturbation expansion. However, the disadvantage here is that in making the binomial expansion we introduce the approximate convergence criterion

$$\delta < 0.5 \quad (3.33)$$

for all possible site energies. This restriction rules out unbounded distributions such as the exponential and the gaussian. We would have to look at these using the r formalism.

3.4 Analytical Solutions

As we have seen the problem of finding the moments of the distribution of reflection coefficients is essentially one of finding the eigenvalues and vectors of the ensemble average RTM. Calculation of the average RTM may either be done directly by numerical averaging or by using truncations of the perturbation expansions 3.25 or 3.30. The eigenvalues and vectors may then be found either using a suitable numerical package or by using perturbation theory. We will concentrate here on looking for analytic solutions using perturbation theory.

3.4.1 Perturbation Theory

We consider a perturbation about the ordered state. At first sight this may seem strange since the introduction of disorder has such an extreme effect on the transport properties of a system, particularly in the infinite length limit where an infinitesimal amount of disorder causes every state to become localized making every chain $\mathbb{Z}$ completely reflective. However the quantities which we are calculating, the moments of the reflection coefficient, hardly change with the introduction of disorder, since at weak disorder their phases are completely random whatever their modulus.

The ordered state is described by the matrix

$$(\mathbf{D}^{(0)})_{m,m'} = e^{2ikm} \delta_{m,m'} \quad (3.34)$$

This matrix clearly has infinite degeneracy for any wavevector rationally related to π

$$k = \frac{q\pi}{u} \quad (3.35)$$

where q and u are two coprime integers. We will therefore need to consider a degenerate perturbation theory. The eigenvalue equation for the ordered state takes the form

$$\mathbf{D}^{(0)}|sp\rangle = \varepsilon_{sp}^{(0)}|sp\rangle \quad (3.36)$$

where

$$\varepsilon_{s,p}^{(0)} = \exp(2i\frac{q\pi}{u}(su + p)) = \varepsilon_p \quad (3.37)$$

and the vector $|sp\rangle$ is a right vector of the form

$$(|sp\rangle)_j = \delta_{j,su+p} \quad (3.38)$$

Introducing the perturbation, the eigenvector equation takes the form

$$(\mathbf{D}^{(0)} + \alpha \mathbf{D}) \underline{\mathcal{L}}_{sp}^{(r)} = E_{sp} \underline{\mathcal{L}}_{sp}^{(r)} \quad (3.39)$$

where[†]

$$\mathbf{D} = \sum_{n=1}^{\infty} \sigma^{(n)} \mathbf{D}^{(n)} \text{ and } \alpha = 1 \quad (3.40)$$

In order to solve this equation we will consider first order in α only so that we can write

$$\underline{\mathcal{L}}_{sp}^{(r)} = \underline{\mathcal{L}}_{sp}^{r(0)} + \alpha \underline{\mathcal{L}}_{sp}^{r(1)} \quad (3.41)$$

$$E_{sp} = \varepsilon_p + \alpha \varepsilon_{sp}^{(1)} \quad (3.42)$$

Substituting these expressions into the eigenvector expression we get the standard form

$$(\mathbf{D}^{(0)} - \varepsilon_p) \underline{\mathcal{L}}_{sp}^{r(1)} = (\varepsilon_{sp}^{(1)} - \mathbf{D}) \underline{\mathcal{L}}_{sp}^{r(0)} \quad (3.43)$$

The zero order term is a superposition of the degenerate unperturbed eigenstates

$$\underline{\mathcal{L}}_{sp}^{r(0)} = \sum_{s'=0}^{\infty} c_{sp,s'p}^r |s'p\rangle \quad (3.44)$$

[†] Definition of $\sigma^{(n)}$ is given in 3.32.

and the first order term is a superposition of all other eigen states

$$\psi_{sp}^{r(1)} = \sum_{s'=0}^{\infty} \sum_{\substack{p'=0 \\ p' \neq p}}^{u-1} a_{sp,s'p'}^r |s'p' \rangle \quad (3.45)$$

If we now substitute these forms into 3.43 and take the scalar product with the left vector $\langle s''p|$ we derive the secular equation

$$0 = \sum_{s'=0}^{\infty} c_{sp,s'p}^r \left(\varepsilon_{sp}^{(1)} \delta_{s''s'}^c - (D_u)_{s''p,s'p} \right) \quad (3.46)$$

where we have written

$$(D_u)_{s''p,s'p} = D_{s''u+p,s'u+p} \quad (3.47)$$

Looking at the form of the matrices D_u we see that

$$D_{2n-1} = \mathcal{O}(\sigma^{(1)})T_1 + \mathcal{O}(\sigma^{(n)})T_2 + \mathcal{O}(\sigma^{(2n)})T_3 + \dots \quad (3.48)$$

$$D_{2n} = \mathcal{O}(\sigma^{(1)})T_1 + \mathcal{O}(\sigma^{(n)})T_2 + \mathcal{O}(\sigma^{(2n+1)})T_3 + \dots \quad (3.49)$$

where the T_n are banded matrices with $2n-1$ diagonals and the terms $\mathcal{O}(\sigma^{(n)})$ are series of leading order $\sigma^{(n)}$. Hence, the elements of D_u which mix the unperturbed states are of order $\mathcal{O}(\sigma^{(n)})$ where $n = \text{int}((u+1)/2)$. For large u or at a generic position in the band, not rationally related to π , this mixing is insignificant and we can truncate the moment expansion to order $m \leq n-1$ making the secular equation diagonal. This reduces the problem to one of non-degenerate perturbation theory. We will come back to the noticeable effects of the degeneracy, the so called ‘anomalies’, in the last section of this chapter.

3.4.2 Non-Degenerate P.T.

In the non-degenerate case, the solution to the secular equation has the form

$$c_{sp,s'p}^r = \delta_{s's}^c \quad (3.50)$$

$$\varepsilon_{sp}^{(1)} = (D'_u)_{sp,sp} \quad (3.51)$$

where $\mathbf{D}'_u$ represents a truncated form of the matrix $\mathbf{D}_u$. Substituting these forms into 3.43 and taking the scalar product with the left vector $\langle s''p''|$ we find

$$a_{sp,s'p'}^r = -\frac{(\mathbf{D}'_u)s'p',sp}{\varepsilon_{p'} - \varepsilon_p} \quad (3.52)$$

The corresponding left eigenvector may be found in a similar manner giving

$$a_{sp,s'p'}^l = a_{s'p',sp}^r \quad (3.53)$$

The approximations we have made so far suggest that our results are correct in the weak disorder limit for short chains and for infinitely long chains so we will re-express our eigenvalues in a way which expresses this

$$(E_{sp})^L = (\varepsilon_p)^L \exp\left(L \frac{\varepsilon_{sp}^{(1)}}{\varepsilon_p}\right) \quad (3.54)$$

Hence, substituting our analytical forms for the eigenvectors and eigenvalues into equation 3.11 the moments of the reflection coefficient take the form

$$\langle R_L^{su+p} \rangle = \delta_{sp,00}^c + \frac{(\mathbf{D}'_u)_{sp,00}}{1 - \varepsilon_p} \left(1 - (E_{ps})^L\right) (1 - \delta_{p0}^c) \quad (3.55)$$

To leading order in $\sigma^{(n)}$ these expressions simplify to

$$\begin{aligned} \langle R_L^{2n-1} \rangle &\approx \frac{(2n-1)\sigma^{(n)}}{1 - e^{2ik(2n-1)}} \left(1 - \exp\left((2ik(2n-1) - 3(2n-1)^2\sigma^{(1)})L\right)\right) \\ \langle R_L^{2n} \rangle &\approx \frac{\sigma^{(n)}}{1 - e^{2ik(2n)}} \left(1 - \exp\left((2ik(2n) - 3(2n)^2\sigma^{(1)})L\right)\right) \end{aligned} \quad (3.56)$$

Figures 3.4 (a) shows the locus of the moment $\langle R_L \rangle$ with wave vector $k = [0.52\pi, 0.95\pi]$ in the complex plain. for binary disorder with $\sigma^{(1)} = 0.1$ and $L = 10$. The dotted line is the exact numerical result of chapter 2 and the full line is the first order perturbation theory result from 3.56. (b) shows the locus of $\langle R^2 \rangle$ for the same parameters. The symmetrical distribution of disorder we have chosen implies the simple symmetry of equation 2.10 so that these plots only need show half the band.

Figures 3.5 (a,c) show $P(\theta)$ for $\sigma^{(1)} = 0.1$ at three different positions in the band (a) $k = 7\pi/8$ (b) $k = 3\pi/4$ and (c) $k = 5\pi/8$. The solid line is the

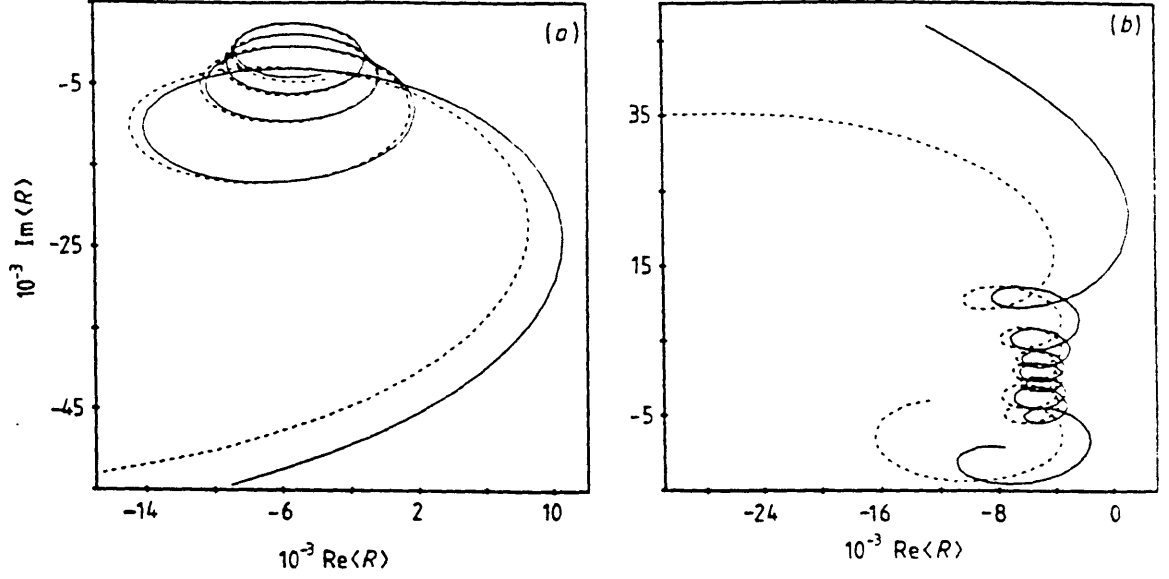


Figure 3.4: (a) Locus of $\langle R \rangle$ for $k = [0.52\pi, 0.95\pi]$, $L = 10$ and $\sigma^{(1)} = 0.1$. (b) Same as (a) for $\langle R^2 \rangle$.

first order perturbation theory result, calculated using 3.55 with $L \rightarrow \infty$ and summing 3.13, and the dashed line is the random sampling result of chapter 2 with $N = 10^9$. In the infinite length limit the symmetry 2.10 leads to

$$P(k^+; \theta) = P(k^-; \theta) \quad (3.57)$$

so that these plots also give the corresponding plots in the other half of the band by mirror symmetry about $\theta = 0$.

3.4.3 Anomalies

We have shown that at a generic position in the band the effects of degeneracy in $\mathbf{D}^{(0)}$ may be ignored. For instance, the elements of the eigenvector corresponding to the ejected unit eigenvalue have leading order

$$(\underline{U}_{00}^r)_m \sim \mathcal{O}\left(\sigma^{\text{int}(\frac{m+1}{2})}\right) \quad (3.58)$$

since the zero order term does not contribute for $m > 1$. However, this simple behaviour is modified for resonant values of the wavevector $k = q\pi/u$. The zero

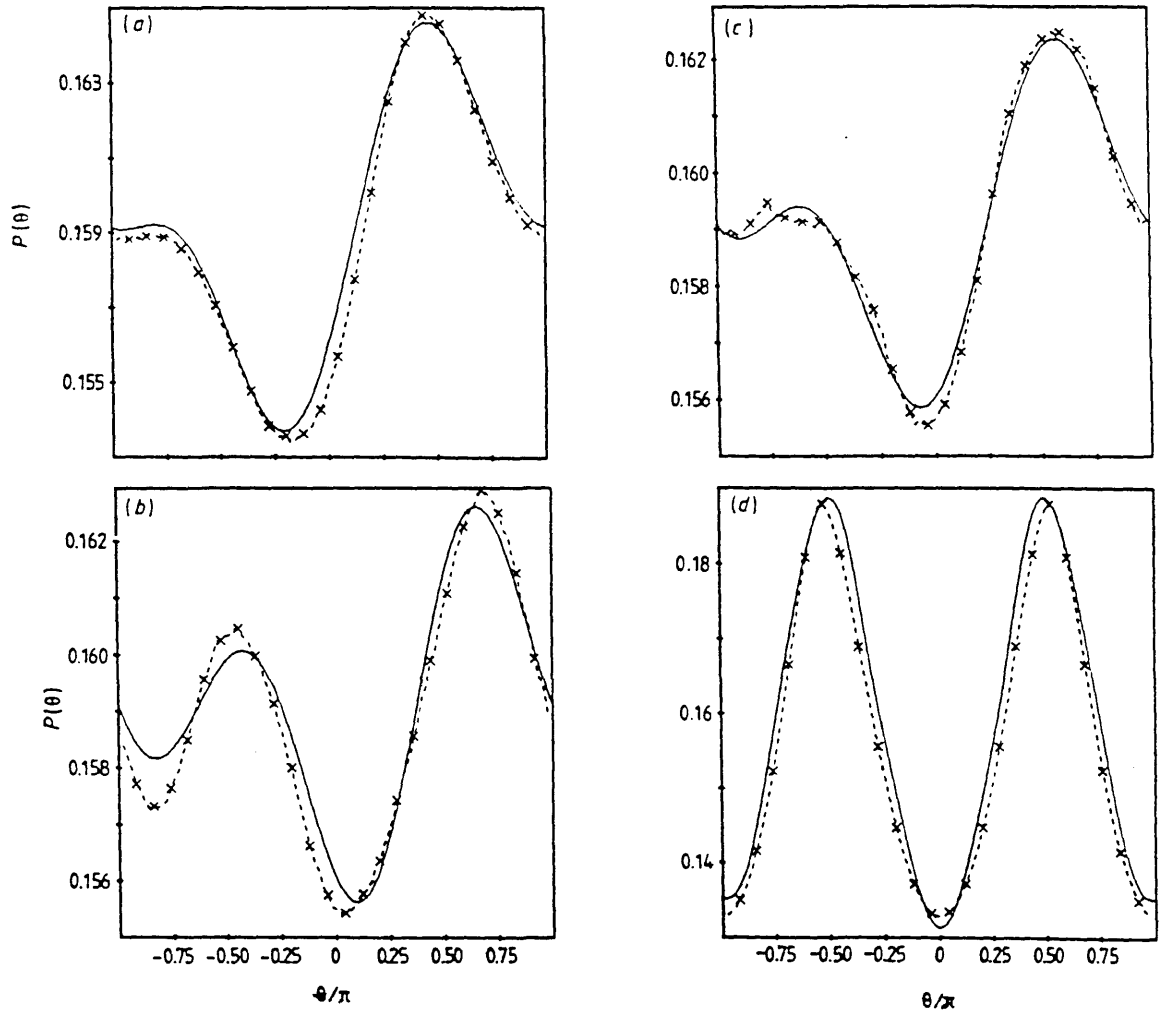


Figure 3.5: $P(\theta)$ for $\sigma^{(1)} = 0.1$ with (a) $k = 7\pi/8$ (b) $k = 3\pi/4$ and (c) $k = 5\pi/8$ and (d) $k = \pi/2$.

order terms for $m = s'u$ are no longer equal to zero (s' is any positive integer) and are determined by the secular equation

$$0 = \sum_{s'=0}^{\infty} c_{00,s'u}^r \left(\mathcal{O}(\sigma^{(1)})(T_1)_{s''0,s'u} + \mathcal{O}(\sigma^{(n)})(T_2)_{s''0,s'u} + \dots \right) \quad (3.59)$$

where

$$n = \text{int} \frac{u+1}{2} \quad (3.60)$$

The solution to this equation gives

$$c_{00,s'u}^r \sim \mathcal{O}(\sigma^{s'(n-1)}) \quad (3.61)$$

to leading order and therefore the leading order of the eigenvector element $(\underline{L}_{00}^r)_{s'u}$ is decreased since

$$s' \left(\text{int} \left(\frac{u+1}{2} \right) - 1 \right) < \text{int} \left(\frac{s'u+1}{2} \right) \quad (3.62)$$

The most striking effect produced by these zero order terms is at the band center $u = 2$ where

$$c_{00,s'u}^r \sim \mathcal{O}(\sigma^{(0)}) \quad (3.63)$$

independent of disorder. This fact explains the band center anomaly in $P(\theta)$ since if, in the limit of zero disorder, its fourier components do not vanish, it will not become completely random. Figure 3.5(d) shows a comparison between the random sampling result for the band center anomaly in $P(\theta)$, for $\sigma^{(1)} = 0.1$, and the result of numerically solving the secular equation 3.59, for which the moment expansion was truncated at $n = 2$ and the size of the matrix was increased until no change was seen in $P(\theta)$. We will come back to this anomaly in chapter 4 using an exact solution for $P(\theta)$.

3.5 Conclusion

In this chapter, we have established a formalism involving an infinite transfer matrix, which in principle, allows us to calculate the moments of the distribution of reflection coefficients $\langle R_L^n \rangle$ to desired accuracy, for any ensemble of disordered chains. We have concentrated on the weak disorder limit and used

perturbation theory to calculate analytic expressions for $\langle R_L'' \rangle$. We find that, at a generic position in the band we can use non-degenerate perturbation theory but for wavevectors which are rationally related to π , we must use degenerate perturbation theory to account for certain moments being anomalously large. The strongest anomaly occurs at the band center. Figures 3.4(a,b), give a comparison between the perturbation theory result and the exact numerical result of chapter 2, for the first two moments $\langle R_L \rangle$ and $\langle R_L^2 \rangle$. Figures 3.5(a,b,c,d) show a similar comparison, this time between the perturbation theory and the random sampling method of chapter 2, for $P(\theta)$ the stationary distribution of the phase of the reflection coefficient, at various positions in the band. $P(\theta)$ in the last figure (d) clearly has a larger amplitude than the other plots thus illustrating the band center anomaly.

Chapter 4

Dyson Equation Methods

4.1 Introduction

In this chapter, we will take a closer look at the distribution of the phase of the reflection coefficient. We limit this to the tight-binding model with diagonal disorder, i.e. random site potentials, in the strongly localised regime, where the length of the disordered region of the sample is much larger than the localisation length. In this regime, the reflection phase reaches a nontrivial stationary, or invariant, distribution. We investigate in particular the regularity properties of this distribution, as well as its dependence both on energy and on the strength of disorder. The present approach is a global one, which does not rely on perturbation theory, nor on any approximation scheme.

In section 4.2, we show that the distribution of the reflection coefficient, and of related quantities, obeys a linear integral equation, of a type first studied by Dyson [49] in the context of one-dimensional random systems. We also derive expressions for the Lyapunov exponent and the integrated density of states of the problem, in terms of the invariant phase distribution. Section 4.3 is devoted to the case of a binary distribution of the random site potentials. This case is special, since the distribution of the reflection phase usually contains an infinity of power-law singularities, which appear as infinitely high peaks when the strength of disorder exceeds some energy-dependent threshold. This novel phenomenon is related to the occurrence of divergences in the density of states of

e.g. harmonic chains with random masses, first described by Halperin [50]. By adapting an approach used by Nieuwenhuizen and Luck [51], to study Halperin's 'island frequencies', we obtain a complete labelling and quantitative description of the power-law singularities in the present problem. Section 4.4 presents what is certainly the only nontrivial distribution of potentials for which the problem is exactly soluble. For this symmetric exponential distribution, with an arbitrary width, we can derive the distribution of the reflection phase in an exact way. Some of the applications of this result are discussed. Section 4.5 presents a short summary and conclusion.

4.2 Generalities

In this section, we derive an integral Dyson equation [49] for the invariant distribution of the reflection phase in the long length limit. This formalism will be used extensively in the next sections. We will rely on definitions given in chapter 2 for a description of the model we look at to avoid repetition.

When the sample length L becomes large, the reflection phase θ_L is asymptotically distributed according to a probability density $P(\theta)$. This density is stationary, i.e. independent of L , and hence invariant under the reflection recursion relation (2.9) of chapter 2. This invariant probability measure can be alternatively described in terms of the Riccati Y -variable or the t -variable,

$$t = \tan \frac{\theta}{2} = \frac{\cos k - Y}{\sin k} \quad (4.1)$$

Hence if $S(Y)$ and $Q(t)$ denote the corresponding densities. Eq. 4.1 implies that these quantities are simply related through

$$Q(t) = (1 + \cos \theta)P(\theta) = \sin k S(Y) \quad (4.2)$$

The existence of an invariant measure for the one-dimensional Anderson model, as well as some of its regularity properties, have been investigated rigorously in ref. [52]. The present work clearly does not pretend at any mathematical rigour on this point.

We will use the t -variable in the technical developments throughout the following, in order to avoid dealing with complex numbers, and to benefit from

the simplicity of the transform

$$t_L = 2\delta_L + \frac{t_{L-1} + \tau}{1 - t_{L-1}\tau} \quad (4.3)$$

for which

$$\delta_L = \frac{\epsilon_L}{2 \sin k} \quad \text{and} \quad \tau = \tan k \quad (4.4)$$

as derived in chapter 2.

The distribution $Q(t)$ obeys an integral equation, of a type first derived by Dyson [49], which expresses its invariance under the random transformation 4.3. This Dyson equation has the form

$$Q(t) = \int \rho(\epsilon) d\epsilon \int Q(u) du \delta_D \left(t - 2\delta - \frac{u + \tau}{1 - u\tau} \right) \quad (4.5)$$

where t and u represent t_L and t_{L-1} , respectively. δ_D denotes the Dirac delta function, which enforces the condition

$$u = g_\delta(t) = \frac{t - 2\delta - \tau}{1 + (t - 2\delta)\tau} \quad (4.6)$$

so that performing the integral over u we are left with

$$Q(t) = \int \rho(\epsilon) d\epsilon |g'_\delta(t)| Q[g_\delta(t)] \quad (4.7)$$

where the accent denotes differentiation w.r.t. t . Eq. 4.7 will be referred to as the Dyson equation of the problem.

It will be shown in section 4.3 that the probability densities $P(\theta)$ and $Q(t)$ are very singular quantities when the site potentials have a binary distribution. Therefore we introduce the following integrated densities, or distribution functions now:

$$W_P(\theta) = \int_{-\pi}^{\theta} P(\varphi) d\varphi, \quad W_Q(t) = \int_{-\infty}^t Q(u) du \quad (4.8)$$

These quantities are always continuous functions but not differentiable when the densities themselves are divergent.

This section ends with a discussion of the relationship between the probability density $P(\theta)$ - or its equivalent formulations $Q(t)$ and $S(Y)$ - and two other quantities of much physical interest, namely the Lyapunov exponent and

the integrated density of states. We begin by defining, for a complex energy E , a characteristic function (or complex Lyapunov exponent) $\Omega(E)$ [53] through

$$\Omega(E) = \lim_{M \rightarrow \infty} \frac{1}{M} \sum_{L=1}^M \ln Y_L \quad (4.9)$$

where the principle branch of the complex logarithm is used. It can be shown (see e.g. ref. [53]) that the limit of this quantity as E goes to the real axis has the form

$$\Omega(E \pm i0) = \gamma(E) \pm i\pi H(E) \quad (4.10)$$

where $\gamma(E)$ is the Lyapunov exponent (inverse localisation length) of the problem, and $H(E)$ denotes its integrated density of states (IDOS), i.e. the fraction of energy eigenvalues in the spectrum which are *larger* than some E . This rather unconventional definition is required by the fact that the off-diagonal terms in the tight-binding Schrödinger equation (2.1) have a positive sign.

The above relations between the variables Y_L , θ_L , and t_L yield the following expressions

$$\begin{aligned} \Omega(E) &= \int \ln Y^* S(Y^*) dY^* \\ &= \int \ln \frac{\epsilon^{-ik} + \epsilon^{ik+i\theta}}{1 + \epsilon^{i\theta}} P(\theta) d\theta \\ &= \int \ln(\cos k - t \sin k) Q(t) dt \end{aligned} \quad (4.11)$$

where it is understood that the invariant probability densities are evaluated for an energy E with an infinitesimal imaginary part.

4.3 The Binary Alloy

In this section we study the distribution $P(\theta)$ of the reflection phase in the case of a binary symmetric distribution of the site potentials: $\epsilon_n = \pm\epsilon$ with equal probabilities $1/2$.

As we discussed in chapter 2, for binary disorder, $P(\theta)$ is a very singular quantity containing an infinity of power-law singularities under generic circum-

stances. The mechanism responsible for this novel singular behaviour is closely related to a phenomenon, first discussed by Halperin [50], who considered binary random harmonic chains, made of light and heavy atoms. The density of states of this system becomes infinite at the eigenfrequencies of finite clusters or 'islands' of light masses in a 'sea' of heavy ones. These singularities occur at high frequency, where heavy masses damp excitations, and only yield divergences of the density of states when the disorder strength (here, the mass difference) exceeds some threshold.

A similar effect occurs in the present problem, where the two different site energies $\pm\epsilon$ play in some sense the part of the atomic masses. We will first present a heuristic and descriptive study of the phenomenon, before going to a more rigorous analysis, based on the Dyson equation 4.7.

Consider the periodic chain $+ - + - + - \dots$ made from an infinite repetition of the simple cell or pattern $(+ -)$. Throughout this section, the symbols $+$ and $-$ denote the signs of the site potentials ϵ_n . This simplest example of a pattern with period 2 will turn out to be physically the most important one. Provided the energy E lies in a gap of this periodic structure, the infinite periodic chain exhibits only two well-defined reflection angles: θ_+ and θ_- , corresponding to whether the atom at the surface has a site energy of $\pm\epsilon$. These phases are entirely determined by the structure of the basic pattern, and by the energy E . The simplest way of looking at this is to introduce the usual transfer-matrix formalism in which the tight-binding Schrödinger equation (2.1) is recast in the following form

$$\begin{pmatrix} \phi_{n+1} \\ \phi_n \end{pmatrix} = \mathbf{M}_n \begin{pmatrix} \phi_n \\ \phi_{n-1} \end{pmatrix} \quad (4.12)$$

The transfer matrix $\mathbf{M}_n$ has the form

$$\mathbf{M}_n = \begin{pmatrix} E - \epsilon_n & -1 \\ 1 & 0 \end{pmatrix} \quad (4.13)$$

Hence the propagation of a wave function along the chain is described by a product of non-commuting 2x2 transfer matrices. The transfer matrix $\mathbf{M}$ of the cell $(+ -)$ is then the product of the two elementary transfer matrices of the form 4.13 associated with the atoms of the cell

$$\mathbf{M} = \begin{pmatrix} E^2 - \epsilon^2 - 1 & \epsilon - E \\ \epsilon + E & -1 \end{pmatrix} \quad (4.14)$$

Since M has unit determinant, its eigenvalues are determined by its trace: $\text{tr} M = E^2 - \epsilon^2 - 2$. If the energy is such that $|\text{tr} M| > 2$, the eigenvalues of M are $\exp(\pm K)$, up to a sign, where K is defined by

$$|\text{tr} M| = 2 \cosh K \quad (4.15)$$

Hence the wave function grows essentially like $\phi_n \sim \exp(nK)$, with two different amplitudes, according to the parity of the site label n . The Riccati variable defined in eq. 2.6 therefore admits two limit values, namely Y_+ and Y_- , which are related to the values $\theta_{\pm}$ of the reflection phase by eqn. 4.1.

Consider now all chains for which the disordered region ends up with the repetition of any finite number N of contiguous cells $(+-)$. It is expected that, for N large enough, the reflection phase θ of such a chain will be very close to either θ_+ or θ_- . In a more quantitative way, since the eigenfunction inside the segment made of the N cells $(+-)$ is a linear combination of $\exp(nK)$ and $\exp(-nK)$, it can be argued that the difference $|\theta - \theta_{\pm}|$ is of the order of the ratio of both solutions, taken at the end of the segment, namely $\exp(-2KN)$. On the other hand, the probability of having such a configuration is proportional to 2^{-2N} . By eliminating the number N of cells between the above estimates, we predict that the distribution function $W_P(\theta)$, defined by eq. 4.8, has a power-law singularity

$$W_{P,sg}(\theta) \sim |\theta - \theta_{\pm}|^{\alpha}, \quad \text{with} \quad \alpha = \frac{\ln 2}{K} \quad (4.16)$$

Such a singularity corresponds, via a formal differentiation, to a power-law behaviour $|\theta - \theta_{\pm}|^{\alpha-1}$ for $P(\theta)$ itself. Hence the probability density exhibits a divergency—an infinitely high peak—only when we have $\alpha < 1$, i.e. $K > \ln 2$. Since the magnitude of K is a measure of randomness, this means that there is a threshold in the disorder strength for peaks to appear. When the exponent α is larger than unity, only some derivative of $P(\theta)$ diverges at $\theta = \theta_{\pm}$.

The heuristic argument just described also predicts that the distribution of the phase exhibits similar but weaker singularities, characterised by the same exponent α , at all the values of the phase corresponding to adding one, two, etc. atoms of any type at the end of the large region made of $(+-)$ cells. We will come back to this point in a more detailed way later in this section.

The periodic arrangements of larger patterns, such as for instance $(+--)$ and $(++-)$, which have period $p = 3$, up to a cyclic permutation, also produce their own sets of singularities, whenever the energy lies in a gap of the associated spectra. These are also power-law singularities, with an exponent α given by

$$\alpha = \frac{p \ln 2}{2K} \quad (4.17)$$

where p denotes the period of the cell, and K is still related to the trace of the associated product of p transfer matrices through eq. 4.15. It is nevertheless expected on physical grounds that the singularities connected with the $(+-)$ cell will be the most important ones. The numerical work presented below fully confirms this assertion.

We now turn to a more accurate analysis, based on the Dyson equation 4.7, of the singularities in the distribution $P(\theta)$, or equivalently $Q(t)$ or $S(Y)$. Here again, we prefer to use the language of the t -variable, for sake of simplicity. The present study is an adaptation of the work by Nieuwenhuizen and Luck [51] on the density of states of harmonic chains. We will present the full derivation in the case of the $(+-)$ cell, which is both the simplest and the most important case.

For the binary distribution of site potentials under consideration, eq. 4.7 has the form

$$2Q(t) = |g'_+(t)| Q[g_+(t)] + |g'_-(t)| Q[g_-(t)] \quad (4.18)$$

where $g_{\pm}(t)$ denote the function $g_s(t)$ defined in eq. 4.6. The transcription of the above heuristic argument goes as follows. The limit reflection angles θ_+ and θ_- correspond to variables t_+ and t_- via eq. 4.1 such that

$$t_+ = g_-(t_-), \quad t_- = g_+(t_+) \quad (4.19)$$

A direct evaluation yields in the present case

$$t_{\pm} = \pm\delta \pm \left[\frac{\tau\delta \pm 1}{\tau\delta \mp 1} (\delta^2 + 1) \right]^{1/2} \quad (4.20)$$

Let us also introduce the notation

$$\lambda_+ = g'_+(t_+), \quad \lambda_- = g'_-(t_-) \quad (4.21)$$

Both of these quantities are positive. The occurrence of singularities in $Q(t)$ at $t = t_{\pm}$ appears clearly through the following argument, inspired from ref.[51]. Since all values of the probability density $Q(t)$ are necessarily positive, the Dyson equation 4.18 implies that we have $2Q(t_+) \geq \lambda_+ Q(t_-)$ and $2Q(t_-) \geq \lambda_- Q(t_+)$, and hence $4Q(t_{\pm}) \geq \lambda_+ \lambda_- Q(t_{\pm})$. Therefore, if the product

$$\Lambda = \lambda_+ \lambda_- \quad (4.22)$$

is larger than 4, both values of Q must either be zero or infinite!

A quantitative description of the actual behaviour of $Q(t)$ is obtained by linearising the Dyson equation around $t = t_{\pm}$ as follows. If $Q_{sy}(t)$ denotes the singular parts of $Q(t)$ around $t_{\pm}$, eq. 4.18 implies that we have, up to first order in the variations x and y

$$\begin{aligned} 2Q_{sy}(t_+ + x) &\approx \lambda_+ Q_{sy}(t_- + \lambda_+ x), \\ 2Q_{sy}(t_- + y) &\approx \lambda_- Q_{sy}(t_+ + \lambda_- y) \end{aligned} \quad (4.23)$$

The general asymptotic solution of these equations has the form of a power-law, modulated by periodic amplitudes, namely

$$\begin{aligned} Q_{sy}(t_+ + x) &\approx |x|^{\alpha-1} A^{\pm} \left(\frac{\ln |x|}{\ln \Lambda} \right), \\ Q_{sy}(t_- + y) &\approx \frac{1}{2} \lambda_-^{\alpha} |y|^{\alpha-1} A^{\pm} \left(\frac{\ln |\lambda_- y|}{\ln \Lambda} \right) \end{aligned} \quad (4.24)$$

where the value of the exponent α

$$\alpha = \frac{2 \ln 2}{\ln \Lambda} \quad (4.25)$$

can be rewritten after a good deal of manipulations as

$$\begin{aligned} \alpha &= \frac{\ln 2}{K}, \\ \text{with} \\ \epsilon^2 - E^2 &= 2(\cosh K - 1) = 4 \sinh^2(K/2) \end{aligned} \quad (4.26)$$

in full agreement with the previous result 4.16.

The amplitudes $A^\pm$ are two periodic functions of their argument, with unit period, and the superscript $\pm$ denotes the sign of x or y . The occurrence of periodic amplitudes is a common feature of a large variety of disordered systems with a discrete, e.g. binary, distribution of the random couplings [51,54,55,56]. As usual, the above linear analysis predicts their existence and their period, but not their specific form.

An integration of eq. 4.24 shows that the distribution function $W_Q(t)$ of the t -variable, defined in eq. 4.8, also has a power-law singular component around $t_\pm$

$$\begin{aligned} W_{Q,sg}(t_+ + x) &\approx |x|^\alpha B^\pm \left(\frac{\ln |x|}{\ln \Lambda} \right), \\ W_{Q,sg}(t_- + y) &\approx \frac{1}{2} |y|^\alpha B^\pm \left(\frac{\ln |\lambda - y|}{\ln \Lambda} \right) \end{aligned} \quad (4.27)$$

The $B^\pm$ are two periodic amplitudes, with unit period, which are essentially primitives of the $A^\pm$. Hence the $B^\pm$ are slightly more regular mathematical objects. It can indeed be argued, in analogy with ref. [54], that they are always continuous functions, but they are nowhere differentiable when $\alpha < 1$. Some plots of these amplitudes will be presented later on.

The results 4.24 and 4.27 show that the distribution $Q(t)$ is never a smooth function, even at weak disorder ($\epsilon \rightarrow 0$). Indeed, for any small value ϵ of the site potentials, the energy interval $|E| < \epsilon$ around the band center lies in a gap of the infinite $(+-)$ structure. In this whole range, eqs. 4.25, 4.26 predict a finite value of the exponent α . Hence the distribution functions $W_P(\theta)$ and $W_Q(t)$ are not $n(\alpha)$ times differentiable, where $n(\alpha)$ denotes the integer part of $\alpha+1$. The derivatives of that order are indeed infinite at $t_\pm$. In particular, at the band center ($E = 0$), eq. 4.26 reads $\epsilon = 2 \sinh(K/2)$. Hence the order $n(\alpha)$ of the singularities blows up at weak disorder as $(\ln 2)/\epsilon$.

As mentioned previously, the distributions $P(\theta)$ and $Q(t)$ exhibit a divergence, or a 'peak', only when $\alpha < 1$. This condition can be recast in the form of a threshold value for the disorder ϵ , namely $\epsilon > \epsilon_0$, with $\epsilon_0^2 = E^2 + 1/2$. At the band center, we have a threshold of $\epsilon_0 = 1/\sqrt{2}$.

Let us now show how ‘secondary peaks’ arise. There are actually an infinity of values of t , besides $t_{\pm}$, where the distribution $Q(t)$ has singularities with the same exponent α , modulated by similar periodic amplitudes. Indeed, by inserting the singular behaviour 4.24 into the r.h.s. of the Dyson equation 4.18, we can show that a similar singular component is present at $t = t_{++} = f_+(t_+)$, and $t = t_{--} = f_-(t_-)$, where the $f_{\pm}$ denote the inverses of the $g_{\pm}$

$$f_{\pm}(t) = \pm 2\delta + \frac{t + \tau}{1 - t\tau} \quad (4.28)$$

These functions coincide, as they should, with the transforms entering the recursion relation 4.3. The singularities at these two values are caused by chains for which the disordered region ends up with $(+-)^N++$, and $(-+)^N--$, respectively, for large N , whence the notation. By iterating the procedure, we obtain analogous singularities at an infinity of values, such as $t_{--+} = f_+(f_-(t_-))$, $t_{+-++} = f_+(f_+(f_-(t_+)))$, etc. These values of t describe the reflection phases of patterns of the form $(+-)^{\infty}U$ or $(-+)^{\infty}V$, where U and V denote arbitrary finite ‘binary words’ made of the symbols $+$ and $-$.

We now compare the above analytical results with some numerical data which have been obtained by the exact enumeration method described chapter 2.

Figure 4.1 shows a histogram of the distribution $P(\theta)$ of the reflection phase in a typical case with an exponent α smaller than unity. The values $k = 0.45\pi$ and $\epsilon = 1$ yield $\alpha = 0.7556$. A large number of deeply pronounced peaks are clearly visible: besides the largest two peaks corresponding to θ_+ and θ_- , all of them are ‘secondary peaks’ as defined previously. We have labelled the largest of them according to the notation explained above.

Figures 4.2 and 4.3 show plots of the periodic amplitude B^- of the singularity of the integrated distribution function $W_Q(t)$, defined in eq. 4.27, against its argument $\xi = \ln(-x)/\ln \Lambda$, extracted from data for t around t_+ . In both cases we have $\alpha < 1$, in such a way that the plotted functions are continuous but nowhere differentiable. Such curves always seem esthetically appealing, at least to the author.

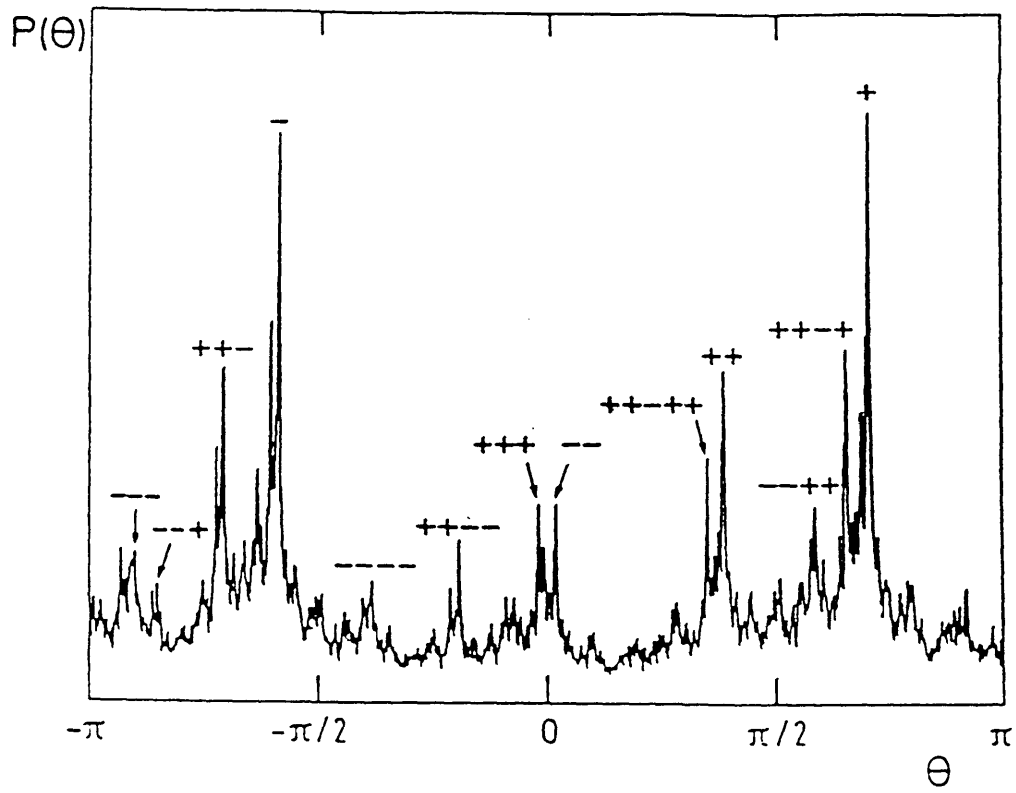


Figure 4.1: Histogram of $P(\theta)$ for binary disorder with $\epsilon = 1$, and $k = 0.45\pi$ and $\alpha = 0.7556$.

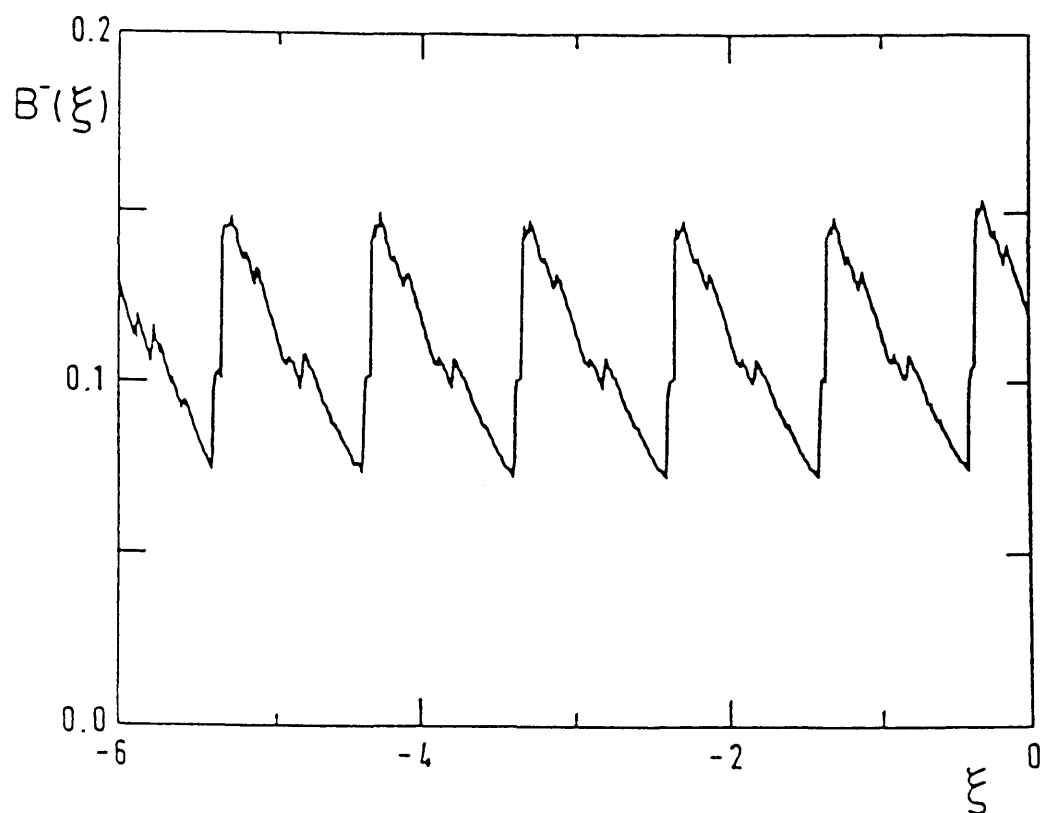


Figure 4.2: Plot of the periodic amplitude B^- , against its argument $\xi = \ln(-x)/\ln \Lambda$. The parameters $k = 0.45\pi$, and $\epsilon = 1.4$, are such that $\alpha = 0.5431$.

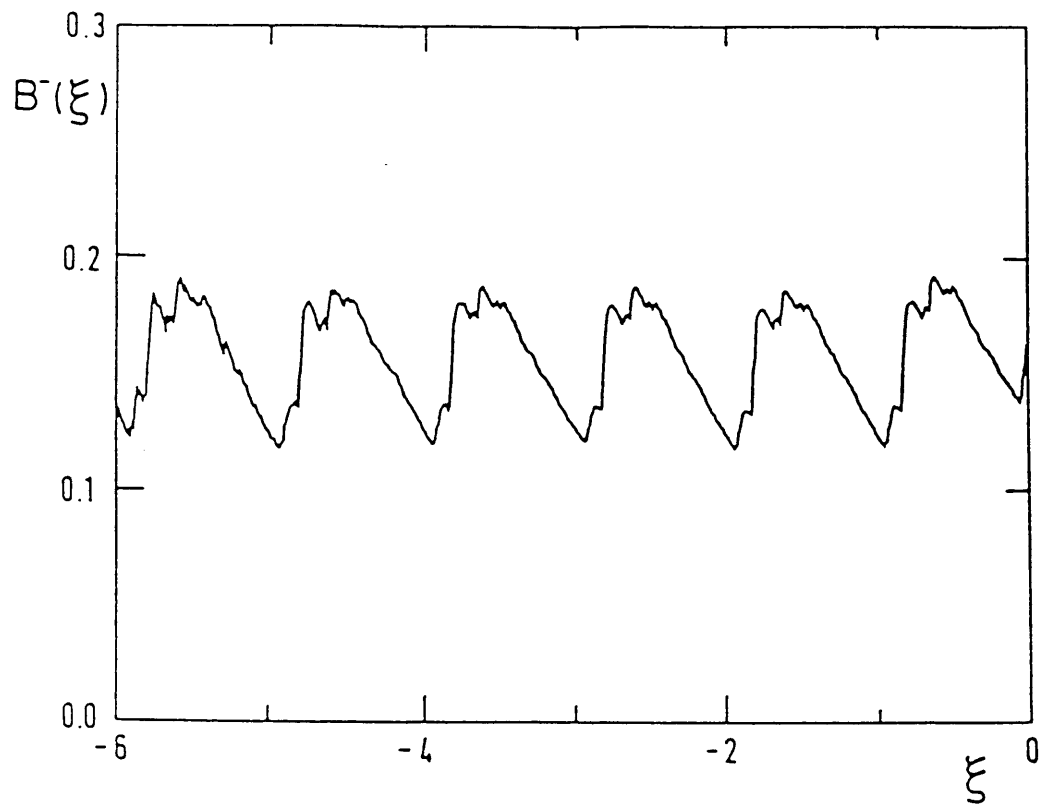


Figure 4.3: Same as Figure 4.2 , for $k = 0.27\pi$, and $\epsilon = 1.7$, so that $\alpha = 0.6777$.

4.4 An Exactly Solvable Model

This section is devoted to the case where the site energies ϵ_N have a symmetric exponential distribution of width W

$$\rho(\epsilon) = \frac{1}{2W} e^{-|\epsilon|/W} \quad (4.29)$$

The remarkable property of this distribution is that all the quantities of interest: the distribution of the reflection phase $P(\theta)$, the Lyapunov exponent $\gamma(E)$, and the IDOS $H(E)$, can be evaluated exactly, following a technique introduced by Nieuwenhuizen [57], which consists of an exact integration over the given random variables (here, the site energies). This powerful method has been applied to a large variety of disordered physical systems in one dimension (see e.g. refs. [58,59,60,61]).

For reasons that will become clear in the following we will work with the logarithmic transform

$$D(z) = \int Q(t) dt \ln(z - t) \quad (4.30)$$

of $Q(t)$, the invariant probability density introduced in section 4.2. Here again, the principle branch of the complex logarithm is used. This definition ensures that $D(z)$ is analytic in the upper half plane ($\text{Im} z > 0$), and continuous as z approaches the real axis. Furthermore, as a direct consequence of eq. 4.5, we have

$$D(z) = \int \rho(\epsilon) d\epsilon \int Q(t) dt \ln \left(z - 2\delta - \frac{t + \tau}{1 - t\tau} \right) \quad (4.31)$$

By rewriting the differential element $\rho(\epsilon) d\epsilon = r(\delta) d\delta$, with

$$r(\delta) = \frac{\beta}{2} e^{-\beta|\delta|} \quad \text{and} \quad \beta = \frac{2 \sin k}{W} \quad (4.32)$$

then reshuffling the argument of the logarithm, we obtain the following integral equation for the function $D(z)$

$$D(z) + D(1/\tau) = \int r(\delta) d\delta \left[D \left(\frac{z - 2\delta - \tau}{1 + (z - 2\delta)\tau} \right) + \ln(z - 2\delta + 1/\tau) \right] \quad (4.33)$$

The key point which allows an exact solution is as follows. δ only enters the integrand through the combination $z - 2\delta$. Hence, if we evaluate $D'(z)$ from

eq. 4.33, the differentiation w.r.t. z can be converted into a differentiation w.r.t. δ inside the integral, which can in turn be compensated by an integration by parts. More explicitly, if we define the partial integral over positive values of δ

$$D_+(z) = \int_0^{+\infty} \beta e^{-\beta\delta} d\delta \left[D \left(\frac{z - 2\delta - \tau}{1 + (z - 2\delta)\tau} \right) + \ln(z - 2\delta + 1/\tau) \right] \quad (4.34)$$

the procedure just described leads to

$$D'_+(z) = \frac{\beta}{2} \left[D \left(\frac{z - \tau}{1 + z\tau} \right) + \ln(z + 1/\tau) - D_+(z) \right] \quad (4.35)$$

This equation can be iterated to get an expression for D''_+ . An analogous formula holds for the integral $D_-(z)$ over negative values of δ . We end up with the second-order differential-difference equation for $D(z)$

$$D''(z) = \frac{\beta^2}{4} \left[D(z) - D \left(\frac{z - \tau}{1 + z\tau} \right) + D(1/\tau) - \ln(z + 1/\tau) \right] \quad (4.36)$$

We have thus reduced the whole problem of the determination of the distribution $P(\theta)$ to that of solving eq. 4.36. Fortunately, this equation can be further simplified as follows. Since it relates values of the unknown function D at z and at $z_1 = (z - \tau)/(1 + z\tau)$, we are led to perform the change of variable

$$y = \frac{z - i}{z + i}, \quad z = i \frac{1 + y}{1 - y} \quad (4.37)$$

which maps the upper half plane ($\text{Im} z > 0$) onto the unit disc ($|y| < 1$), and maps z_1 onto $y_1 = e^{-2ik}y$, where k is the wavevector. We also define a new unknown function $E(y)$ by

$$D(z) = E(y) - \ln(1 - y) - \ln \frac{1 - e^{-2ik}}{2i} \quad (4.38)$$

The asymptotic behaviour $D(z) = \ln z + \mathcal{O}(1/z)$ for large z leads to

$$E(1) = \ln(2i \sin k) - ik \quad (4.39)$$

On the other hand, eq. 4.11 implies

$$\Omega = D(1/\tau) - \ln \sin k = E(e^{-2ik}) - \ln(2i \sin k) + 2ik \quad (4.40)$$

Eqs. 4.39, 4.40 allow us to show that eq. 4.36 is fully equivalent to

$$(1-y)^4 E''(y) - 2(1-y)^3 E'(y) - (1-y)^2 = -\beta^2 \left[E(y) - E(\epsilon^{-2ik} y) + \Omega_r \right] \quad (4.41)$$

where

$$\Omega_r = \Omega - ik \quad (4.42)$$

denotes the ‘random part’ of the characteristic function Ω , i.e. the difference between Ω and its value $\Omega_0 = ik$ in the absence of disordered site potentials.

The requirement that $E(y)$ is analytic in the unit disc and continuous at its boundary determines in a unique way both the function E and the complex constant Ω_r . If we insert into eq. 4.41 the —necessarily convergent— series expansion

$$E(y) = E(0) + \sum_{n \geq 1} \frac{1}{n} c_n y^n \quad (4.43)$$

we obtain the following recursion relation

$$\Delta c_n = (1 - \beta^2 \Omega_r) \delta_{n,0} - 2\delta_{n,1} + \delta_{n,2} - \beta^2 \frac{1 - \epsilon^{-2ik}}{n} c_n \quad (4.44)$$

Here $\delta_{m,n}$ is the Kronecker symbol, and Δc_n denotes the following five-term difference operator acting on the c_n

$$\Delta c_n = (n+1)c_{n+2} + (n-1)c_{n-2} - 2(2n+1)c_{n+1} - 2(2n-1)c_{n-1} + 6nc_n \quad (4.45)$$

with the convention that $c_n = 0$ for $n \leq 0$.

Four boundary conditions are therefore necessary to specify the c_n entirely. Eq. 4.44 taken for $n = 0, 1$, and 2 —the three cases where the equation is not homogeneous— provides two boundary conditions, and determines Ω_r as well. The two missing conditions come from considering the behaviour of c_n for $n \rightarrow \infty$. Indeed, assuming that c_n is a slowly varying function of n for large n , and forgetting about oscillatory terms proportional to ϵ^{-2ik} , we approximate eqs. 4.44, 4.45 as

$$n \Delta c_n \approx n^2 \frac{d^4 c_n}{dn^4} \approx -\beta^2 c_n \quad (4.46)$$

Four independent solutions of this homogeneous equation read asymptotically

$$c_n \sim \exp(\omega \sqrt{n}), \quad \omega = (\pm 1 \pm i) \sqrt{2\beta} \quad (4.47)$$

where both $\pm$ signs are independent of each other. The two values of ω with a positive real part yield a growing solution, and have to be discarded. The requirement of regularity at infinity thus fixes the last two boundary conditions.

We have therefore shown that eqs. 4.44, 4.45 determine the function E in a unique way. We now have to express the quantity of main interest, namely the distribution of the reflection phase, in terms of $E(y)$. The definition 4.30 of $D(z)$ implies that the distribution $Q(t)$ is given by the following boundary value

$$-\pi Q(t) = \text{Im} D'(z = t + i0^+) \quad (4.48)$$

This value of z corresponds to $y = -\epsilon^{i\theta}$. Expressing $Q(t)$ in terms of $P(\theta)$ according to eq. 4.2, and $D(z)$ in terms of $E(y)$ according to eq. 4.38, we obtain the final result

$$2\pi P(\theta) = 1 + 2 \sum_{n \geq 1} (-1)^{n-1} \text{Re} (c_n \epsilon^{in\theta}) \quad (4.49)$$

Hence the c_n are essentially the Fourier coefficients of the distribution of the reflection phase. These complex quantities are defined as the unique solution of eqs. 4.44, 4.45, with the appropriate boundary conditions, as discussed above. We shall now examine analytically some properties of this exact solution, and present some numerical illustrations of it.

Our exact solution provides an analytical form for the fall-off of the c_n , and hence of the regularity properties of the probability density $P(\theta)$. The behaviour of the c_n at large n is given by eq. 4.47, where, as explained above, only the two decreasing solutions have to be considered. Hence the c_n decay more rapidly than any power of the index n , and the distribution $P(\theta)$ is very smooth (differentiable infinitely many times), in strong contrast with the case of the binary alloy studied in section 4.3. To be complete, let us mention that $P(\theta)$ is not an analytic function at $\theta = \pm\pi$. It can be shown by inserting the estimate 4.47 into eq. 4.49 and evaluating the sum by the saddle-point method, that the distribution of the reflection phase has the following singular part around $\theta = \pm\pi$

$$P_{sg}(\theta) \sim \exp \left(-\frac{2 \sin k}{|\theta \pm \pi| W} \right) \quad (4.50)$$

This exponentially small singularity lies 'on top of' a very smooth background. The mechanism responsible for this singular contribution is in fact quite simple.

If the N^{th} atom has a very large site energy ϵ_N , either positive or negative, then the reflection phase θ_N differs from $\pm\pi$ only by a small amount $(2 \sin k)/|\epsilon_N|$; such an event occurs at any site with probability $\exp(-|\epsilon_N|/W)$. Eq. 4.50 is recovered by eliminating ϵ_N between these two estimates. We are therefore led to expect an analytic distribution of the reflection phase whenever the site energies are bounded, and have a rather smooth (e.g. continuous) probability distribution.

The exact solution derived above also permits us to study the distribution $P(\theta)$ in the weak disorder limit ($W \rightarrow 0$) in a simple and systematic way. This regime has already been studied in chapter 3 using perturbation theory but we will include it here, at the risk of a little repetition, because the exact solution sheds some new light. The prefactors $(1 - e^{-2ik})$ in the r.h.s. of eq. 4.44, require that values of the wavevector k which are rational multiples of π have to be considered separately. These are the cases where the wave function in absence of randomness is commensurate to the lattice.

Consider first a generic value of the wavevector, not rationally related to π . It can easily be shown from eqs. 4.44, 4.45 that c_1 and c_2 are proportional to W^2

$$\begin{aligned} c_1 &\approx \frac{-2}{\beta^2(1 - e^{-2ik})} = \frac{i\epsilon^{ik}W^2}{4\sin^3 k}, \\ c_2 &\approx \frac{2}{\beta^2(1 - e^{-4ik})} = \frac{-i\epsilon^{2ik}W^2}{8\sin^3 k \cos k} \end{aligned} \quad (4.51)$$

that c_3 and c_4 are proportional to W^4 , and more generally c_{2m-1} and c_{2m} are proportional to W^{2m} for a small disorder width W as derived in chapter 3.

This simple behaviour at weak disorder is modified for resonant values of the wavevector, rationally related to π . It is already known that the Lyapunov exponent and the density of states present anomalies [62,63,64,65,66] in their weak disorder expansion in such cases.

The strongest anomaly occurs at the band center ($E = 0, k = \pi/2$). It is indeed clear from eq. 4.51 that the expansion of c_2 is singular at that point. The band center is actually the only case for which the c_n do not vanish in the

$W \rightarrow 0$ limit. Thus the distribution $P(\theta)$ does not become trivial (uniform) at weak disorder. More precisely, it can be derived from eqs. 4.44, 4.45 that the c_n are proportional to W^{-2} for odd values of n , but have non-vanishing limits for even n . These nontrivial values are given by the following three-term recursion

$$(n+1)c_{n+2} + (n-1)c_{n-2} + 6nc_n = \delta_{n,2} \quad (4.52)$$

with $c_n = 0$ for $n \leq 0$, as previously. The solution of eq. 4.52 gives the universal distribution

$$2\pi P_0(\theta) = 1 - 2 \sum_{n \geq 2} c_n \cos n\theta \quad (4.53)$$

of the reflection phase at the band center for any weak disorder. The first few values of the c_n read

$$c_2 = 8.611110^{-2}, c_4 = -1.109410^{-2}, c_6 = 1.587210^{-3} \quad (4.54)$$

The c_n fall off as $(-1)^{n/2} (1 + \sqrt{2})^{-n}$ for large n , implying in particular that $P_0(\theta)$ is an analytic function.

For other resonant values $k = \pi p/q$ of the wavevector, where p and q are two coprime integers, some of the coefficients c_n vanish as a smaller power of W than generically. The smallest index which exhibits an anomaly is $n = q$: the leading power of W^{-2} in c_q is less by one unit than generically, in agreement with a recent systematic study of anomalies [66].

We end this section with some numerical illustrations of our exactly soluble model. It is indeed easy to solve the central equations 4.44, 4.45 numerically. Firstly we find two independent general solutions, say $c_{n,1}$ and $c_{n,2}$, of the homogeneous equations 4.44 4.45 (for all $n \geq 3$), which decay for $n \rightarrow \infty$. Then we find a linear combination of these solutions $c_n = a_1 c_{n,1} + a_2 c_{n,2}$ which satisfy the inhomogeneous cases: $n = 0, 1$, and 2 . These are three equations for the three unknowns, namely a_1 , a_2 , and Ω_r , the ‘random part’ of the characteristic function. As explained in section 4.2, this last quantity yields, according to eq. 4.9, the Lyapunov exponent and the integrated density of states of the problem as by-products of the computation, for any energy E in the spectrum $[-2, +2]$ of the perfect leads. Let us just mention that the characteristic function Ω for E outside this interval could also be obtained through a slight adaptation of the present analysis.

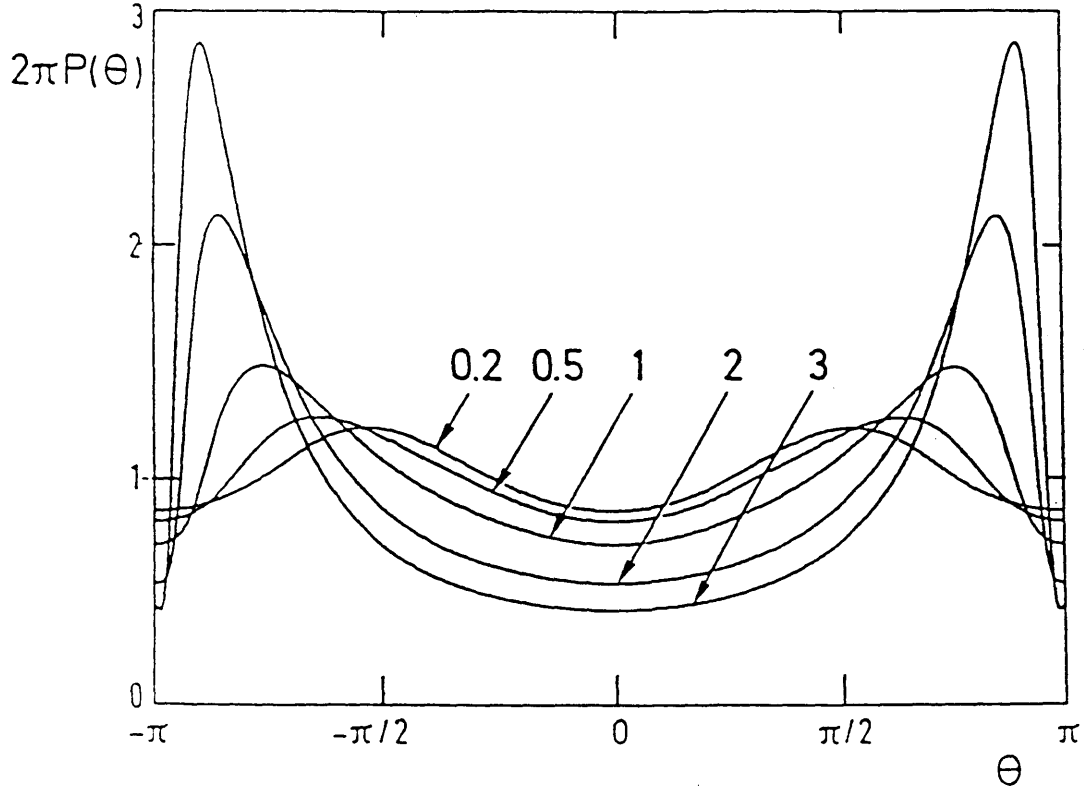


Figure 4.4: Histogram of $P(\theta)$ at $k = \pi/2$ for different values W , indicated on the curves.

Figure 4.4 shows plots of the distribution $P(\theta)$ for different values of the disorder strength W , at the band center ($E = 0$). In this case, the Fourier coefficients c_n are real, and $P(\theta)$ is an even function of θ .

Figure 4.5 shows an analogous series of plots for a generic value of energy, corresponding to $k/\pi = 0.13$. As disorder becomes stronger, the distribution becomes more and more peaked towards $\pm \pi$ this general property holds for any distribution of the site potentials. In order to illustrate the phenomenon of the anomalies present in the weak disorder limit, Figure 4.6 presents plots of the first two (real) Fourier coefficients c_1 and c_2 , at the band center, against the width W . In agreement with the above discussion of anomalies, c_1 vanishes as W^2 , whereas c_2 has a nontrivial anomalous $W \rightarrow 0$ limit, given by eq. 4.54. Also note however that this coefficient does vanish for some finite value of W . The arrow in the plot indicates the ‘anomalous’ limit.

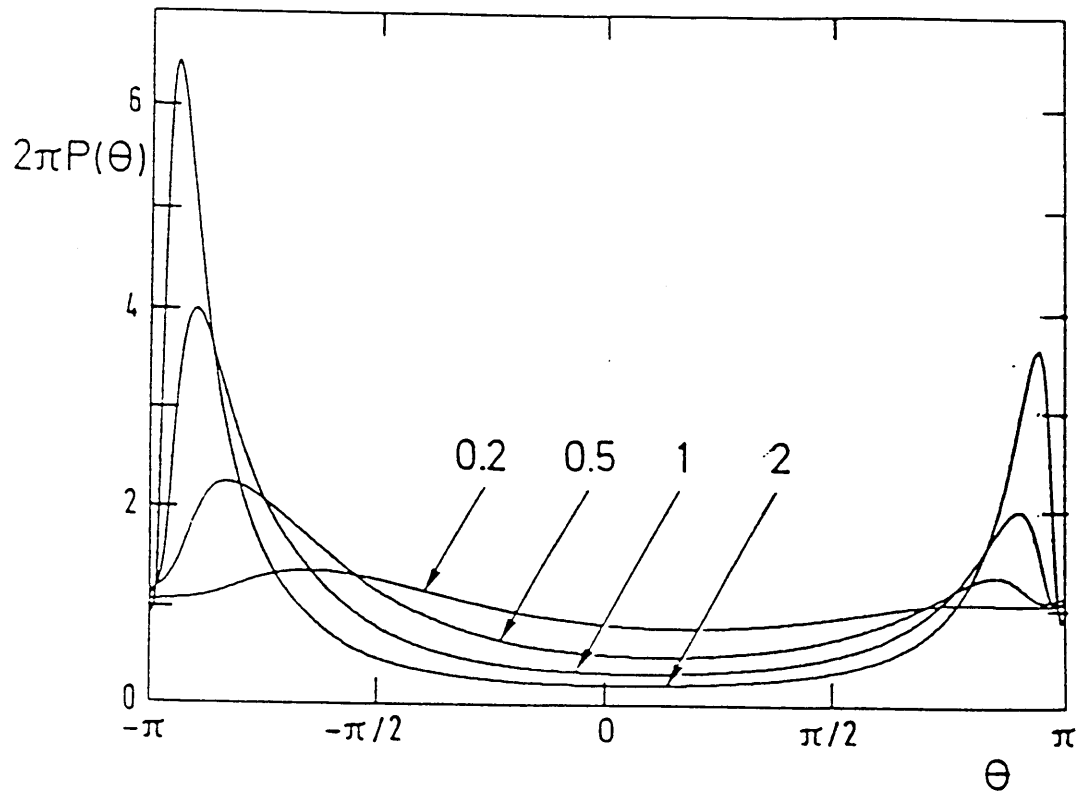


Figure 4.5: Same as Figure 4.4, for a generic point of the spectrum: $k = 0.13\pi$.

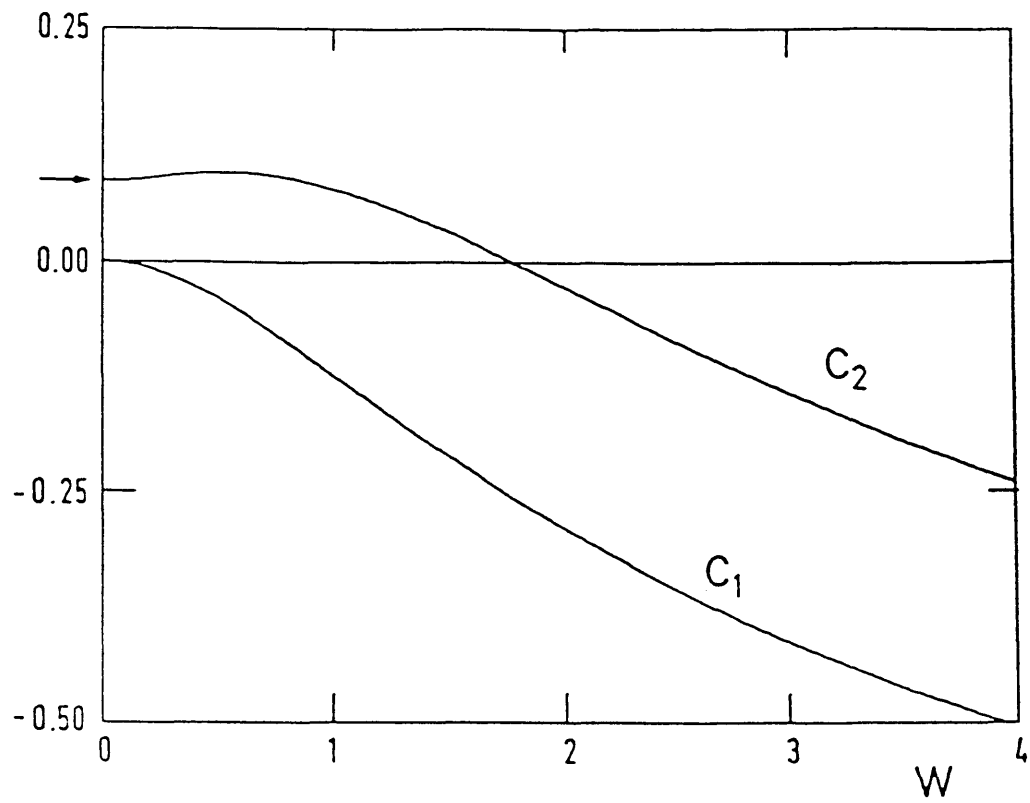


Figure 4.6: Plot of the first two Fourier coefficients c_1 and c_2 of $P(\theta)$ at the band center against W .

4.5 Conclusion

In this chapter, we have used the tight-binding formalism of chapter 2 to derive a linear integral equation for $P(\theta)$, or rather, for an equivalent quantity $Q(t)$, of a type studied first by Dyson [49]. We have also shown that $P(\theta)$ has a simple relation to the Lyapunov exponent $\gamma(E)$ and the integrated density of states $H(E)$ of the problem, provided the energy E is in the spectrum of the perfect leads.

We then proceeded to examine $P(\theta)$ for two special types of disorder, namely the binary alloy, with site potentials $\pm\epsilon$, and an exactly soluble model, with a symmetric exponential distribution of potentials.

The case of the binary alloy, where the site potentials assume the values $\pm\epsilon$, with probability $1/2$, is considered in section 4.3. We have shown that long repetitions of periodic patterns of potentials are responsible for the existence of an infinity of power-law singularities in the reflection phase distribution. This effect is similar to the phenomenon, first described by Halperin [50], which affects the density of states of random harmonic chains, with light and heavy atomic masses. The predominant singularities are associated with repetitions $+ - + - + - \dots$ of the pattern $(+-)$ with period two. Patterns with higher periods produce much weaker singular contributions. The exponent α which characterises these sets of singularities is obtained in an exact way. It depends both on the disorder strength ϵ and on energy, so that divergences, ‘peaks’, in $P(\theta)$ are actually observed only when disorder exceeds some energy-dependent threshold. The results of an exact enumeration procedure show that the positions of all the most visible peaks present in this data are explained by the analytic approach. We also present plots of the periodic amplitudes, which modulate the power-law singularities. This singular behaviour of $P(\theta)$ occurs whenever the distribution of the site potentials contains some discrete component.

We consider in section 4.4, a special class of distributions for the site potentials, namely the symmetric exponentials, for which the whole problem is exactly soluble. The solution, namely the determination of the Fourier coeffi-

cients of the distribution $P(\theta)$, as well as $\gamma(E)$ and $H(E)$, follows a method introduced by Nieuwenhuizen [57]. This method, which reduces the problem to solving a difference equation can in principle be extended to a wider class of potential distributions $\rho(\epsilon)$, symmetric or not, where a polynomial in ϵ multiplies the exponential distribution.

This exact solution allows a detailed investigation of various properties of the phase distribution. We find that $P(\theta)$ is differentiable infinitely many times, and fails to be analytic only because of an essential singularity at $\theta = \pm\pi$, related to the occurrence of arbitrarily large site potentials. It is therefore expected that $P(\theta)$ is analytic for any bounded and continuous distribution of the site potentials. We also investigate the behaviour of the Fourier coefficients c_n of $P(\theta)$ at weak disorder looking in particular at the anomalies which are known to affect the weak disorder expansion of quantities such as the Lyapunov exponent for any wavevector rationally related to π .

Finally, we should mention that some of the present results may generalise to higher dimensional systems. In the strongly localised regime a 3-D wire is totally reflecting, and hence is described by a unitary reflection matrix. The eigenvalues of that matrix are therefore pure phases, and the object of interest is the distribution of these phases.

Chapter 5

Weak Scattering in 3-D.

5.1 Introduction

In this chapter we study the statistics of the elements of the reflection matrix in the weak scattering regime. In this regime, the length of the system is smaller than both the elastic mean free path and the inelastic mean free path and the dominant scattering process is single scattering. Thus making a Born type perturbation series an ideal description for reflection from these systems. We will show how to derive such a series from a recursion relation for the reflection matrix and show the results it gives for the single scattering regime. The weak scattering regime is of some relevance to the study of mesoscopic systems which can even be fabricated such that transport through them may be considered purely ballistic [67].

In section 5.2, we derive a perturbation expansion for the reflection matrix of a disordered wire in terms of tight-binding parameters from a recursion relation for the reflection matrix. In section 5.3 we describe a technique for finding the ensemble average of combinations of elements from the reflection matrix for arbitrary types of disorder using the single scattering approximation. Finally, in section 5.4 we find the exact distribution of each element of the reflection matrix for a Gaussian ensemble in the same approximation.

5.2 Generalities

In this section we derive a 3-D version of the reflection recursion relation (RRR) of chapter 2 using essentially the same method but using matrices. We then show how it may be used to find a weak disorder perturbation expansion for the reflection matrix of a disordered wire.

The first step in deriving the RRR is to define our model of a disordered system and its reflection and transmission matrices. We consider an ensemble of disordered wires described by the tight binding Schrödinger equation

$$\epsilon_{z,\underline{x}}\phi_{z,\underline{x}} + V(\phi_{z,\underline{x}+\underline{x}} + \phi_{z,\underline{x}-\underline{x}} + \phi_{z,\underline{x}+\underline{y}} + \phi_{z,\underline{x}-\underline{y}}) + V'(\phi_{z+1,\underline{x}} + \phi_{z-1,\underline{x}}) = E\phi_{z,\underline{x}} \quad (5.1)$$

In the (x, y) plane the wires are square with side $L \times L$ atoms and have periodic boundary conditions. In the z direction they consist of a central disordered region ($1 \leq z \leq L_z$) connected at either end to semi-infinite crystalline leads. In the leads, the site energies are constant ($\epsilon_{z,\underline{x}} = \epsilon_0$) and in the disordered region, they are independent random variables with a common probability density $\rho(\epsilon)$ symmetrically distributed about ϵ_0 .

The z component of the wavevector of an electron propagating in the leads, K_z , is related to its transverse wave vector $\underline{k}$ and its energy E through

$$E = \epsilon_0 + 2V' \cos(K_z) + 2V(\cos(\underline{k}, \underline{x}) + \cos(\underline{k}, \underline{y})) \quad (5.2)$$

In order for us to consider reflection and transmission of such an electron we require that K_z is real for all transverse modes that an electron could scatter into, which requires that $|(E - \epsilon_0)/2V'| \leq 1 - 2\beta$ where $\beta = V/V'$.

The reflection and transmission matrices $\mathbf{R}_{L_z}$ and $\mathbf{T}_{L_z}$ for a wave incident in the $-z$ direction are defined such that the wave function in the leads may be written in the following **matrix** form (**bold** characters are always matrices in this text).

$$\phi_z = \begin{cases} \psi e^{-(z-L_z)} v^{-1/2} + \psi e^{(z-L_z)} v^{-1/2} \mathbf{R}_{L_z} & \text{for } z \geq L_z \\ \psi e^{-z} v^{-1/2} \mathbf{T}_{L_z} & \text{for } z \leq 1 \end{cases} \quad (5.3)$$

The matrix ϕ_z contains the wave function amplitudes for different sites $\underline{r}$ and transverse modes $\underline{k}$ at the layer z

$$(\phi_z)_{\underline{k},\underline{r}} = \phi_{z,\underline{r}}^{\underline{k}} \quad (5.4)$$

ϕ_z is a product of three matrices; a matrix containing the transverse part

$$\psi_{\underline{r},\underline{k}} = \frac{1}{L} \exp(i\underline{r} \cdot \underline{k}) \quad (5.5)$$

a diagonal matrix containing the longitudinal part

$$e_{\underline{k},\underline{k}'} = \exp(iK) \delta_{\underline{k},\underline{k}'}^c \quad (5.6)$$

and a diagonal matrix containing the group velocity of each transverse mode

$$v_{\underline{k},\underline{k}'} = \frac{1}{2V'} \frac{\partial E}{\partial K} \delta_{\underline{k},\underline{k}'}^c \quad (5.7)$$

δ^c is a Kronecker delta. Including this group velocity term defines the reflection and transmission matrices in the constant current basis.

The Riccati variable, equation 2.5, becomes a Riccati matrix in 3-D defined by

$$Y_z = \phi_{z+1} \phi_z^{-1} \quad (5.8)$$

In terms of this matrix the tight binding schrödinger equation 5.1 takes the form

$$Y_z = M_0 - \epsilon_z - Y_{z-1}^{-1} \quad (5.9)$$

where

$$(M_0)_{\underline{r},\underline{r}'} = \frac{E - \epsilon_0}{V'} \delta_{\underline{r},\underline{r}'}^c - \beta(\delta_{\underline{r}+\underline{x},\underline{r}'}^c + \delta_{\underline{r}-\underline{x},\underline{r}'}^c + \delta_{\underline{r}+\underline{y},\underline{r}'}^c + \delta_{\underline{r}-\underline{y},\underline{r}'}^c) \quad (5.10)$$

and

$$(\epsilon_z)_{\underline{r},\underline{r}'} = \frac{\epsilon_{z,\underline{r}} - \epsilon_0}{V'} \delta_{\underline{r},\underline{r}'}^c \quad (5.11)$$

Using relations 5.3 and 5.8 the relationship between the reflection matrix R_{L_z} and the Riccati matrix Y_{L_z} has the form

$$Y_{L_z} = \psi v^{-1/2} (e^{-1} + e R_{L_z}) (\mathbf{1} + R_{L_z}) v^{-1/2} \psi \quad (5.12)$$

so that by substituting 5.12 into 5.9 we can derive the reflection recursion relation

$$\mathbf{R}_{L_z} = (\mathbf{e}\mathbf{R}_{L_z-1}\mathbf{e} + i\delta_{L_z}(\mathbf{1} + \mathbf{e}\mathbf{R}_{L_z-1}\mathbf{e}))(\mathbf{1} - i\delta_{L_z}(\mathbf{1} + \mathbf{e}\mathbf{R}_{L_z-1}\mathbf{e}))^{-1} \quad (5.13)$$

where the disorder matrix δ_{L_z} takes the form

$$\delta_{L_z} = \frac{1}{2}\mathbf{v}^{-1/2}\psi^*\epsilon_{L_z}\psi\mathbf{v}^{-1/2} \quad (5.14)$$

As we have demonstrated in chapter 2, the RRR is a useful expression as it stands. It allows us to find, by numerical iteration, the reflection matrix of any disordered wire. This in turn allows us to investigate the reflection statistics of any ensemble of disordered wires. In 3-D the numerical effort is much increased due to the matrix inversion required for each iteration but the process should be quite stable numerically. We will not do any numerical work here but will concentrate on finding a perturbation expansion for the weak scattering regime.

In the weak scattering regime the disorder matrices δ_z are ‘small’ quantities and can be used to write the reflection matrix a series of increasingly small terms in the following way

$$\mathbf{R}_{L_z} = \mathbf{R}_{L_z}^{(1)} + \mathbf{R}_{L_z}^{(2)} + \mathbf{R}_{L_z}^{(3)} + \dots \quad (5.15)$$

where $\mathbf{R}_{L_z}^{(j)}$ contains terms of order j in δ_{L_z} . Each of these terms may be derived from a binomial expansion of the RRR in terms of δ_{L_z} which has the following form

$$\mathbf{R}_{L_z} = \mathbf{e}\mathbf{R}_{L_z-1}\mathbf{e} + (\mathbf{1} + \mathbf{e}\mathbf{R}_{L_z-1}\mathbf{e}) \sum_{j=1}^{\infty} (i\delta_{L_z}(\mathbf{1} + \mathbf{e}\mathbf{R}_{L_z-1}\mathbf{e}))^j \quad (5.16)$$

This series converges if the eigenvalues of the matrix $i\delta_{L_z}(\mathbf{1} + \mathbf{e}\mathbf{R}_{L_z-1}\mathbf{e})$ are all less than unity, a condition which is true for weak disorder. An alternative expansion in terms of the reflection matrix $\mathbf{r} = i\delta(1 - i\delta)^{-1}$ is absolutely convergent but for weak scattering $\mathbf{r} \approx i\delta$ and δ is a more convenient parameter to average, as we shall see. Considering just the first order term it is clear that $\mathbf{R}_{L_z}^{(1)}$ must obey the simple recursion relation

$$\mathbf{R}_{L_z}^{(1)} = \mathbf{e}\mathbf{R}_{L_z-1}^{(1)}\mathbf{e} + i\delta_{L_z} \quad (5.17)$$

which may be iterated using the boundary condition $\mathbf{R}_0 = \mathbf{o}$, the condition that the leads are non-reflective. The result of this iteration is

$$\mathbf{R}_{L_z}^{(1)} = \sum_{j=1}^{L_z} e^{|L_z-j|} i \delta_j e^{|L_z-j|} \quad (5.18)$$

This expression can be thought of as a sum of single scattering events at each layer and is therefore equivalent to the Born approximation. We may write 5.18 in the short hand notation

$$\mathbf{R}_{L_z}^{(1)} = (\boldsymbol{\eta} i \boldsymbol{\Omega} \boldsymbol{\eta})_{L_z, L_z} \quad (5.19)$$

where

$$\boldsymbol{\Omega}_{j_1, j_2} = \delta_{j_1} \delta_{j_1, j_2}^* \quad (5.20)$$

and

$$\boldsymbol{\eta}_{j_1, j_2} = e^{|j_1-j_2|} \quad (5.21)$$

Both $\boldsymbol{\Omega}$ and $\boldsymbol{\eta}$ are matrices of matrices.

The second order term may be found in the same way. The recursion relation for this term has the form

$$\mathbf{R}_{L_z}^{(2)} = e \mathbf{R}_{L_z-1}^{(2)} e + e \mathbf{R}_{L_z-1}^{(1)} e i \delta_{L_z} + i \delta_{L_z} e \mathbf{R}_{L_z-1}^{(1)} e + (i \delta_{L_z})^2 \quad (5.22)$$

We can substitute for $\mathbf{R}_{L_z}^{(1)}$ from 5.18 and iterate using the same boundary condition as before to get

$$\mathbf{R}_{L_z}^{(2)} = \sum_{j_1, j_2=1}^{L_z} e^{|L_z-j_1|} i \delta_{j_1} e^{|j_1-j_2|} i \delta_{j_2} e^{|L_z-j_2|} \quad (5.23)$$

which maybe thought of as a sum of double scattering events for every pair of layers in the wire. Subsequent terms follow the same pattern so that the n^{th} order term will be a sum over all scattering events involving n layers giving the following series

$$\mathbf{R}_{L_z} = (\boldsymbol{\eta} i \boldsymbol{\Omega} \boldsymbol{\eta} + \boldsymbol{\eta} i \boldsymbol{\Omega} \boldsymbol{\eta} i \boldsymbol{\Omega} \boldsymbol{\eta} + \boldsymbol{\eta} i \boldsymbol{\Omega} \boldsymbol{\eta} i \boldsymbol{\Omega} \boldsymbol{\eta} i \boldsymbol{\Omega} \boldsymbol{\eta} + \dots)_{L_z, L_z} \quad (5.24)$$

This series is equivalent to the Born series and interestingly enough may be summed to give

$$\mathbf{R}_{L_z} = (\boldsymbol{\eta} i \boldsymbol{\Omega} \boldsymbol{\eta} (\mathbf{1} - \boldsymbol{\eta} i \boldsymbol{\Omega})^{-1})_{L_z, L_z} \quad (5.25)$$

Unfortunately evaluating a reflection matrix from equation 5.25 is not easy since it involves inverting a matrix of size $L_z L^2 \times L_z L^2$ a more costly operation than simply iterating the original recursion relation. For the rest of this chapter we will concentrate on the first order term, representing a sum over single scattering events, the dominant scattering mechanism in the weak scattering regime.

5.3 Moments

In this section we illustrate a method for finding the ensemble average of any combination of elements from the reflection matrix for arbitrary ensembles of wires using the first term in the perturbation expansion for $\mathbf{R}_{L_z}$ equation 5.18. We will do this by evaluating explicitly $\langle |(\mathbf{R}_{L_z})_{\underline{k}, \underline{k}'}|^{2n} \rangle$ for $n = 1, 2, 3$, the reflected intensities into each channel.

The first term in equation 5.24 takes the form

$$(\mathbf{R}_{L_z})_{\underline{k}, \underline{k}'} = \sum_{j=1}^{L_z} \epsilon^{i(K_{\underline{k}} + K_{\underline{k}'})(L_z - j)} i(\delta_j)_{\underline{k}, \underline{k}'} \quad (5.26)$$

We will use the simplified notation $R = (\mathbf{R}_{L_z})_{\underline{k}, \underline{k}'}$, $K = (K_{\underline{k}} + K_{\underline{k}'})/2$, the average z component wavevector and $\delta_j = (\delta_{L_z})_{\underline{k}, \underline{k}'}$ from now on to avoid making the calculations look more complicated than they really are. As we see, this first term splits the problem of calculating the elements of the reflection matrix into $L^2 \times L^2$ 1-D problems, one for each possible scattering event $\underline{k}' \rightarrow \underline{k}$. However this separation isn't as simple as considering a wire made from a collection of unconnected 1-D wires, this would only occur for $\beta = 0$.

In order to calculate $\langle |R|^2 \rangle$ we multiply 5.26 by its complex conjugate and take an ensemble average.

$$\langle |R|^2 \rangle = \sum_{j_1, j_2=1}^{L_z} \epsilon^{2iK(j_2 - j_1)} \langle \delta_{j_1} \delta_{j_2}^* \rangle \quad (5.27)$$

where the notation $\langle \dots \rangle$ represents an ensemble average over all site energies $\epsilon_{z, \underline{r}}$. Different layers are statistically independent so that we may write

$$\langle \delta_{j_1} \delta_{j_2}^* \rangle = \langle |\delta|^2 \rangle \delta_{j_1, j_2}^c \quad (5.28)$$

-Ve +Ve j_1 j_2 j_3 j_4	No of equivalent Diagrams	Ensemble Average Quantities
	1	$\sigma_3^4 = \langle \delta ^4 \rangle$
	1	$\sigma_2^4 = \langle (\delta)^2 \rangle^2$
	2	$\sigma_1^4 = (\langle \delta ^2 \rangle)^2$

Figure 5.1: Diagrams for fourth moment

Hence carrying out the sum in 5.27 we find

$$\langle |R|^2 \rangle = L_z \sigma^2 \quad (5.29)$$

where $\sigma^2 = \langle |\delta|^2 \rangle$.

The next moment has the form

$$\langle |R|^4 \rangle = \sum_{j_1 \dots j_4}^{L_z} e^{2iK(j_4+j_3-j_2-j_1)} \langle \delta_{j_1} \delta_{j_2} \delta_{j_3}^* \delta_{j_4}^* \rangle \quad (5.30)$$

The averages in this sum which are not zero must have pairs of j 's identical since each layer is statistically independent. This may occur in three different ways which we express in the simple diagrams of figure 5.1 summing the contributions due to each of these diagrams we get

$$\langle |R|^4 \rangle = 2L_z(L_z - 1)\sigma_1^4 + L_z\sigma_3^4 + (S - L_z)\sigma_2^4 \quad (5.31)$$

where

$$S = \frac{\sin^2(2KL_z)}{\sin^2(2K)} \quad (5.32)$$

The next order is more complicated as we are considering the average quantity $\langle \delta_{j_1} \delta_{j_2} \delta_{j_3} \delta_{j_4}^* \delta_{j_5}^* \delta_{j_6}^* \rangle$. The distinct diagrams for this case are shown in figure 5.3, summing these diagrams we derive

-Ue			+Ue			No of equivalent Diagrams	Ensemble Average Quantities
J ₁	J ₂	J ₃	J ₄	J ₅	J ₆		
						1	$\sigma_3^6 = \langle \delta ^6 \rangle$
						6	$\sigma_1^6 = (\langle \delta ^2 \rangle)^3$
						9	$\sigma_4^6 = \langle \delta^2 \rangle^2 \langle \delta ^2 \rangle$
						9	$\sigma_2^6 = \langle \delta ^2 \rangle \langle \delta ^4 \rangle$
						3	$\sigma_5^6 = \langle \delta^2 \rangle \langle \delta ^2 \delta^{*2} \rangle$
						3	$\sigma_6^6 = \langle \delta^{*2} \rangle \langle \delta ^2 \delta^2 \rangle$

Figure 5.2: Diagrams for sixth moment

$$\begin{aligned}
\langle |R|^6 \rangle = & 6L_z(L_z - 1)(L_z - 2)\sigma_1^6 + 9L_z(L_z - 1)\sigma_2^6 + L_z\sigma_3^6 \\
& + 9(L_z - 2)(S - L_z)\sigma_4^6 + 6(S - L_z)\text{Re}(\sigma_5^6) \quad (5.33)
\end{aligned}$$

Each σ in equations 5.29, 5.31 and 5.33 may be evaluated in terms of moments of the site energies using equation 5.14. In 1-D, for Gaussian disorder this leads to results of Heinrichs [33] and as he notes give corrections to a random phase assumption.

5.4 Gaussian Disorder

In this section, we find an exact expression for the distribution of each element of the reflection matrix for a gaussian ensemble of disordered wires in the single scattering limit by adapting a technique due to Heinrichs [33].

The joint probability distribution for the real and imaginary parts of a particular reflection amplitude $(\mathbf{R}_{L_z})_{\underline{k}, \underline{k}'} = R = X + iY$ has the form

$$P(X, Y) = \langle \delta^d(X - X') \delta^d(Y - Y') \rangle \quad (5.34)$$

where δ^d is a Dirac delta function and X', Y' are defined by equation 5.26 to be

$$X' = \text{Re}(R) = - \sum_{j=1}^{L_z} (\delta_j^I \cos(2K(L_z - j)) + \delta_j^R \sin(2K(L_z - j))) \quad (5.35)$$

$$Y' = \text{Im}(R) = \sum_{j=1}^{L_z} (\delta_j^R \cos(2K(L_z - j)) - \delta_j^I \sin(2K(L_z - j))) \quad (5.36)$$

δ_j^R and δ_j^I are the real and imaginary parts of δ_j .

In order to find $P(X, Y)$ we re-write 5.34 using the integral representation of the Dirac delta functions so that

$$P(X, Y) = \frac{1}{(2\pi)^2} \int \int_{-\infty}^{\infty} dk_1 dk_2 \exp(i(k_1 X + k_2 Y)) \langle \exp(-i(k_1 X' + k_2 Y')) \rangle \quad (5.37)$$

and write the part to be averaged in terms of the random site energies

$$-i(k_1 X' + k_2 Y') = \sum_{j, \underline{L}} i a_{j, \underline{L}} (\epsilon_j)_{\underline{L}} \quad (5.38)$$

where

$$a_{j,\underline{L}} = c_{\underline{k},\underline{k}'}(k_1 \sin(2K(L_z - j) + (\underline{k}' - \underline{k})_{\underline{L}}) - k_2 \cos(2K(L_z - j) + (\underline{k}' - \underline{k})_{\underline{L}})) \quad (5.39)$$

and

$$c_{\underline{k},\underline{k}'} = \frac{1}{2L^2} \sin^{-1/2}(K_{\underline{k}}) \sin^{-1/2}(K_{\underline{k}'}) \quad (5.40)$$

So far, the analysis is true for any type of disorder since we have not explicitly performed the ensemble average. In general, this averaging is quite complicated but for Gaussian disorder where the site energies $\epsilon = (\epsilon_j)_{\underline{L}}$ have the probability density

$$\rho(\epsilon) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{\epsilon^2}{2\sigma^2}\right) \quad (5.41)$$

it may be done exactly giving the result

$$\langle \exp(\sum_{j,\underline{L}} i a_{j,\underline{L}}(\epsilon_j)_{\underline{L}}) \rangle = \exp\left(-\frac{\sigma^2}{2} \sum_{j,\underline{L}} (a_{j,\underline{L}})^2\right) \quad (5.42)$$

where

$$\sum_{j,\underline{L}} (a_{j,\underline{L}})^2 = S_{11}k_1^2 - 2S_{12}k_1k_2 + S_{22}k_2^2 \quad (5.43)$$

and

$$\begin{aligned} S_{11} &= (c_{(\underline{k},\underline{k}')})^2 \left(\frac{L_z}{2} - \lambda \right) L^2 \\ S_{22} &= (c_{(\underline{k},\underline{k}')})^2 \left(\frac{L_z}{2} + \lambda \right) L^2 \\ S_{12} &= (c_{(\underline{k},\underline{k}')})^2 \mathcal{C} L^2 \end{aligned} \quad (5.44)$$

The correction terms have the form

$$\begin{aligned} \lambda &= \frac{1}{2} + \frac{\cos(2KL_z) \sin(2K(L_z - 1))}{2 \sin(2K)} \Delta_{\underline{k},\underline{k}'} \\ \mathcal{C} &= \frac{\sin(2KL_z) \sin(2K(L_z - 1))}{2 \sin(2K)} \Delta_{\underline{k},\underline{k}'} \end{aligned} \quad (5.45)$$

with

$$\Delta_{\underline{k},\underline{k}'} = \sum_{\underline{g}} \delta_{\underline{k}' - \underline{k} - \underline{g}/2} \quad (5.46)$$

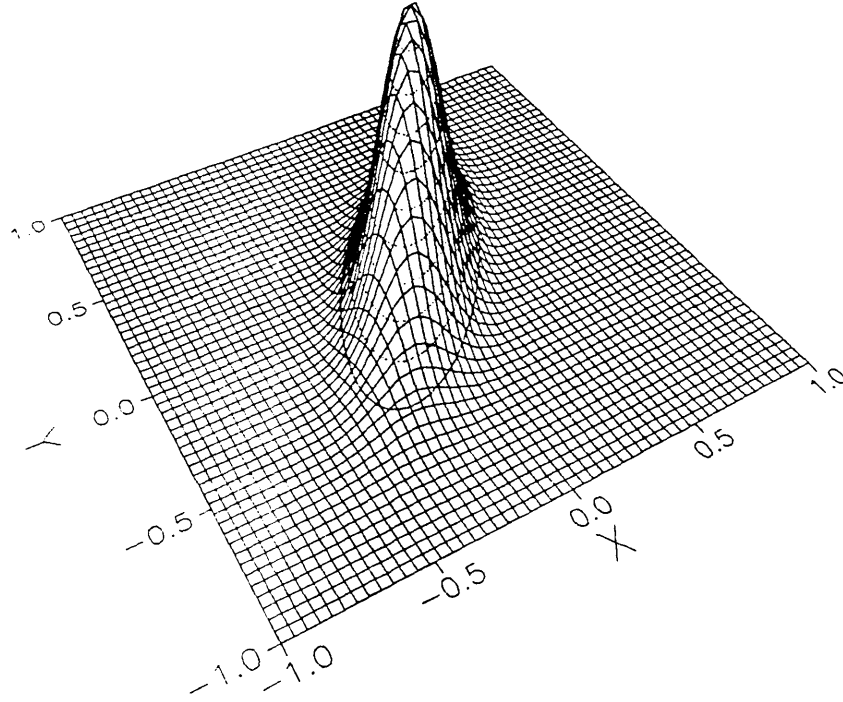


Figure 5.3: $P(X, Y)$ in the specular direction for $K = 0.498\pi$ and $\sigma^2\lambda = 0.1$

where the vector $\underline{g}$ is a 2-D reciprocal lattice vector. Carrying out the Gaussian integral over k_1, k_2 in equation 5.37 we find $P(X, Y)$ has the form of an elliptical 2-D gaussian

$$P(X, Y) = \frac{1}{2\pi\sigma^2\lambda} \exp\left(-\frac{1}{2\sigma^2\lambda^2} (S_{22}X^2 + 2S_{12}XY + S_{11}Y^2)\right) \quad (5.47)$$

where

$$\lambda^2 = S_{11}S_{22} - S_{12}^2 \quad (5.48)$$

It is only in the specific directions dictated by Δ and for $|K - \pi/2| < L_z^{-1}$ that $P(X, Y)$ takes this explicitly elliptical form. For instance, figure 5.3 shows the specular term $\underline{g} = 0$ for $K = 0.498\pi$ and $\sigma^2\lambda = 0.1$. For generic direction $\underline{k}' - \underline{k}$ and wave vector K $P(X, Y)$ simplifies to

$$P(X, Y) = \frac{1}{2\pi\sigma^2\lambda} \exp\left(-\frac{1}{2\sigma^2\lambda} (X^2 + Y^2)\right) \quad (5.49)$$

where

$$\lambda = \frac{L_z}{8L^2} \sin^{-1}(K_{\underline{k}}) \sin^{-1}(K_{\underline{k}'}) \quad (5.50)$$

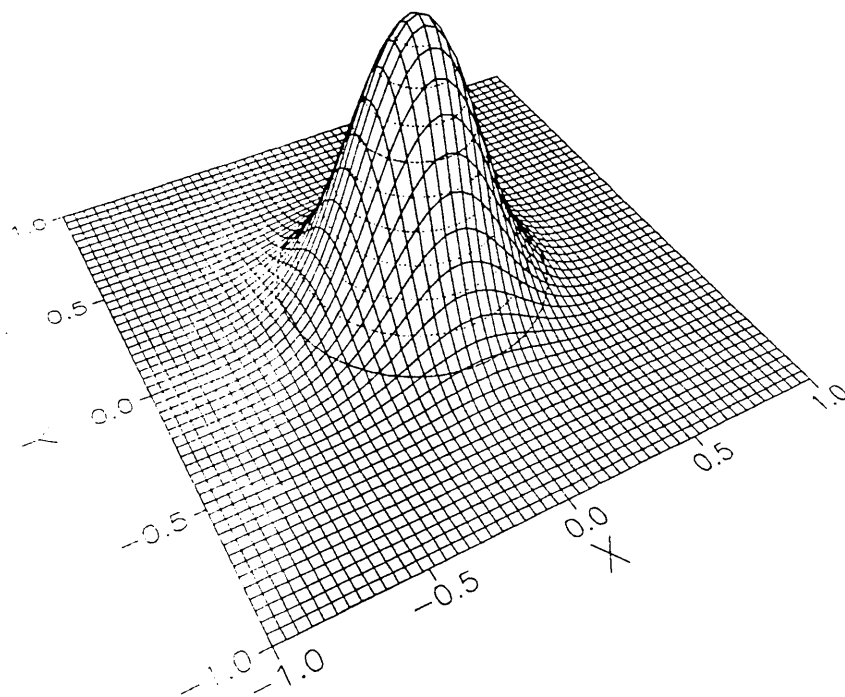


Figure 5.4: General form of $P(X, Y)$

Figure 5.4 shows a plot of $P(X, Y)$ for $\sigma^2\lambda = 0.1$. Thus, under generic conditions, the phase of each element of the reflection matrix is completely randomly distributed and scattering into different directions is only modulated by the group velocity terms in equation 5.50. The back scattering peak which normally characterises weak disorder does not appear here since it arises from time reversed paths not included in the single scattering approximation. In order to find this peak we would have to consider higher order terms in the perturbation expansion 5.24.

5.5 Conclusion

In this chapter, we have extended the tight-binding formalism of chapter 2 to 3-D. We consider a wire of cross-section $L \times L$ atoms with a central disordered region in the z direction of L_z layers, containing diagonal disorder. We have derived a recursion relation for the reflection matrix of these wires and shown how it gives rise to a perturbation expansion for the reflection matrix. This expansion has the same form as the Born series. We have then concentrated on the first term in the expansion, corresponding to single scattering. In section 5.3, we have calculated moments of the reflected intensity $\langle |R_{\underline{k}, \underline{k}'}|^{2n} \rangle$ into each channel for arbitrary disorder type. In section 5.4, we have used an adaptation of a method due to Heinrichs [33] to calculate the exact distribution of each element of the reflection matrix for Gaussian disorder $P(X, Y)$. These distributions are elliptical Gaussians (or bivariate Gaussians). However, their explicitly elliptical nature only appears for directions which are commensurate with the underlying lattice in some way, as in Bragg scattering, and for values of the average wave vector K close to $\pi/2$. In general, they appear perfectly cylindrical indicating that the phase of each reflection matrix element is randomly distributed.

Chapter 6

Transport properties and the RTM in 1-D

6.1 Introduction.

In this chapter we will show how an adaptation of the RTM used in chapter 3 may be used to find the moments of the transmission amplitude $\langle |T_L|^{2n} \rangle$ for weak disorder. As an application to this formalism we then give a very simple derivation of these moments for the tight-binding model of disorder and show that their dependence on n is that of the maximal fluctuation theorem of Pendry *et al* [68]. This work has the advantage that the formalism is simple to grasp but still gives the same results as earlier workers Abrikosov and Ryzhkin [69,70] and Kirkman and Pendry [2].

In section 6.2, we recall the transfer matrix formalism of chapter 3 and derive a new transfer matrix containing reflected intensities. In section 6.3, we use the new transfer matrix to calculate the moments of the transmitted intensity $\langle |T_L|^{2n} \rangle$ for the tight-binding model.

6.2 Generalities

The reflection transfer matrix $\mathbf{M}$ contains all the powers of the reflection coefficient in its first column. $M_{i0} = R^i$. A fact which, in chapter 3, enabled us to study the reflection coefficient of disordered chains. However, this property is useful for determining more than just surface effects. We can also look at transmission simply by working with a matrix which is the direct product of the RTM with its complex conjugate

$$\mathbf{W} = \mathbf{M} \odot \mathbf{M}^* \quad (6.1)$$

which contains, as elements, all the products $M_{ij}M_{i'j'}^*$ and hence the moduli $|R|^{2n}$. These moduli are simply related to the transmission moduli $|T_L|^{2n}$ through conservation of probability $|T_L|^2 + |R_L|^2 = 1$ giving

$$|T_L|^{2n} = \sum_{i=0}^n \binom{n}{i} |R_L|^{2i} \quad (6.2)$$

We can therefore use $\mathbf{W}$ to look at the transmitted intensity through disordered systems.

The direct product 6.1 is quite a complicated object, it has four indices, each of which run to infinity. However if we wish to use standard techniques of matrix manipulation and perturbation theory we must order it in the form of a standard $N \times N$ matrix with the largest terms in the top left hand corner. In an ensemble of systems where the disorder is weak the distribution of reflection phases is, as we have discussed in chapters 2–5, essentially random so that quantities which depend on it average to zero. Hence for such an ensemble it makes sense to order the matrix by writing it as a matrix of ‘smaller’ matrices $\mathbf{W}_{\alpha\beta}$ of the form

$$(\mathbf{W}_{\alpha\beta})_{ij} = M_{ij}M_{\alpha+i,\beta+j}^* \quad (6.3)$$

This ordering gives, in the top left hand corner, the matrix $\mathbf{W}_{00}$ which contains all the moduli of the elements of the RTM appearing in the same places as the corresponding elements in the RTM. The other matrices $\mathbf{W}_{\alpha\beta}$ contain elements which depend on the reflection phase in some way and will therefore, after averaging, for an ensemble of weakly disordered systems, be comparatively much smaller than the moduli.

The matrix $\mathbf{W}$ is a transfer matrix so that for a system of L units

$$\mathbf{W}_L = \prod_{n=1}^L \mathbf{w}_n \quad (6.4)$$

Where the $\mathbf{w}_n$ are the transfer matrices representing the individual units. This kind of linear relationship has the tremendous advantage that, for a system of statistically independent units, the transfer matrix can be averaged by simply averaging the matrices representing individual units.

$$\langle \mathbf{W}_L \rangle = \langle \mathbf{w}_n \rangle^L \quad (6.5)$$

The problem of finding $\langle \mathbf{W}_L \rangle$ then amounts to finding the L^{th} power of the individual ensemble average matrix $\langle \mathbf{w}_n \rangle$. This is done by diagonalising the matrix, raising its eigenvalues to the L^{th} power, and finally recombining the matrix.

Both the reflection transfer matrix and the new transfer matrix have an isolated unit eigenvalue which determines the properties of a system in the strongly localised regime. For the reflection transfer matrix this limit is not trivial, the right eigenvector corresponding to this unit eigenvalue contains the fourier components of the distribution of reflection phases. But for the transport matrix $\mathbf{W}$ this limit is trivial and gives

$$\lim_{L \rightarrow \infty} |R_L|^{2n} = 1 \quad (6.6)$$

every modulus equal to unity. Indicating the fact that in the strongly localised limit every chain is completely reflective. Hence, in order to gain more information we must consider the whole spectrum of eigenvalues. Here though the eigen values form a continuum and are therefore not amenable to the simple perturbation theory used in chapter 3.

6.3 An application.

In this section, we will derive approximate analytic expressions for the moments of the distribution of transmitted intensities $\langle |T_L|^{2n} \rangle$ using the tight binding model. We do this for weak disorder in the strongly localised regime.

Using the tight binding formalism of chapter 3, we may approximate $\mathbf{w}$ in the weak disorder limit by expanding it to second order in $i\delta$. The lowest order in $i\delta$ for which $\langle \mathbf{w} \rangle$ is not trivially the identity matrix. In this approximation $\langle \mathbf{w}_{00} \rangle$ has a tridiagonal form:

$$\begin{aligned} (\langle \mathbf{w}_{00} \rangle)_{l,l+1} &= \delta'^2 l^2 \\ (\langle \mathbf{w}_{00} \rangle)_{l,l} &= 1 - 2\delta'^2 l^2 \\ (\langle \mathbf{w}_{00} \rangle)_{l,l-1} &= \delta'^2 l^2 \end{aligned} \tag{6.7}$$

Where

$$\delta'^2 = \langle (\delta)^2 \rangle \tag{6.8}$$

Off diagonal matrices which make up $\langle \mathbf{w} \rangle$ are at least of order δ'^2 and hence coupling to these, in perturbation theory, is of order δ'^4 which we have assumed to be zero. Also, for wavevectors not rationally related to π mixing with other matrices on the diagonal may be ignored and hence we may work solely with $\langle \mathbf{w}_{00} \rangle$ from now on.

6.3.1 Eigenvalues and Vectors

Equations 6.7 clearly show that the right eigenvector which corresponds to the unit eigenvalue in $\langle \mathbf{w}_{00} \rangle$ gives the trivial limit in equation 6.6 for the reflection amplitudes.

The eigenvalues of $\langle \mathbf{w}_{00} \rangle$ form a continuum, but are nevertheless quite simple to find. We do this by re-writing the matrix in the form of a differential equation and then solve that.

Writing the right eigenvectors in the form

$$v^r = \begin{pmatrix} c(0) \\ c(1) \\ c(2) \\ \vdots \end{pmatrix} \tag{6.9}$$

we see that their elements obey the second order recursion relation

$$\delta'^2 l c(l+1) + (1 - 2\delta'^2 l) c(l) + \delta'^2 l c(l-1) = \lambda c(l) \quad (6.10)$$

where λ is an eigenvalue of the matrix. If we now make the assumption that they vary smoothly and continuously as a function of l we can replace $c(l \pm 1)$ by

$$c(l \pm 1) = c(l) \pm c'(l) + \frac{1}{2} c''(l) \quad (6.11)$$

where the $'$ represents a derivative w.r.t l . Giving equation 6.10 in the differential form

$$l^2 c''(l) = -\mu c(l) \quad (6.12)$$

Where

$$\mu = (1 - \lambda) / \delta'^2 \quad (6.13)$$

The general solutions to this equation have the log-sinusoidal form:

$$c(l) = A l^{\frac{1}{2}} \sin(\alpha \ln(l) + \beta) \quad (6.14)$$

Where

$$\alpha = \frac{1}{2} \sqrt{4\mu - 1} \quad (6.15)$$

The constants of integration α and β are respectively, an eigenvalue and a phase shift, the values of which are determined by the boundary conditions imposed by the matrix and physical considerations. A is a normalization factor which will be determined after finding the left eigenvectors of the matrix.

We get one boundary condition from the recursion relation 6.10 for $l = 0, 1$

$$\lambda c(0) = c(0)$$

$$\lambda c(1) = \delta'^2 c(0) + (1 - 2\delta'^2) c(1) \quad (6.16)$$

which for $\lambda \neq 1$ give $c(0) = 0$ and

$$\tan(\beta) = \frac{2^{\frac{1}{2}} \sin(\alpha \ln(2))}{2 - \frac{1}{4} + \alpha^2 + 2^{\frac{1}{2}} \cos(\alpha \ln(2))} \quad (6.17)$$

We get a second boundary condition from $l \rightarrow \infty$ which we impose by assuming that the matrix $\langle w_{00} \rangle$ may be truncated at some arbitrarily large value of $l = N$ then take the limit $N \rightarrow \infty$. This boundary condition is

$$c(N) = 0 \quad (6.18)$$

From physical considerations this is reasonable, since the modulus of all reflection phases must be less than unity and therefore their moments for increasing n must converge to zero. This second boundary condition gives rise to a condition on the eigenvalue spectrum:

$$\alpha_n \ln(N) + \beta_n = n\pi \quad \text{for} \quad n = 1, N \quad (6.19)$$

A discrete spectrum for finite N going over to a continuum for infinite N . Looking at equations 6.17 and 6.19 it is clear that for $n \ll \ln N$ we may approximate α_n by

$$\alpha_n = \frac{n\pi}{\ln(N)} \quad (6.20)$$

which gives

$$\lambda_n = 1 - \frac{\delta'^2}{4} \left(1 + 4 \left(\frac{n\pi}{\ln(N)} \right)^2 \right) \quad (6.21)$$

For increasing n the exact form for these eigenvalues quickly diminishes [1] and we may approximate the full spectrum by

$$\lambda_n = \exp \left(-\frac{\delta'^2}{4} \left(1 + 4 \left(\frac{n\pi}{\ln(N)} \right)^2 \right) \right) \quad (6.22)$$

The left eigenvectors

$$c^l = (d(0), d(1), d(2) \dots) \quad (6.23)$$

obey a different recursion relation from 6.10. However close inspection of ^(6.7) shows that they are related through

$$\begin{aligned} d(l) &= \frac{c(l)}{l^2} \quad \text{for } l \neq 0 \\ d(0) &= -\frac{\delta'^2}{1-\lambda} d(1) \text{ for } l = 0 \end{aligned} \quad (6.24)$$

Using equations 6.24 together with the right eigenvectors:

$$c^n(j) = A_n j^{\frac{1}{2}} \sin \left[\frac{n\pi}{\ln(N)} \ln(j) + \beta_n \right] \quad (6.25)$$

the normalization condition is simply

$$1 = \sum_{j=1}^N A_n^2 \frac{j}{j^2} \sin^2 \left[\frac{n\pi}{\ln(N)} \ln(j) + \beta_n \right] \quad (6.26)$$

If we make j a continuous variable, thereby changing the sum to an integral, the normalization factor for $n \ll \ln N$ has the form:

$$A_n = \frac{2}{\sqrt{(\ln(N))}} \quad (6.27)$$

6.3.2 Finding the Moments.

We are now in a position to evaluate the moments $\langle |R_L|^{2n} \rangle$. The expression for these moments in terms of the eigenvalues and vectors of $\langle \mathbf{w}_{00} \rangle$ takes the standard form

$$\langle |R_L|^{2n} \rangle = \sum_{i=0}^N \lambda_i^L c^i(n) d^i(0) \quad (6.28)$$

The $i = 0$ term is unity since $\lambda_0 = 1$, $d^0(0) = 1$ and $c^0(n) = 1$. The other terms are given by the values we have derived for the eigenvectors and values so that

$$1 - \langle |R_L|^{2n} \rangle = \frac{8n^{\frac{1}{2}}}{y_0} \exp\left(-\frac{\delta'^2 L}{4}\right) \sum_{p=1}^N \exp(-\delta'^2 L x^2) \frac{1}{1 + 4x^2} \sin(x \ln(n) + \beta_p) \sin(\beta_p) \quad (6.29)$$

where

$$x = \frac{p\pi}{\ln N} \quad (6.30)$$

If we now take the limit $N \rightarrow \infty$ and change the sum over p to an integral over x the expression simplifies to

$$1 - \langle |R_L|^{2n} \rangle = \frac{8n^{\frac{1}{2}}}{\pi} \exp\left(-\frac{\delta'^2 L}{4}\right) \int_0^\infty \exp(-\delta'^2 L x^2) \frac{1}{1 + 4x^2} \sin(x \ln(n) + \beta) \sin(\beta) dx \quad (6.31)$$

In order to evaluate this integral we shall assume that the exponential decays sufficiently fast that we can expand all terms to its right only to second order

in x , thus restricting the region of validity to the strongly localised regime $\delta'^2 L \gg 1$. The integral then takes the form

$$\int_0^\infty \exp(-\delta'^2 L x^2) (\ln(n) + k) k x^2 dx \quad (6.32)$$

where

$$k = \frac{2^{\frac{1}{2}} \ln(2)}{2 - \frac{1}{4} - 2^{\frac{1}{2}}} \quad (6.33)$$

which is simply done and yields for the moments

$$\langle |R_L|^{2n} \rangle = 1 - \frac{1}{(\delta'^2 L)^{\frac{3}{2}}} \exp\left(-\frac{\delta'^2 L}{4}\right) \frac{2n^{\frac{1}{2}}}{\sqrt{\pi}} k (\ln(n) + k) \quad (6.34)$$

Finally, averaging equation 6.2 and substituting for the moments from 6.34 we find that even in this approximation we retrieve the maximal fluctuation theorem of Pendry *et al* ref [68].

$$\langle |T_L|^{2n} \rangle = C(n) \langle |T_L| \rangle \quad (6.35)$$

6.4 Conclusion.

In this chapter, we described a new formalism for calculating the moments of the transmitted intensity $\langle |T_L|^{2n} \rangle$. The formalism is an extension of that used in chapter 3 and involves a matrix which is the direct product of the reflection transfer matrix with its complex conjugate $\mathbf{W} = \mathbf{M} \oplus \mathbf{M}^*$. As an application we have calculated an analytic expression for the moments of the transmitted $\langle |T_L|^{2n} \rangle$ for weak disorder in the strongly localised regime and shown that their form is consistent with the more generally valid maximal fluctuation theorem of Pendry *et al* [68].

Chapter 7

Generalised Transfer Matrices

7.1 Introduction

As a result of the clear similarity between the RTM of chapter 3 and the generalised transfer matrices $\mathbf{X}^N$ of Kirkman and Pendry [1,2] the question of their exact relation arises. This investigation has led to an exciting new development, at least to the present author, a simplified derivation and a greater understanding of the generalised transfer matrices for any dimension. These matrices have been used extensively to look at such things as densities of states, decay lengths and fluctuations in disordered systems. In 1-D their complete history maybe found in a series of papers by Pendry [4,71,72,73,74,75], Pendry and Kirkman [76,77], Kirkman and Pendry [1,2] Pendry *et al* [78,68] Slevin and Pendry [79], Pendry and Barnes [80,81] and in 3-D Pendry [82,83] Pendry and Castaño [3].

In section 6.2, we describe a general formalism for reflection and transmission from disordered systems in 3-D. In section 6.3, we derive $\mathbf{X}^N$ in 1-D by a new method and compare it to the derivation in ref [1,2]. In section 6.4, we derive a new generalised transfer matrix for 3-D and compare its form with that of Pendry and Castaño [3].

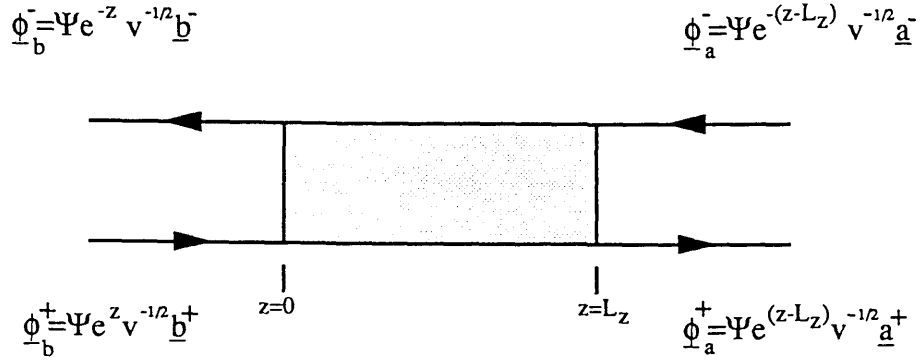


Figure 7.1: Boundary conditions for reflection from and transmission through a disordered system.

7.2 Generalities

In this section, we describe formalism for reflection and transmission from disordered 3-D systems. We consider the same model as in chapter 5 but will not restrict ourselves to the tight-binding Hamiltonian. Instead, we will consider wires made from statistically independent units (or layers) with transverse boundary conditions which obey conservation of probability and time reversal symmetry

Figure 6.1 shows the form of the wave function in the leads. Where ψ , ϵ and v have the definitions given in equations 5.5–5.7 of chapter 5. The vectors $\underline{\phi}^\pm$ contain site amplitudes and $\underline{a}/\underline{b}$ contain current amplitudes.

The relationships between the current amplitudes of the waves on either side of the disordered region define a scattering matrix $\mathbf{S}$ which characterizes the disordered region the elements of which are the reflection and transmission matrices:

$$\begin{pmatrix} \underline{a}^+ \\ \underline{b}^- \end{pmatrix} = \mathbf{S} \begin{pmatrix} \underline{a}^- \\ \underline{b}^+ \end{pmatrix} \quad (7.1)$$

where

$$\mathbf{S} = \begin{pmatrix} \mathbf{R}^{+-} & \mathbf{T}^{++} \\ \mathbf{T}^{--} & \mathbf{R}^{-+} \end{pmatrix} \quad (7.2)$$

Each element of a reflection or transmission matrix is an amplitude coupling one transverse mode to another. For instance, for a wave incident along $(\underline{k}', -K')$,

with unit amplitude, the amplitude of the wave reflected into $(\underline{k}, K)$ will be $(\mathbf{R}^{+-})_{\underline{k}, \underline{k}'}$.

Conservation of probability is satisfied if the current amplitudes obey

$$\begin{pmatrix} \underline{a}^{+\ast} & \underline{b}^{-\ast} \end{pmatrix} \begin{pmatrix} \underline{a}^+ \\ \underline{b}^- \end{pmatrix} = \begin{pmatrix} \underline{a}^{-\ast} & \underline{b}^{+\ast} \end{pmatrix} \begin{pmatrix} \underline{a}^- \\ \underline{b}^+ \end{pmatrix} \quad (7.3)$$

This implies that the $\mathbf{S}$ matrix must be unitary

$$\mathbf{S}\mathbf{S}^\dagger = \mathbf{S}^\dagger\mathbf{S} = \mathbf{1} \quad (7.4)$$

which leads to the following relationships between the elements of $\mathbf{S}$:

$$\mathbf{R}^{+-\dagger}\mathbf{R}^{+-} + \mathbf{T}^{--\dagger}\mathbf{T}^{--} = 1 \quad (7.5)$$

$$\mathbf{T}^{++\dagger}\mathbf{R}^{+-} + \mathbf{R}^{-+\dagger}\mathbf{T}^{--} = 0 \quad (7.6)$$

$$\mathbf{R}^{-+\dagger}\mathbf{R}^{-+} + \mathbf{T}^{++\dagger}\mathbf{T}^{++} = 1 \quad (7.7)$$

Time reversal symmetry is satisfied if the complex conjugate of the solutions shown in figure 7.1 are also solutions with the same eigen value this leads to the new relations

$$\begin{pmatrix} \underline{a}^- \\ \underline{b}^+ \end{pmatrix} = \tilde{\mathbf{S}} \begin{pmatrix} \underline{a}^+ \\ \underline{b}^- \end{pmatrix} \quad (7.8)$$

with

$$\tilde{\mathbf{S}} = \begin{pmatrix} \tilde{\mathbf{R}}^{+-} & \tilde{\mathbf{T}}^{++} \\ \tilde{\mathbf{T}}^{--} & \tilde{\mathbf{R}}^{-+} \end{pmatrix} \quad (7.9)$$

where the tilde is defined for *any* matrix by

$$\tilde{\mathbf{R}}_{\underline{k}, \underline{k}'} = \mathbf{R}_{-\underline{k}, -\underline{k}'}^\ast \quad (7.10)$$

Comparing equation 7.1 with 7.8 and using relation 7.4 we see that $\tilde{\mathbf{S}} = \mathbf{S}^\dagger$ which leads to further relations between the elements of $\mathbf{S}$.

$$\begin{aligned} \tilde{\mathbf{R}}^{-+} &= \mathbf{R}^{-+\dagger} \\ \tilde{\mathbf{R}}^{+-} &= \mathbf{R}^{+-\dagger} \end{aligned} \quad (7.11)$$

$$\tilde{\mathbf{T}}^{++} = \mathbf{T}^{--\dagger} \quad (7.12)$$

The complex conjugates of equations 7.11 are statements of the reciprocity theorem in the constant current basis.

We are now in a position to derive the transfer matrix M which relates the amplitudes of the waves on the left hand side of the disordered region to those on the right.

$$\begin{pmatrix} \underline{a}^- \\ \underline{a}^+ \end{pmatrix} = M \begin{pmatrix} \underline{b}^- \\ \underline{b}^+ \end{pmatrix} \quad (7.13)$$

So far we have not assumed that the number of states on either side of the sample is the same however in order to re-arrange equation 7.1 to give the elements of M it is convenient to do so since it avoids having to consider generalised inverses. The result is

$$M = \begin{pmatrix} (\mathbf{T}^{--})^{-1} & \tilde{\mathbf{R}}^{+-}(\tilde{\mathbf{T}}^{--})^{-1} \\ \mathbf{R}^{+-}(\mathbf{T}^{--})^{-1} & (\tilde{\mathbf{T}}^{--})^{-1} \end{pmatrix} \quad (7.14)$$

where we have used relations 7.6, 7.11 and 7.12 to give it in a convenient form.

This matrix is a transfer matrix and therefore obeys the recursion relation

$$M_{L_z+1} = \mathbf{m}_{L_z+1} M_{L_z} \quad (7.15)$$

where $\mathbf{m}_{L_z+1}$ the transfer matrix representing the layer L_z and M_{L_z} is the transfer matrix representing L_z connected layers.

Using equation 7.15 we are now in a position to derive the recursion relation between the reflection matrices $\mathbf{R}_{L_z+1}$ and $\mathbf{R}_{L_z}$. The first step is to recognize that the matrix relation 7.15 implies the following recursion relations:

$$\mathbf{T}_{L_z+1}^{-1} = (\mathbf{m}_{11} + \mathbf{m}_{12}\mathbf{R}_{L_z})\mathbf{T}_{L_z}^{-1} \quad (7.16)$$

and

$$\mathbf{R}_{L_z+1}\mathbf{T}_{L_z+1}^{-1} = (\mathbf{m}_{21} + \mathbf{m}_{22}\mathbf{R}_{L_z})\mathbf{T}_{L_z}^{-1} \quad (7.17)$$

where for convenience we have written $\mathbf{R}^{+-}$ as $\mathbf{R}$ and $\mathbf{T}^{--}$ as $\mathbf{T}$. The matrix elements $\mathbf{m}_{ij}$ are those of $\mathbf{m}_{L_z+1}$. Combining 7.16 and 7.17 we can eliminate the transmission matrix and derive the reflection recursion relation:

$$\mathbf{R}_{L_z+1} = (\mathbf{m}_{21} + \mathbf{m}_{22}\mathbf{R}_{L_z})(\mathbf{m}_{11} + \mathbf{m}_{12}\mathbf{R}_{L_z})^{-1} \quad (7.18)$$

It is quite simple to show that relations 7.16 and 7.18 are completely equivalent to those derived from the multiple scattering picture figure 3.3. In fact for the new work which we derive in this chapter we could have simply used the relations for $\mathbf{R}_{L_z+1}$ and $\mathbf{T}_{L_z+1}$ from the multiple scattering picture and skipped to this point. However, part of the aim of the chapter is to make a comparison with previous work and for that reason it is most convenient to work on both with the same formalism.

7.3 The 1-D case

In this section, we will show how to derive the generalised transfer matrix $\mathbf{X}^N$ by a new method using relations 7.16 and 7.18, then compare this method with that used in ref [1.1].

In 1-D both $\mathbf{R}$ and $\mathbf{T}$ become complex numbers so that the usual rules of commutivity apply and we can derive the RTM from 7.18 in the same manner as in subsection 3.2.1 giving the same result. However, just as we were able to eliminate $\mathbf{T}$ from equations 7.16 and 7.17 and hence derive the RTM we can also deliberately re-introduce it to make a transfer matrix containing the transmission coefficient. Multiplying each row of the RTM by the N^{th} power of equation 7.16 we get:

$$\mathbf{R}_{L_z+1}^i \mathbf{T}_{L_z+1}^{-N} = (\mathbf{m}_{21} + \mathbf{m}_{22} \mathbf{R}_{L_z})^i (\mathbf{m}_{11} + \mathbf{m}_{12} \mathbf{R}_{L_z})^{N-i} \mathbf{T}_{L_z}^{-N} \quad (7.19)$$

both powers may be expanded binomially and are absolutely convergent: the first because i is an integer and the second for any value of N because $|\frac{\mathbf{m}_{12}}{\mathbf{m}_{11}} \mathbf{R}_{L_z}| \leq 1$. Hence using the Cauchy sum rule we can derive the transfer matrix relation:

$$\underline{\mathbf{x}}_{L_z+1}^N = \mathbf{x}_{L_z+1}^N \underline{\mathbf{x}}_{L_z}^N \quad (7.20)$$

where

$$\mathbf{x}_{ij}^N = \sum_{n=0}^{\min(i,j)} \binom{i}{n} \binom{N-i}{j-n} \mathbf{m}_{11}^{N-i-j+n} \mathbf{m}_{12}^{i-n} \mathbf{m}_{21}^{j-n} \mathbf{m}_{22}^n \quad (7.21)$$

and

$$(\underline{\mathbf{x}}_{L_z}^N)_j = \mathbf{R}_{L_z}^j \mathbf{T}_{L_z}^{-N} \quad (7.22)$$

This matrix is identical with that of ref [1,2].

We now compare the new method above for finding $\mathbf{X}^N$ with that used in ref [1,2]. There, we work with the relation

$$\underline{v}_{L_z+1} = \mathbf{m}_{L_z+1} \underline{v}_{L_z} \quad (7.23)$$

where

$$\underline{v}_{L_z} = \begin{pmatrix} \mathbf{T}_{L_z}^{-1} \\ \mathbf{R}_{L_z} \mathbf{T}_{L_z}^{-1} \end{pmatrix} \quad (7.24)$$

derived from equations 7.14 and 7.15. The first step is to take the N^{th} direct product of 7.23 making a new relation of the same form as 7.23. The new column vectors $\underline{v}_{L_z}^N$ are of length 2^N and contain all possible permutations of length N of the two elements $\mathbf{T}_{L_z}^{-1}$ and $\mathbf{R}_{L_z} \mathbf{T}_{L_z}^{-1}$ of $\underline{v}_{L_z}$. The permutations which are identical, due to commutivity, are then removed by adding identical terms and dividing by their number. After removal of the permutation symmetry the new column vectors $\underline{v}_{L_z}^N$ contain only *combinations* of length N of the two elements

$$\underline{v}_{L_z}^N = \begin{pmatrix} \mathbf{T}_{L_z}^{-N} \\ \mathbf{R}_{L_z} \mathbf{T}_{L_z}^{-N} \\ \mathbf{R}_{L_z}^2 \mathbf{T}_{L_z}^{-N} \\ \vdots \\ \mathbf{R}_{L_z}^N \mathbf{T}_{L_z}^{-N} \end{pmatrix} \quad (7.25)$$

In this derivation the matrix $\mathbf{x}^N$ which relates $\underline{v}_{L_z}^N$ to $\underline{v}_{L_z+1}^N$ is identical to the matrix in equation 7.21 except that it is only defined for integer N and is finite. However, our new method is true for any value of N but here we are left with a conceptual difficulty if we wish to consider arbitrary N , since a combination of a non-integer number of elements is hard to imagine let alone a *complex* number of elements. The pragmatic solution is simple, we analytically continue the factorials in the definition of $\mathbf{x}^N$ to gamma functions giving the exact same form as 7.21 but with the insight of the new method it is clear why we can make this continuation.

7.4 Transfer Matrices in Higher Dimensions

In this section we extend the simple analysis which gave us generalised transfer matrices in 1-D to the higher dimensional case. We start by looking for a

RTM. The complication here is that the reflection and transmission matrices do not commute so that it is no longer possible to derive a RTM which relates only the powers of the reflection matrix. Instead it must relate combinations of the elements of $\mathbf{R}_{L_z+1}$ to combinations of the elements of $\mathbf{R}_{L_z}$. The reflection recursion relation 7.18 implies that any element of the reflection matrix $\mathbf{R}_{L_z+1}$ is a function of all the elements of $\mathbf{R}_{L_z}$, therefore it may be expanded as a multi-dimensional Taylor series in these elements.

$$R'_{ij} = X_{ij}^{(0)} + \sum X_{ij,j_1j_1}^{(1)} \mathbf{R}_{i_1j_2} + \sum X_{ij,j_1j_1i_2j_2}^{(2)} \mathbf{R}_{i_1j_1} \mathbf{R}_{i_2j_2} + \dots \quad (7.26)$$

where we have written $\mathbf{R}' = \mathbf{R}_{L_z+1}$ and $\mathbf{R} = \mathbf{R}_{L_z}$ for simplicity. In the Taylor expansion permutation symmetry is already factored out but due to reciprocity symmetry the number of elements of the reflection matrix which are different is reduced to $d(d+1)/2$, where d is the number of transverse modes, and this symmetry may also be factored out. This expansion is absolutely convergent since it is simply a sum of all reflected multiple scattering paths figure 3.3.

Expression 7.26 can now be used to find an expansion of the same form as 7.26 but with different coefficients X , for any combination of the elements of $\mathbf{R}_{L_z+1}$. We do this simply by multiplying the series representing each element and expanding. In simplified notation this may be written as

$$\mathbf{R}_{L_z+1}^{(i)} = \sum_{j=0}^{\infty} \mathbf{X}_{ij} \mathbf{R}_{L_z}^{(j)} \quad (7.27)$$

where $\mathbf{R}_{L_z}^{(j)}$ is a column vector containing the different combinations of the elements of $\mathbf{R}_{L_z}$ of length j . Each element $\mathbf{X}_{ij}$ is a matrix, with its dimensions determined by i and j , containing the coefficients of the Taylor expansion. The matrix $\mathbf{X}$ is therefore the 3-D reflection transfer matrix where

$$\underline{\mathbf{v}}_{L_z+1} = \mathbf{X}_{L_z+1} \underline{\mathbf{v}}_{L_z} \quad (7.28)$$

with $(\underline{\mathbf{v}}_{L_z})_i = \mathbf{R}_{L_z}^{(i)}$.

In 3-D we have not yet found a way to make a generalised transfer matrix containing the transmission matrix itself and its direct product powers by our new method. We have however been able to find one which contains $\det^N(\mathbf{T}^{-1})$.

a quantity which is related to the mean decay rate $\langle l^{-1}(E) \rangle$ and integrated density of states $\langle H(E) \rangle$ through

$$\begin{aligned}\langle l^{-1}(E) \rangle &= \lim_{N \rightarrow 0} \operatorname{Re} \left[\frac{d}{dN} \det^N(\mathbf{T}^{-1}) \right] \\ \langle H(E) \rangle &= \lim_{N \rightarrow 0} -\operatorname{Im} \left[\pi^{-1} \frac{d}{dN} \det^N(\mathbf{T}^{-1}) \right]\end{aligned}\quad (7.29)$$

The method is essentially the same as in 1-D : we take the determinant of equation 7.16 then raise the result to the N^{th} power and include it as a power series in each row of the reflection transfer matrix as follows:

$$\det^N(\mathbf{T}_{L_z+1}^{-1}) = \det^N(\mathbf{M}_{11} + \mathbf{M}_{12}\mathbf{R}_{L_z})\det^N(\mathbf{T}_{L_z}^{-1}) \quad (7.30)$$

the first determinant on the rhs may be expanded as a taylor series in the elements of $\mathbf{R}_{L_z}$ as we did in deriving the expansion 7.26

$$\det^N(\mathbf{M}_{11} + \mathbf{M}_{12}\mathbf{R}_{L_z}) = \sum_{i=0}^{\infty} \alpha_{(i)} \mathbf{R}_{L_z}^{(i)} \quad (7.31)$$

This series is also absolutely convergent for any value of N for the same reason the expansion of the RRR was. Hence, multiplying both sides of equation 7.27 by equation 7.31 we arrive at the higher dimensional extension of $\mathbf{X}^N$:

$$\underline{\mathbf{v}}_{L_z+1} = \mathbf{X}_{L_z+1}^N \underline{\mathbf{v}}_{L_z} \quad (7.32)$$

where

$$\underline{\mathbf{v}}_{L_z} = \mathbf{R}_{L_z}^{(j)} \det^N(\mathbf{T}_{L_z}^{-1}) \quad (7.33)$$

This matrix has not been derived before. Pendry and Castaño [3] used a different matrix which we will describe below.

In the 3-D case, simply taking the N^{th} direct product of equation 7.23 does not yield a very interesting matrix, as it did in 1-D, it simply contains combinations of the elements of $\mathbf{T}^{-1}$ and $\mathbf{R}\mathbf{T}^{-1}$. Hence, Pendry and Castaño [3] worked with a new transfer matrix $\mathbf{Y}$ containing as elements all the d^{th} order minor determinants of $\mathbf{M}$, and hence the determinant of the transmission coefficient. The relations equivalent to 7.23 and 7.24 are then:

$$\underline{\mathbf{v}}_{L_z+1}^p = \mathbf{Y}_{L_z+1} \underline{\mathbf{v}}_{L_z}^p \quad (7.34)$$

where

$$\underline{c}_{L_z}^p = \begin{pmatrix} \det(\mathbf{T}_{L_z}^{-1}) \\ \det_1(\mathbf{R}_{L_z})\det(\mathbf{T}_{L_z}^{-1}) \\ \det_2(\mathbf{R}_{L_z})\det(\mathbf{T}_{L_z}^{-1}) \\ \vdots \\ \det_d(\mathbf{R}_{L_z})\det(\mathbf{T}_{L_z}^{-1}) \end{pmatrix} \quad (7.35)$$

here $\det_i$ represents a column vector containing as elements all the minor determinants, of order i , of its argument. If we now take the N^{th} order direct product of 7.34 and remove the permutation symmetry the new column vector will be a vector containing all the different possible combinations of minor determinants of $\mathbf{R}$ up to $\det^N(\mathbf{R})$ each multiplied by $\det^N(\mathbf{T}^{-1})$. Again here $\mathbf{R}$ separates completely from $\mathbf{T}$ so that it is possible to carry out the analytic continuation to arbitrary N . This matrix is clearly quite different from that in equation 7.32. firstly it is much bigger and secondly it contains far more degeneracy in the zero disorder matrix (see chapter 3).

7.5 Conclusion

In this chapter, we have shown how the generalised matrices of Kirkman and Pendry [1,2] and Pendry and Castaño [3] may be derived in a very simple manner, using the reflection recursion relation and following the method of chapter 3. In particular, this new method shows that the analytic continuation used in [1] is the correct one and that all series involved converge absolutely. In 3-D, we have also found a new matrix which contains far less degeneracy than that of [3] making it easier to deal with, either using perturbation theory or numerically.

Chapter 8

Conclusion

This conclusion is simply a collection of the conclusions from each chapter and has been included to draw all the results together in one place.

In chapter 2, we reported on the study of the distribution of the reflection coefficient for ensembles of disordered systems, described by the tight-binding model and considered chains made from a central region containing arbitrary diagonal disorder, connected to two semi-infinite perfect leads.

We derived a recursive numerical procedure to calculate the distribution of reflection coefficients $P(X, Y)$ and its moments and used it to find the generic behaviour of $P(X, Y)$ as a function of the length of the system L , the incident wave vector k , the strength of disorder σ and the type of disorder ρ . The results of our investigation are shown in a series of figures 2.1 to 2.9 and set the basis for the analytical investigations of further chapters.

In chapter 3, we established a formalism involving an infinite transfer matrix, which in principle, allows us to calculate the moments of the distribution of reflection coefficients $\langle R_L^n \rangle$ to desired accuracy, for any ensemble of disordered chains. We concentrated on the weak disorder limit and used perturbation theory to calculate analytic expressions for $\langle R_L^n \rangle$. We found that, at a generic position in the band we could use non-degenerate perturbation theory but for wavevectors rationally related to π , we must use degenerate perturbation theory to account for certain moments being anomalously large. The

strongest anomaly occurs at the band center. Figures 3.4(a,b), give a comparison between the perturbation theory result and the exact numerical result of chapter 2, for the first two moments $\langle R_L \rangle$ and $\langle R_L^2 \rangle$. Figures 3.5(a,b,c,d) show a similar comparison, this time between the perturbation theory and the random sampling method of chapter 2, for $P(\theta)$ the stationary distribution of the phase of the reflection coefficient, at various positions in the band. $P(\theta)$ in the last figure (d) clearly has a larger amplitude than the other plots, illustrating the band center anomaly.

In chapter 4, we used the tight-binding formalism of chapter 2 to derive a linear integral equation, of a type studied first by Dyson [49], for $P(\theta)$, or rather, for an equivalent quantity $Q(t)$. We also found that $P(\theta)$ has a simple relation to the Lyapunov exponent $\gamma(E)$ and the integrated density of states $H(E)$ of the problem, provided the energy E is in the spectrum of the perfect leads.

We then proceeded to examine $P(\theta)$ for two special types of disorder, namely the binary alloy, with site potentials $\pm\epsilon$, and an exactly soluble model, with a symmetric exponential distribution of potentials.

The case of the binary alloy, where the site potentials assume the values $\pm\epsilon$, with probability $1/2$, is considered in section 4.3. We found that long repetitions of periodic patterns of potentials are responsible for the existence of an infinity of power-law singularities in the reflection phase distribution. This effect is similar to the phenomenon, first described by Halperin [50], which affects the density of states of random harmonic chains, with light and heavy atomic masses. The predominant singularities are associated with repetitions $+ - + - + - \dots$ of the pattern $(+-)$ with period two. Patterns with higher periods produce much weaker singular contributions. The exponent α which characterises these sets of singularities is obtained in an exact way. It depends both on the disorder strength ϵ and on energy, so that divergences, ‘peaks’, in $P(\theta)$ are actually observed only when disorder exceeds some energy-dependent threshold. The results of an exact enumeration procedure show that the positions of all the most visible peaks present in this data are explained by the analytic approach. We also present plots of the periodic amplitudes, which

modulate the power-law singularities. This singular behaviour of $P(\theta)$ occurs whenever the distribution of the site potentials contains some discrete component.

In section 4.4, we considered a special class of distributions for the site potentials, namely the symmetric exponentials, for which the whole problem is exactly soluble. The solution, namely the determination of the Fourier coefficients of the distribution $P(\theta)$, as well as $\gamma(E)$ and $H(E)$, follows a method introduced by Nieuwenhuizen [57]. This method, which reduces the problem to solving a difference equation can in principle be extended to a wider class of potential distributions $\rho(\epsilon)$, symmetric or not, where a polynomial in ϵ multiplies the exponential distribution.

This exact solution allows a detailed investigation of various properties of the phase distribution. We found that $P(\theta)$ is differentiable infinitely many times, and fails to be analytic only because of an essential singularity at $\theta = \pm\pi$, related to the occurrence of arbitrarily large site potentials. It is therefore expected that $P(\theta)$ is analytic for any bounded and continuous distribution of the site potentials. We also investigated the behaviour of the Fourier coefficients c_n of $P(\theta)$ at weak disorder looking in particular at the anomalies which are known to affect the weak disorder expansion of quantities such as the Lyapunov exponent for any wavevector rationally related to π .

Finally, we should mention that some of the results in this chapter may generalise to higher dimensional systems. In the strongly localised regime a 3-D wire is totally reflecting, and hence is described by a unitary reflection matrix. The eigenvalues of that matrix are therefore pure phases, and the object of interest would be the distribution of these phases.

In chapter 5, we extended the tight-binding formalism of chapter 2 to 3-D. We consider a wire of cross-section $L \times L$ atoms with a central disordered region in the z direction of L_z layers, containing diagonal disorder. We derived a recursion relation for the reflection matrix of these wires and have shown that it gives rise to a perturbation expansion for the reflection matrix. This expansion has the same form as the Born series. We then concentrated on the first term in the expansion, corresponding to single scattering. In section 5.3, we

calculated moments of the reflected intensity $\langle |R_{\underline{k},\underline{k}'}|^{2n} \rangle$ into each transverse channel for arbitrary disorder type. In section 5.4, we used an adaptation of a method due to Heinrichs [33] to calculate the exact distribution of each element of the reflection matrix for Gaussian disorder $P(X, Y)$. These distributions are elliptical Gaussians (or bivariate Gaussians). However, their explicitly elliptical nature only appears for directions which are commensurate with the underlying lattice in some way, as in Bragg scattering, and for values of the average wave vector K close to $\pi/2$. In general, they appear perfectly cylindrical indicating that the phase of each reflection matrix element is randomly distributed.

In chapter 6, we derived a new formalism for calculating the moments of the transmitted intensity $\langle |T_L|^{2n} \rangle$. The formalism is an extension of that used in chapter 3 and involves a matrix which is the direct product of the reflection transfer matrix with its complex conjugate $\mathbf{W} = \mathbf{M} \otimes \mathbf{M}^*$. As an application we calculated an analytic expression for the moments of the transmitted intensity $\langle |T_L|^{2n} \rangle$ for weak disorder in the strongly localised regime and found that their form is consistent with the more generally valid maximal fluctuation theorem of Pendry *et al* [68].

In chapter 7, we reported on a simplified derivation of the generalised matrices of Kirkman and Pendry [1.2] and Pendry and Castaño [3] using the reflection recursion relation and following the method of chapter 3. In particular, this new derivation shows that the analytic continuations used in [1.2] and [3] are the correct ones and that all series involved converge absolutely. In 3-D, we found a new transfer matrix containing far less degeneracy than that of [3] making it easier to deal with either using perturbation theory or numerically.

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