ELECTRONS IN DISORDERED ONE DIMENSIONAL SYSTEMS

by

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Thesis submitted for the degree of

Doctor of Philosophy of the University of London

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London

July 1989

Abstract

A theoretical investigation of electron transport in disordered materials is presented. In particular we study the low temperature and/or small system size regime where inelastic scattering can be neglected and quantum interference dominates the physics.

After a brief review of the subject in Chapter I we begin by considering purely one dimensional systems in Chapters II and III. The problem is formulated in terms of transfer matrices which describe the scattering properties of the system. We are then able using direct products of transfer matrices, their symmetry properties under permutation group operations and an analytic continuation to obtain a general expression for $\langle -\ln t \rangle$. Here t is the transmission coefficient for electrons propagating through a one dimensional disordered system and angular brackets represent an average over all possible microscopic disorder configurations. We apply the solution to both substitutional (diagonal) and topological (off diagonal) disorder and compare our theoretical results with a numerical simulation.

In Chapter III we obtain a general expression for all the cumulants of $-\ln|t|^2$ and Θ where $t=|t|\exp(i\Theta)$ is the transmission coefficient defined in Chapter II. We deduce from the system size dependence of the cumulants that both variables are normally distributed in the limit of infinite system size. This predicts in general a two parameter scaling for both distributions. We examine the Anderson model in detail and compare our theoretical results with numerical simulations for this model.

In Chapters IV and V we extend the analysis to one dimensional systems of finite cross section. The symmetry analysis and the analytic continuation are developed in Chapter IV to obtain expressions for the Lyapunov exponents of such systems. We make a specific application to a two channel system and find that under certain conditions the analytic continuation breaks down. In Chapter V we develop self consistent approximations for the exponents using a perturbative technique.

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Acknowledgements

I wish to express my sincere gratitude to Professor John Pendry for his help and supervision over my three years at Imperial College. I would also like to thank Ele Castano, Angus MacKinnon and Spiros Evangelou for many helpful and stimulating discussions.

I acknowledge the Science and Engineering Research Council of Great Britain for financial support.

1. The Semi-Classical theory of Transport

The starting point for the semi-classical treatment of transport is Bloch's theorem for electrons in the periodic potential of a crystal lattice. This states that the solutions of the Schroedinger equation for such systems are of the form

$$\Phi_{\mathbf{k}}(\mathbf{r}) = \exp(i\mathbf{k}.\mathbf{r})\ u(\mathbf{r}) \qquad (1)$$

where $u(\mathbf{r})=u(\mathbf{r}+\mathbf{R})$ for all lattice vectors $\mathbf{R}$. The Bloch states are labelled by a crystal momentum vector $\mathbf{k}$ which is related to the energy ε of the state

$$\varepsilon \equiv \varepsilon(\mathbf{k}) \qquad (2)$$

The motion of an electron wave packet formed from Bloch states in the vicinity of wave vector $\mathbf{k}$ is governed by [1]

$$\hbar \frac{d\mathbf{k}}{dt} = e(\mathbf{E} + \mathbf{v}(\mathbf{k}) \times \mathbf{B}) \qquad (3)$$

Here $\mathbf{v}(\mathbf{k})$ is the group velocity of the wave packet

$$\mathbf{v}(\mathbf{k}) = \frac{1}{\hbar} \frac{d\,\varepsilon(\mathbf{k})}{d\mathbf{k}} \qquad (4)$$

These are essentially the same dynamics as in free space except that the periodic potential of the crystal lattice alters the inertia of the electron and leads to the introduction of a mass tensor $\mathbf{m}^*$

$$\mathbf{m}^* \frac{d\mathbf{v}}{dt} = e\ (\mathbf{E} + \mathbf{v}(\mathbf{k}) \times \mathbf{B}) \qquad (5)$$

where

$$[\ \mathbf{m}^*\ ]^{-1} = \frac{1}{\hbar^2} \frac{d^2}{d\mathbf{k}d\mathbf{k}} \varepsilon(\mathbf{k}) \qquad (6)$$

The presence of impurities in the lattice, electron-electron and electron-phonon interactions are treated as

perturbations which cause scattering between Bloch states. The conductivity is derived using the Boltzmann formalism with the effect of scattering included by introducing a relaxation time τ. The final result for the conductivity tensor σ is [1]

$$\sigma_{ij} = \frac{1}{2\pi^2} \frac{e^2\tau}{\hbar} \int \frac{v_i(\mathbf{k})v_j(\mathbf{k})}{|\mathbf{v}(\mathbf{k})|} dS \qquad (7)$$

where the integral is over the fermi surface. If we assume that the band structure is isotropic, that is $\varepsilon \equiv \varepsilon(|\mathbf{k}|)$ then were obtain the well known Drude result for the conductivity

$$\sigma_B = \frac{ne^2\tau}{m^*} \qquad (8)$$

In this case both the conductivity and effective mass tensors are isotropic and can be written as scalars. If the fermi surface is not spherical the conductivity will depend on the orientation of the applied field relative to the crystal structure. A good example here is graphite where the conductivity is dramatically different perpendicular to as opposed to in the plane of the carbon layers.

The motion of the electrons in the semi-classical model is diffusive and in fact the conductivity is related to the diffusion constant D by the Einstein relation

$$\sigma = e^2 n(\varepsilon_F) D \qquad (9)$$

where $n(\varepsilon_F)$ is the density of states at the fermi energy. The essence of the semi-classical approximation is to treat the periodic potential of the crystal lattice quantum mechanically but to treat the scattering classically. In general it is possible to distinguish between two types of scattering. Coherent scattering, usually elastic scattering by impurities, which maintains the phase coherence of the wave function and incoherent scattering, usually inelastic scattering of electrons by other electrons or phonons which destroys the phase coherence of the wavefunction.

The effects of electron-electron interactions can often be neglected. This is quite reasonable if the carrier density is low as in for example a lightly doped semiconductor. However even when the carrier concentration is high as in for example a metal the electron-electron scattering is greatly reduced as a consequence of the Pauli exclusion principle and the related Fermi-Dirac statistics. Nevertheless it is important to realise that under certain circumstances electron-electron interactions can radically alter the ground state (and excitation spectrum) of the system so that it no longer resembles that of a set of noninteracting electrons in Bloch states inside the fermi surface. This can have profound physical consequences, as in for example phenomena of superconductivity and the fractional quantum hall effect. The electron-phonon scattering rate depends on temperature since this determines the occupancy of the phonon gas. In general the electron-phonon scattering rate tends to zero as a power of T as T->0. In two dimensional systems the mean free path for all inelastic scattering can be measured using the weak localisation correction to the Boltzmann conductivity. The weak localisation correction will be discussed in section 2.1.1, for details of the experimental observations the reader is referred to the review by Lee and Ramakrishnan [2].

The importance of impurity scattering depends on the concentration of impurities. The semiclassical theory treats each impurity as isolated and neglects the interference between partial waves scattered from different impurities. This is quite reasonable if the impurity concentration is low (so that the elastic scattering length L_e is large compared with the lattice spacing), or if the inelastic scattering length L_i is comparable with the elastic length L_e. In the latter case interference effects due to multiple scattering between impurities can be neglected since the wavefunctions are not phase coherent on this length scale.

In general we shall distinguish two scattering lengths. The first is the coherent scattering length, which we identify with the elastic mean free path L_e. The second is the phase coherence length L_ϕ which we identify with the inelastic

mean free path L_i. We shall assume that L_ϕ is effectively infinite or at least very much longer than L_e which is usually the case at very low temperatures. Under these conditions interference effects due to coherent scattering should be apparent. In some cases these interference effects can be masked at finite temperature by "energy averaging" over a range k_BT near the fermi level. Interactions of the electron spin with magnetic impurities or length scales associated with magnetic fields may also be important.

2. Quantum Transport

2.1 Weak Localisation

An obvious starting point for the systematic calculation of corrections to the Boltzmann conductivity is the Kubo formula. A number of authors have calculated the corrections to σ_B due to the interference effects arising form coherent backscattering. The corrections are computed by summing over a subset of diagrams known as maximally crossed diagrams, the contributions of other diagrams being neglected. The results depend on the physical dimension of the system [2]

$$\sigma_{3D}(L) = \sigma_B - \frac{2e^2}{h\pi^2}\left[\frac{1}{L_e} - \frac{1}{L}\right] \qquad (10)$$

$$\sigma_{2D}(L) = \sigma_B - \frac{2e^2}{h\pi}\ln[L/L_e]$$

$$\sigma_{1D}(L) = \sigma_B - \frac{2e^2}{h}[L - L_e]$$

These results apply at zero temperature. At finite temperatures it can be argued that the system size L should be replaced by the inelastic length[1] L_i. The power law variation of this length against T implies a logarithmic dependence of the conductivity on temperature for a two

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[1] In general L will be replaced by L_ϕ but in the experiments on metal films this is identified as L_i.

dimensional system. This is confirmed in experiments on thin metal films at low temperatures. Bergmann [3] has proposed a physical interpretation of the maximally crossed diagrams in terms of the constructive interference of time reversed scattering paths. This constructive interference is broken by the application of a magnetic field, a fact which has been used to explain anomalies in the low temperature magneto-resistance of thin metal films.

Coherent back scattering does not alter the diffusive nature of the electron motion, at least in three dimensions. For this reason the logarithm temperature dependence of σ and the magneto-resistance anomalies are known as weak localisation phenomena. This is in contrast to Anderson localisation (section 2.2) which occurs for high impurity concentrations where the electronic motion is not diffusive. Intriguingly in one and two dimensions the perturbation theory breaks down if the system size L is large enough. This is an indication of how the nature of electron motion in disordered system depends on the dimensionality of the system.

2.2 Universal Conductance Fluctuations

The weak localisation effects described above arise from interference on length scales less than the inelastic length L_i but are observable in macroscopic samples where $L \gg L_i$. In recent years it has become possible to fabricate semiconductor devices whose dimensions are smaller than the inelastic length at temperatures of a few degrees Kelvin. It is predicted theoretically [4-9] that the conductance G of such a system is sensitive to the exact arrangement of impurities within the sample and that on averaging over all possible impurity configurations

$$\mathrm{var}(G) \approx e^2/h \qquad (11)$$

independent of the exact sample size provided $L_e << L << L_i$ and the mean conductance.[2] In early experiments on MOSFETS [10] which confirmed (11) it was not possible to change the microscopic arrangement of impurities and so the fluctuations in the conductance were observed against fermi level (gate voltage) and magnetic field. Theoretical work showed that fluctuations in these cases are equivalent to averaging over impurity configurations. In more recent work [11-12] it has been possible to change the impurity configurations by populating and depopulating electron traps in GaAlAs/GaAs hetero-junctions providing further confirmation of (11).

2.3 Magnetic Effects

In experiments on small metal rings and cylinders [13-14] whose dimensions are smaller than the L_ϕ it is observed that the conductance exhibits periodic oscillations as a function of the flux enclosed by the ring or cylinder. Coherent back scattering, responsible for weak localisation, produces oscillation with period h/2e. Direct interference of electron waves scattered around the different arms of ring structure gives rise to oscillations with period h/e. There is also an aperiodic background fluctuation of the conductance known as a "magnetofingerprint" This variation is found to be exactly reproducible at a fixed temperature. The fundamental explanation of these phenomena is to be found in the dependence of the momentum operator **p** on the electromagnetic vector potential **A**

$$\mathbf{p} = i\hbar \frac{d}{d\mathbf{r}} + e\mathbf{A} \qquad (12)$$

The periodic oscillations are often called Aharonov-Bohm oscillations because of their close relation to the effect

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[2] It is assumed here that electronic motion is diffusive and that Anderson localisation (see section 2.2) is not important on the length scale L of the sample.

of that name which occurs in the interference of electron beams in vacuum which enclose a magnetic flux.

2.4 Anderson Localisation

In a pioneering work [15] Anderson obtained the startling result that if the interference of the partial waves scattered by the impurities is sufficiently strong the electron motion is no longer diffusive.

Anderson studied a tight binding hamiltonian H

$$H = \sum_n \varepsilon_n |n><n| + V \sum_n \sum_m |n><m| \qquad (13)$$

where the site energies are random with distribution

$$p(\varepsilon) = \frac{1}{W} \qquad |\varepsilon| \leq \frac{W}{2} \qquad (14)$$

$$= 0 \qquad \text{otherwise}$$

and the sum over m in (13) is over the nearest neighbours of the nth lattice site. Consider a state which at t=0 which has non zero amplitude only on a single site, say n=0

$$\Phi(t=0) = |0> \qquad (15)$$

Its time development is governed by the time dependent Schroedinger equation

$$H\Phi = i\hbar \frac{d}{dt} \Phi \qquad (16)$$

Anderson was able to show that if the ratio of W to V is sufficiently large the wavefunction does not diffuse away to infinity as $t \to \infty$ but that at long times it remains exponentially localised over a small region of space. This result shows that random interference can radically alter the character of the eigenstates of a system. In a metallic regime where the electron motion is diffusive the eigenstates of the system are extended and the wavefunctions have appreciable amplitude right across the system. This results is not altered by the the weak random interference

from low impurity concentrations discussed in the last section. However as the impurity concentration is increased a transition occurs to a regime where the eigenstates of the system are exponentially localised in space. This effect is called Anderson localisation.

In a development of the ideas of Anderson localisation Mott [16] argued that when W/V is small states in the band tails will be localised, states at the band centre remaining extended. There will thus be an energy Ec, called the mobility edge, which separates extended from localised states (Figure 1.1). As the disorder or impurity concentration is increased this energy moves toward the band centre until a critical disorder is reached where all states in the band become localised. This is known as the Anderson transition.

In the localised regime where diffusion does not occur the question arises as to how electron transport will take place. At zero temperature the Einstein relation (9) implies that the conductivity will be zero since the diffusion constant D is zero. At finite temperature however transport can occur by thermally assisted hopping between localised states. This process is known as variable range hopping and Mott has shown that it implies a temperature dependence of the conductivity of the form [16]

$$\sigma = A \exp(-B/T^n) \qquad (17)$$

This has been confirmed by experiment, however the exact value of n is difficult to measure and does not always agree with the theoretical prediction of n=1/4.

3. The Scaling Theory of Localisation

Having introduced the idea of Anderson localisation in the last section we outline the most influential theory of this phenomenon which has appeared during the last decade, the scaling theory of Abrahams, Anderson, Licciardello and Ramakrishnan [17].

Figure 1.1

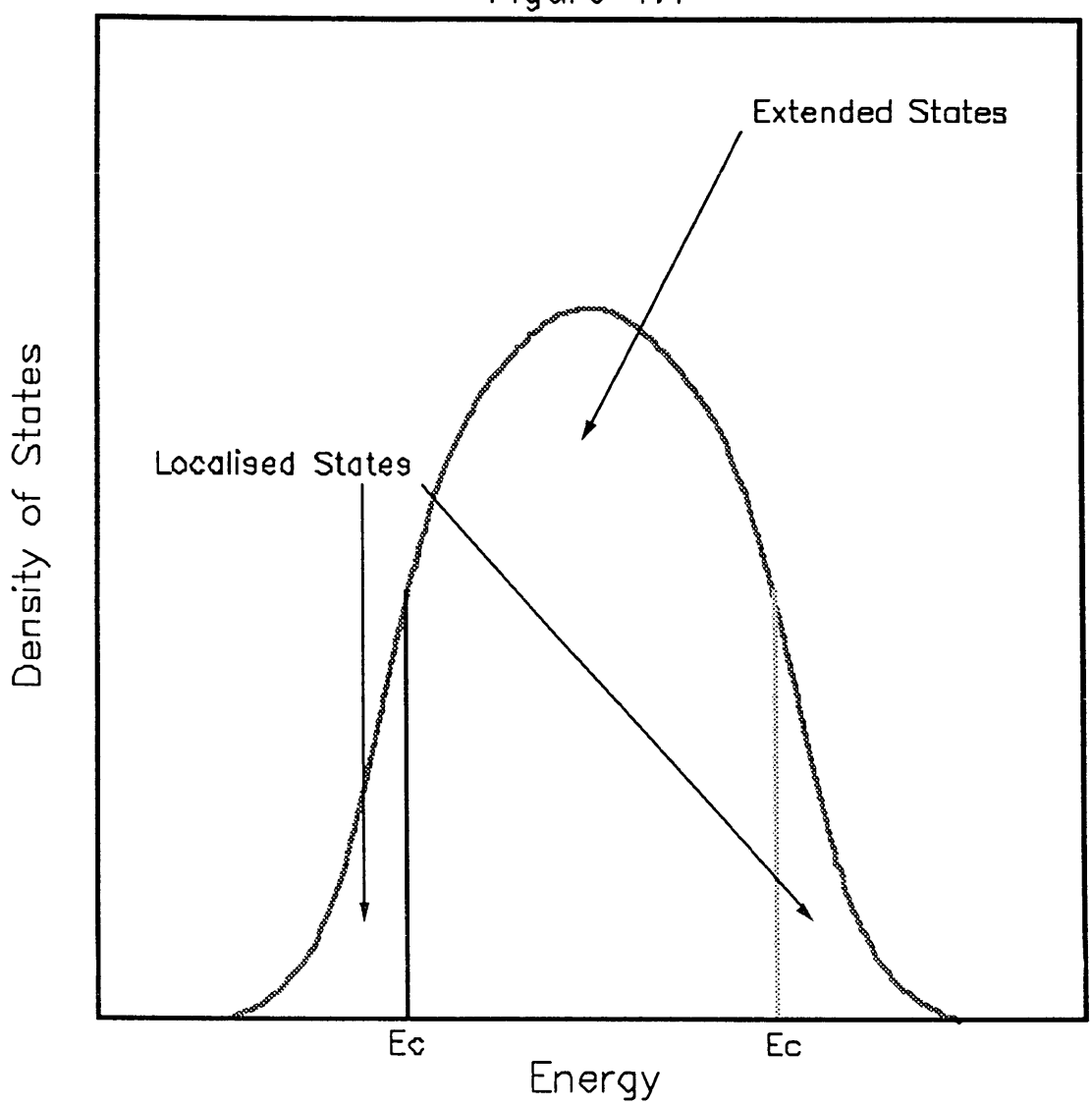

Figure 1.1 - The mobility edge which seperates localised from extended eigenstates.

Consider the conductance g(L) of a d dimensional "hypercube" of size L, where L is much longer than the elastic mean free path. It can be argued using ideas due to Thouless [18] that the the conductance of a similar "hypercube" of size bL is determined solely by the factor b and the dimensionless conductance at size L. This assumption can be expressed as

$$g(bL) = f(g(L),b) \tag{18}$$

or in continuous terms as

$$\frac{d\ ln(g(L))}{dlnL} = ß(g(L)) \tag{19}$$

Here g is related to the usual conductance G by

$$G = \frac{e^2}{h}\ g \tag{20}$$

The function ß should be universal and depend only on the dimension of the system. The form of ß(g) in the metallic regime where g>>1 can be deduced from the weak localisation results (9). A simple calculation gives

$$ß(g) = d-2 \ - \frac{2}{\pi}d-1 \cdot \frac{1}{g} + ... \tag{21}$$

In the strong localisation limit, where g<<1 we expect that the conductance will fall off exponentially with size

$$g(L) = g_0 exp(-\alpha L) \tag{22}$$

where α and g_0 are constants. Here AALR [17] find that

$$ß(g) = ln[g/g_0(d)] \cdot [\ 1 + ag + ...\ ] \tag{23}$$

where a>0. Here α is the mean exponential localisation rate for the electron wavefunctions in the localised regime. The inverse of this quantity is defined as the localisation length Lc

$$Lc \equiv \frac{2}{\alpha} \tag{24}$$

The further assumption that ß(g) is monotonic and continuous between these limit leads to the form of the ß or scaling function given in Figure 1.2.

In one and two dimensions the beta function is always negative and therefore the scaling theory predicts that all states in d=1 and d=2 are localised, even for weak disorder. For d=1 this result was already well known, for a review see Ishii [19]. For d=3 there is a fixed point of the scaling transformation at a critical conductance g_c where

$$ß(g_c) = 0 \tag{25}$$

Scaling up from some arbitrary length $L_0 >> L_e$ two types of behaviour are predicted depending on the conductance at L_0

$$\lim_{L\to\infty} g(L) = \exp(-\alpha L) \qquad g(L_0) < g_c \tag{26}$$

$$\lim_{L\to\infty} g(L) = \sigma L \qquad g(L_0) > g_c \tag{27}$$

The critical value g_c signals a transition between localised and extended states. Thus the scaling theory predicts the existence of a mobility edge in three dimensions.

Strictly the scaling theory applies only at T=0. At finite temperature the conductivity in the localised regime is dominated by the variable range hopping process of Mott. The importance of the scaling theory is that it provides unambiguous answers to fundamental questions. How does the nature of the eigenstates of a random potential depend on the dimensionality of the system? Does $\sigma(T=0)\to 0$ smoothly as we approach the mobility edge or is there a discontinuous change in σ at Ec? The answer to the first question has already been given above so we will focus on the second question. Consider scaling from some initial length L_0 where the conductance g_0 is near the critical value g_c. Near g_c we linearise the beta function

$$ß(g) = s \ln[g/g_c] \tag{28}$$

where s is the slope of ß at $g=g_c$. If $g > g_c$ we obtain in the limit $L\to\infty$ by integration of (19)

Figure 1.2

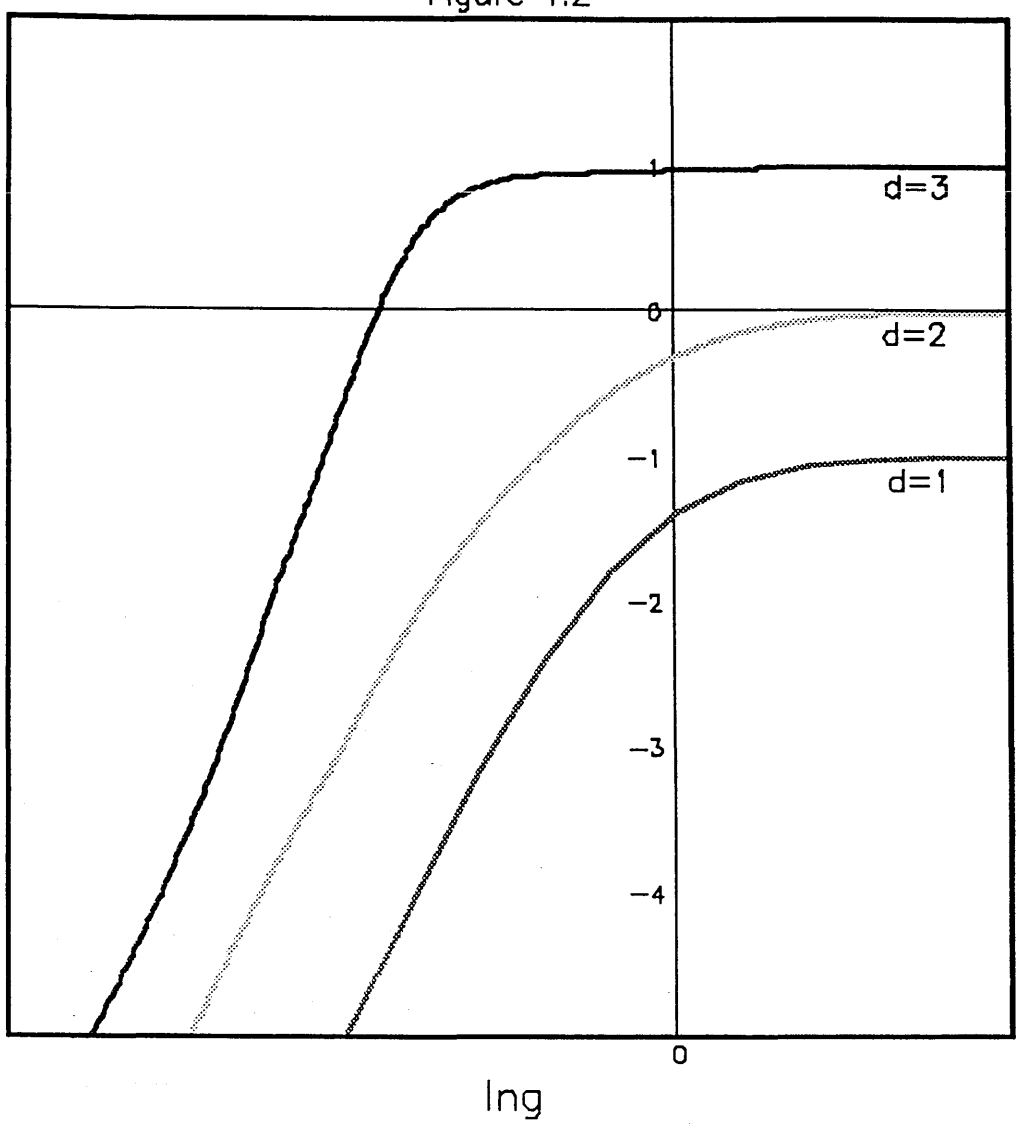

Figure 1.2 - The beta function for the scaling theory of localisation.

$$\sigma \approx \left[\frac{g_0 - g_c}{g_c} \right]^{\nu} \qquad (29)$$

where $\nu=1/s$. The transition is thus continuous. This means that there is no minimum metallic conductivity as had been proposed by Mott [16].

4. Is the Scaling Hypothesis Correct?

The scaling theory is extremely informative but it relies crucially on the single parameter scaling hypothesis of equation (19). The initial motivation for this hypothesis was an heuristic argument due to Thouless [18]. The mean spacing of the energy levels at the fermi level in the d dimensional hypercube is δE where

$$\delta E = \frac{1}{n(\varepsilon_F) L^d} \qquad (30)$$

The sensitivity of the energy of the eigenstates of the cube to boundary conditions Γ can be estimated using the uncertainty relation from the time τ an electron can remain in a state without "noticing" the boundary.

$$\Gamma = \frac{h}{\tau} \qquad (31)$$

$$= \frac{hD}{L^2} = \frac{h\sigma}{L^2 e^2 n(\varepsilon_F)}$$

Here we have used the Einstein relation between the conductivity σ and the diffusion constant D. We now notice that the dimensionless conductance g can be written as a ratio

$$g = \Gamma/\delta E \qquad (32)$$

$$= \frac{h}{e^2} \sigma L^{d-2}$$

It is now argued that if two blocks are placed together the coupling between levels in each block will be of order Γ and the average mismatch between levels of order δE. If we

imagine combining many blocks together we can describe the system using an Anderson type model where

$$W/V \equiv \delta E/\Gamma \qquad (33)$$

In the Anderson model it is only the ratio of W to V which is important and this implies that the only variable which is important in determining the conductance of the combined system is the ratio $\Gamma/\delta E$ for the individual blocks which is equal to the dimensionless conductance at scale L g(L). This argument gives some support to the scaling hypothesis in metallic regime where the electron motion is diffusive. The extension to the localised regime is unclear.

In order to test the predictions of the scaling theory for two and three dimensions numerical studies of the Anderson model for one dimensional systems of finite cross section were made [20-22]. Using a finite size scaling analysis outlined in Chapter IV the localisation length Lc for two and three dimensional systems were deduced as a functions of fermi energy and W/V. Integrating (19) with the initial condition $g_0 < g_c$ using the linear approximation (28) near g_c and identifying the result with (22) we find that the localisation length diverges at the mobility edge as

$$Lc \approx \left[\frac{g_0 - g_c}{g_c} \right]^{-\nu} \qquad (34)$$

In the numerical studies a divergence of Lc for a critical value of W/V dependent on the fermi energy is found for d=3. For d=2 it is found that Lc is always finite. This confirms one of the main results of the scaling theory but provides only indirect evidence for the scaling hypothesis.

Comparing (34) with (29) we see that the exponent for the divergence of Lc at Ec is equal to the exponent for $\sigma(T=0)$ at Ec. This allows a comparison of experimental data for the conductance exponent with numerical work on the Anderson model. Recently doubts have been expressed concerning the widely quoted theoretical value $\nu=1$ which does not agree with experiments on some systems eg Si:P $\nu \approx 1/2$. It is thought that interaction effects may be important here but as yet no consensus has emerged.

Consideration of the statistics of the resistance of one dimensional systems highlights a fundamental difficulty in the scaling hypothesis. The resistance distribution defined on the ensemble of possible microscopic impurity configurations is very broad, the variance of the distribution diverging exponentially with length [23-24]. Nor does the mean of the conductance have the simple exponential form which would be expected from (22) [25-26]. In fact the mean conductance is not dominated by the contributions from "typical" localised states but by contributions from atypical resonance states [27]. Resonance or "necklace" states have much larger transmission coefficients than typical localised states. In an attempt to overcome these problems Anderson, Thouless, Abrahams and Fisher [28] analysed the statistics of ln(1+R) where R is the dimensionless resistance. The average defines the localisation length Lc

$$\langle \ln(1+R) \rangle = 2L/Lc \qquad L \gg Lc \tag{35}$$

The variance of ln(1+R) scales linearly with length so that the distribution is not too broad. It was proposed that the scaling hypothesis should apply to a typical or scale resistance R_s where

$$R_s = \exp[2L/Lc] - 1 \tag{36}$$

Differentiation then gives

$$ß(g_s) = -(1 + g_s) \ln[1 + 1/g_s] \tag{37}$$

where $R_s=1/g_s$. How relevant the scale conductance would be to an actual measurement of conductance will depend of course on the distribution of conductance. For a complete solution of the scaling problem in one dimension we must know how the distribution of conductance scales with length. In particular does the distribution obey a single parameter scaling?

$$p_L(g) \rightarrow p(g, L/Lc) \quad L \rightarrow \infty \tag{38}$$

A detailed solution of this problem is presented in Chapter III. We find that single parameter scaling holds for weak

disorder but that for strong disorder a crossover to two parameter scaling occurs.

In two and three dimensions the scaling of the conductance distribution is not yet fully understood. It is known that the non self averaging of the conductance is not confined either to one dimensional systems or to the localised regime. In the UCF regime the variance of the conductance is independent of system parameters. If p(g) is a normal distribution then this immediately implies a single parameter scaling of the distribution, the only relevant parameter being the mean conductance <g>. In the localised regime the behaviour is expected to be more analogous to the one dimensional case. Recent work by a number of authors [8, 29-31] tends to support the idea that in the weak disorder limit the distribution is determined by a single parameter. There are indications however that this is not so for strong disorder [32].

5. Generalised Transfer Matrices

The basis of the theoretical approach to be presented in Chapters II-V is a scattering formalism. The transmission of electron waves through, and their reflection by, a section of disordered material can be described by a transfer matrix **M**. The transfer matrix **T** for a system composed of L sections will be of the form

$$\mathbf{T} = \prod_{n=1}^{L} \mathbf{M}_n \tag{39}$$

Referring to Appendix I of Chapter II we find that the transfer matrix of a one dimensional system is of the form

$$T = \begin{bmatrix} 1/t^* & r/t \\ r^*/t^* & 1/t \end{bmatrix} \tag{40}$$

The transfer matrix "propagates" 1/t and r/t through the system

$$\mathbf{T}_L \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} r_L/t_L \\ 1/t_L \end{bmatrix} \qquad (41)$$

By the use of a symmetry analysis and an analytic continuation Kirkman and Pendry [33] derived a generalised transfer matrix $\mathbf{X}(\mathbf{T},z)$ which "propagates" $1/t^z$ through the system for z any complex number. This method has also been applied to the study of correlation functions in one dimensional systems of relevance to noise in low dimensional structures [34-35].

In Chapter II we review and extend the analysis of [33]. In particular we apply the method to so called "offdiagonal" disorders in the one dimensional Anderson model. In Chapter III we develop the theory further and obtain a general expression for the statistical cumulants of $-\ln|t|^2$ and Θ (Θ is the phase of t.) From this basic result we obtain the asymptotic form of the distributions of both variables in the limit that $L\to\infty$. This provides an unambiguous answer to the scaling question in one dimension.

In Chapters IV and V we make a start at the generalisation of these ideas to one dimensional systems of finite cross section. As well as being of importance in the understanding of fully two and three dimensional systems, recent experiments on conductance in restricted geometries makes such system of interest in their own right [36-37].

The relation of the scattering properties to the transport properties of the system is not always unambiguous. In one dimension the relation is normally made by way of the Landauer formula [38]

$$g = \frac{|t|^2}{|r|^2} \qquad (42)$$

The generalisation to many channel system is usually given as [39-40]

$$g = \mathrm{tr}(\mathbf{t}^{+}\mathbf{t}) \qquad (43)$$

where $\mathbf{t}$ is now the transmission matrix. There has recently been considerable interest in this point and for a detailed discussion the reader the relevant references. In general the exact relation depends on the experimental conditions and to avoid ambiguities we present the results of the main chapters in terms of the scattering properties.

References

[1] Ziman J M "Principles of the Theory of Solids" Cambridge University Press Cambridge 1972

[2] Lee P and Ramakrishnan T Reviews of Modern Physics 57 287 (1985)

[3] Bergmann G Physics Reports 107 1 (1984)

[4] Stone A Physical Review Letters 54 2692 (1985)

[5] Lee P and Stone A Physical Review Letters 55 1622 (1985)

[6] Lee P, Stone A and Fukuyama H Physical Review B 35 1039 (1987)

[7] Y Imry Europhysics Letters 1 249 (1986)

[8] Muttalib K, Pichard J L, Stone A Physical Review Letters 59 2475 (1987)

[9] Zanon N and Pichard J L Journal of Physics France 49 907 (1988)

[10] Skocpol V Physica Scripta T19 95 (1987)

[11] Mailly D, Sanquer M, Pichard J L and Pari P Europhysics Letters 8 471 (1989)

[12] Debray P, Pichard J L, Vicente J, and Tung P Submitted to Physical Review Letters

[13] Aranov A and Sharvin Yu Reviews of Modern Physics 59 755 (1987)

[14] Laibowitz R, Santhanam P, Umbach C, Washburn S and Webb R Physica Scripta T19 87 (1987)

[15] Anderson P Physical Review 109 1492 (1958)

[16] Mott N "Conduction in Non-Crystalline Materials" Clarendon Press Oxford 1987

[17] Abrahams E, Anderson P, Licciardello D and Ramakrishnan T Physical Review Letters 42 673 (1979)

[18] Thouless D in "Ill Condensed Matter" Editors Balian R et al. North Holland 1979

[19] Ishii K Supplements of Progress of Theoretical Physics 53 77 (1973)

[20] MacKinnon A and Kramer B Zeitshcift fur Physik B 53 1 (1983)

[21] Bulka B, Kramer B and MacKinnon A Zeisshcrift fur Physik B 60 13 (1985)

[22] Schreiber M, Kramer B and MacKinnon A Physica Scripta T25 67 (1989)
[23] Abrikosov A Solid State Communications 37 997 (1981)
[24] Pendry J Journal of Physics C 20 733 (1987)
[25] Abrikosov A and Ryzhkin I Advances in Physics 27 147 (1978)
[26] Kirkman P and Pendry J Journal of Physics C 20 733 (1984)
[27] Pendry J Journal of Physics C 20 733 (1987)
[28] Anderson P , Thouless D, Abrahams E and Fisher D Physical Review B 22 3519 (1980)
[29] Mello P, Pereyra P and Kumar N Annals of Physics 181 290 (1988)
[30] Mello P and Shapiro B Physical Review B 37 5860 (1988)
[31] Mello P and Pichard J Submitted to Physical Review Letters
[32] Cohen A, Roth Y and Shapiro B Physical Review B 38 12125 (1988)
[33] Kirkman P and Pendry J Journal of Physics C 17 4327 (1984)
[34] Pendry J and Kirkman P Journal of Phtsics C 19 207 (1980)
[35] Pendry J, Kirkman P and Castano E Physical Review Letters 57 (1986)
[36] van Wees, van Houten H, Beenakker C, Williamson J, Kouwenhoven L, van der Marel D and Foxon C 60 848 (1988)
[37] Wharam D, Thornton T, Newbury R, Pepper M, Ahmed H, Frost J, Hasko D, Peacock D, Ritchie D and Jones G Journal of Physics C 21 L209 (1988)
[38] Landauer R Philosophical Magazine 21 863 (1970)
[39] Fisher D and Lee P Physical Review B 23 6851 (1981)
[40] Buttiker M, Imry Y, Landauer R and Pinhas S Physical Review B 31 6207 (1985)

Chapter II - Generalised Transfer Matrices and the Calculation of <-lnt> for One Dimensional Disordered Systems

1. Introduction

In this and the following chapter we concentrate our attention on strictly one dimensional systems, leaving the discussion of the quasi one dimensional systems to chapters IV and V.

In this chapter we derive a general expression for <-lnt>, where t is the transmission coefficient for electrons propagating through a disordered one dimensional material and the angular brackets refer to an average of the possible microscopic disorder configurations. The real part of this quantity is equal to the exponential decay rate of the transmission and its imaginary part is proportional to the ensemble average integrated density of states. The basis for our theoretical approach is the generalised transfer matrix method of Kirkman and Pendry [1], which we describe fully in section 2. In section 3.1 we introduce the Anderson model for disordered materials and then in the subsequent sections 3.2-3.4 we apply the generalised transfer matrix method to obtain <-lnt> explicitly for various limiting cases of this model. In particular in section 3.2 we calculate <-lnt> for weak off diagonal disorder[1], we give numerical implementation of the method for arbitrary disorder in 3.3 and study an anomaly present in off diagonally disordered systems at the band centre in 3.4.

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[1]This term will be explained in section 3.2

2. Calculation of <-lnt> for One Dimensional Systems

In this section we obtain a general expression <-lnt> where t is the transmission coefficient for waves travelling through a one dimensional disordered system.[2] We characterise the scattering of the system by a transfer matrix **T** which relates incident and reflected wave amplitudes at the left (a_+ and a_- respectively) to those at the right (b_- and b_+) of the system (see Appendix I),

$$\begin{bmatrix} b_+ \\ b_- \end{bmatrix} = \mathbf{T} \cdot \begin{bmatrix} a_+ \\ a_- \end{bmatrix} \qquad (1)$$

The subscripts + and - denote the direction of propagation of the waves. We suppose our system to be made up of L single channel scatterers each described by an individual transfer matrix $\mathbf{M}_n$ where n=1,..,L. Then **T**, the transfer matrix for the whole system, will be a product of these transfer matrices

$$\mathbf{T} = \prod_{n=1}^{L} \mathbf{M}_n \qquad (2)$$

We shall assume that each $\mathbf{M}_n$ is independently and identically distributed with some probability distribution p(**M**).

We consider systems with time reversal symmetry where T has the explicit form

$$T = \begin{bmatrix} 1/t^* & (r/t) \\ (r/t)^* & 1/t \end{bmatrix} \qquad (3)$$

where t and r are the amplitude transmission and reflection coefficients respectively.

As a first step we write

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[2] In fact we obtain a general expression for $<-\ln t^*>$ which is trivially related to <-lnt>

$$[t^*]^{-N} = [1,0] \otimes .. [1,0] \; \mathbf{T} \otimes .. \mathbf{T} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes .. \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad (4)$$

where each direct product is taken N times. It is easy to show that

$$\mathbf{T} \otimes .. \mathbf{T} = \prod_{n=1}^{L} \mathbf{M}_n \otimes .. \mathbf{M}_n \quad (5)$$

These expressions can be considerably simplified by noticing that any direct product of N identical matrices decomposes into independent subspaces according to the irreducible representations of the permutation group of order N [2]. This considerably simplifies the evolution of vectors under repeated multiplication by operators of this type. This is exactly the situation prevailing in equations (4) and (5). For our purposes here it will be sufficient to notice that any symmetric vector **u**, that is a vector whose components have the property that

$$u_{j1 \; \ldots \; jN} = u_{P(j1 \; \ldots \; jN)} \quad (6)$$

where P is any permutation of the N indices, remains symmetric after multiplication by such an operator. Since both projection vectors in (4) are symmetric their evolution under repeated multiplication is confined within the subspace of all symmetric vectors. To take advantage of this we must first choose a set of ortho-normal basis vectors for the symmetric subspace. The set of vectors $\{\mathbf{v}(i) : i=0,..,N\}$ with components

$$v(i)_{j1....jN} = \sqrt{(i!(N-i)!/N!)} \quad \text{if} \quad j1+... \; jN = N+i$$
$$= 0 \qquad \text{otherwise} \quad (7)$$

and each j = 1 or 2 is easily shown to be such a basis. We then define a symmetry reduced transfer matrix $\mathbf{X}(\mathbf{T},N)$ with elements

$$X_{i,j} = \mathbf{v}(i) \; . \; \mathbf{T} \otimes \ldots \mathbf{T} \; . \; \mathbf{v}(j) \quad (8)$$
$$= \sum_{k=0}^{\min(i,j)} \sqrt{\left({}^{N-i}C_{j-k} \; {}^{N-j}C_{i-k} \; {}^{i}C_{k} \; {}^{j}C_{k} \right)} \cdot T_{1,1}^{\,N-i-j+k} \; T_{1,2}^{\,j-k} \; T_{2,1}^{\,i-k} \; T_{2,2}^{\,k}$$

This definition and the decomposition into independent subspaces guarantee that **X** has the usual multiplicative property of a transfer matrix

$$\mathbf{X}(\mathbf{T},N) = \prod_{n=1}^{L} \mathbf{X}(\mathbf{M}_n,N) \tag{9}$$

We can now obtain the Nth moment of $1/t^*$

$$< [t^*]^{-N} > = \mathbf{w}^T \cdot < \mathbf{X}(\mathbf{M}_n,N) >^L \cdot \mathbf{w} \tag{10}$$

where **w** is a column vector with components $w_j = \delta_{j,0}$ $(0 \leq j \leq N)$, $\mathbf{w}^T$ is the transpose of **w** and angular brackets indicates an average over the distribution $p(\mathbf{M})$.

To proceed further we need an analytic continuation of (10). This can be achieved by generalising the definition of the **X** matrix. We analytic continue the binomial coefficients using the gamma function

$${}^{N}C_{p} = \frac{\Gamma(N+1)}{\Gamma(N-p+1)\ \Gamma(p+1)} \tag{11}$$

for N any complex number and p a positive integer. This is sufficient to allow evaluation of all the coefficients appearing in the definition of the **X** matrix for arbitrary N. To complete the analytic continuation we extend the range of the matrix indices to $0 \leq i,j \leq \infty$. We can see that our continuation is at least consistent with our previous exact result for the positive integer moments of 1/t by noticing that the new **X** matrix becomes block diagonal when N is a positive integer or zero

$$\mathbf{X}(N) = \left[\begin{array}{c|c} 0 \leq i,j \leq N & 0 \\ \hline 0 & N < i,j \leq \infty \end{array}\right] \tag{12}$$

It can also be shown [1] that the continuation gives $<t^{-N}>$ correctly for all N when considering translationally

invariant (ordered) systems. Thus, although there seems to be no reason why this continuation should be unique the above limiting cases and also extensive comparison with numerical simulation [1] give us considerable confidence that the solution given here is exact for nearly all one dimensional systems.

$$<-\ln t^{*}> \quad = \quad \frac{d}{dN} <t^{-N}>| \qquad (13)$$
$$|N=0$$

In the limit that $L\to\infty$ the real part of $<-\ln t^{*}>/L$ defines the localisation length Lc and the imaginary part is equal to the ensemble average integrated density of states per unit length $<\sigma(E)>$

$$\lim_{L\to\infty} \frac{<-\ln t^{*}(E)>}{L} \quad = \quad \frac{1}{Lc} \quad + \quad i\pi<\sigma(E)> \qquad (14)$$

at energy E.

We can find a more explicit expression for $<-\ln t^{*}>$ if we express $<\mathbf{X}>$ in terms of its eigenvalues μ_m and right and left eigenvectors $|m>$ and $<m|$ respectively and write

$$< [t^{*}]^{-N} > \quad = \quad \sum_{m=0}^{\infty} \mu_m(N)^{L}\, \mathbf{w}^{T}|N,m><m,N|\mathbf{w} \qquad (15)$$

We now notice that at N=0 $\mathbf{w}$ and $\mathbf{w}^{T}$ are left and right eigenvectors of $\mathbf{X}$ respectively with eigenvalue unity. If we label these eigenvectors and eigenvalue by m=0 we can write

$$\mathbf{w} \quad = \quad |N=0,m=0> \qquad (16)$$
$$\mathbf{w}^{T} \quad = \quad <m=0,N=0|$$
$$\mu_o(N=0) \quad = \quad 1$$

Using the properties of the eigenvalue spectrum of $\mathbf{X}$ in the interval around N=0 which are explained in Appendix II we find that at large L we have

$$<-\ln t^{*}> = \frac{d}{dN} \left[L\mu_o(N) + \mathbf{w}^{T}|N,0><0,N|\mathbf{w} \right] | \qquad (17)$$
$$|N=0$$

This completes the calculation of <-lnt>. Taking the limit L->∞ we obtain the localisation length and density of states from equation (14) with

$$\lim_{L\to\infty} \frac{\langle -\ln t^{*}\rangle}{L} = \frac{d}{dN}\,\mu_o(N)\,\Big|_{N=0} \qquad (18)$$

The development above is broadly in line with that of Kirkman and Pendry [1] but does differ in the detailed form of the **X** matrix. Here we have used a symmetric normalisation for the basis vectors of the symmetric subspace. This gives a complete block diagonalisation of **X** at positive integer N and a simpler form of equation (17).

We now extend the analysis of Kirkman and Pendry [1] so as to gain some insight into equation (18). We factorise the **X** matrix

$$\mathbf{X}(\mathbf{M},N) = M_{1,1}^{\,N}\,\mathbf{Z}(\mathbf{M},N) \qquad (19)$$

and expand the first factor to order N and obtain

$$\langle \mathbf{X}(M,N)\rangle = \langle \mathbf{Z}(M,N)\rangle + N\,\langle \ln M_{1,1}\,\mathbf{Z}(M,N)\rangle + O(N^2) \qquad (20)$$

If the eigenvalues of <Z> are non degenerate at N=0, which is nearly always the case in the presence of disorder we have

$$\mu_o(N) = \mu_o'(N) + N\,\langle \ln M_{1,1}\rangle + O(N^2) \qquad (21)$$

so that in the limit L->∞

$$\langle -\ln t_L^{*}\rangle \approx L\,\left[\,\langle -\ln t_1^{*}\rangle + \frac{d}{dN}\,\mu_o'(N)\,\Big|_{N=0}\,\right] \qquad (22)$$

where we have neglected the term which is independent of L in equation (17). We see that <-lnt> at length L splits into a sum of two parts, L times <-lnt> for a system of unit length and a correction term arising from the fact that in general the $\mathbf{M}_n$'s do not commute.

3. Application to the Anderson Model

3.1 The Anderson Model

The Hamiltonian **H** for the Anderson model in real space representation is tridiagonal with elements

$$H_{n,n} = \varepsilon_n$$
$$H_{n,n+1} = H_{n+1,n} = -V_n \qquad (23)$$

The corresponding wave function $\Phi(r)$ is

$$\Phi(r) = \sum_{n=-\infty}^{\infty} a_n \Phi_n(r-r_n) \qquad (24)$$

The Schrodinger equation gives us a recurrence relation for the a_n's

$$Ea_n = \varepsilon_n a_n - V_n a_{n+1} - V_{n-1} a_{n-1} \qquad (25)$$

The off diagonal elements V_n are assumed to be real and positive since they can be made so by a simple gauge transformation if they are not.

Physically the model corresponds to a simple tight binding model with nearest neighbour interactions. The wavefunction Φ_n is interpreted as an atomic or molecular orbital centred at the nth site, whose position is r_n. The total wavefunction $\Phi(r)$ is a linear combination of these with coefficients a_n.

The model is completely specified by giving distributions for the diagonal elements ε_n and off diagonal elements V_n which we now do. We suppose that we have a disordered system of length L ($1 \leq n \leq L$) embedded between two semi infinite ordered systems, or leads, ($n<1$ and $n>L$) so that

$$\varepsilon_n = \varepsilon \quad \text{with probability } p(\varepsilon) \text{ for } 1 \leq n \leq L \qquad (26)$$
$$= \langle\varepsilon\rangle \text{ with probability one for } n<1 \text{ and } n>L$$

and

$$V_n = V \quad \text{with probability } p(V) \text{ for } 1 \leq n \leq L \qquad (27)$$

$= 1$ with probability one for $n<1$ and $N>L$

It is implicit in (26) that the ε_n are uncorrelated for different n and similarly the V_n as regards (27). For convenience we choose the zero of energy so that $<\varepsilon>=0$ and the units of energy so that $<\ln(V)>=0$.

We can rewrite the recurrence relation for the coefficients a_n in terms of a real space transfer matrix $\mathbf{M}_n$ as

$$\begin{bmatrix} a_{n+1} \\ a_n \end{bmatrix} = \mathbf{M}_n(\text{r space}) \begin{bmatrix} a_n \\ a_{n-1} \end{bmatrix} \tag{28}$$

where

$$\mathbf{M}_n(\text{r space}) = \begin{bmatrix} (\varepsilon_n - E)/V_n & , & -V_{n-1}/V_n \\ 1 & , & 0 \end{bmatrix} \tag{29}$$

The real space transfer matrix for the disordered section is

$$\begin{bmatrix} a_{L+1} \\ a_L \end{bmatrix} = \mathbf{T}(\text{r space}) \cdot \begin{bmatrix} a_1 \\ a_0 \end{bmatrix} \tag{30}$$

and

$$\mathbf{T}(\text{r space}) = \prod_{n=1}^{L} \mathbf{M}_n(\text{r space}) \tag{31}$$

We now encounter a difficulty in that the $\mathbf{M}_n$'s are not independent since $\mathbf{M}_n$ and $\mathbf{M}_{n+1}$ both contain the variable V_n. We can however solve this problem by making a simple factorisation

$$\mathbf{M}_n = \begin{bmatrix} 1/V_n & , & 0 \\ 0 & , & 1 \end{bmatrix} \begin{bmatrix} \varepsilon_n - E & , & -1 \\ 1 & , & 0 \end{bmatrix} \begin{bmatrix} 1 & , & 0 \\ 0 & , & V_{n-1}/1 \end{bmatrix} \tag{32}$$

We can then re-define $\mathbf{M}_n$ as

$$\mathbf{M}_n = \begin{bmatrix} 1 & 0 \\ 0 & V_n \end{bmatrix} \begin{bmatrix} 1/V_n & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \varepsilon_n - E & -1 \\ 1 & 0 \end{bmatrix} \tag{33}$$

$$= \begin{bmatrix} (\varepsilon_n - E)/V_n & -1/V_n \\ V_n & 0 \end{bmatrix}$$

then the transfer matrix **T** for the disordered system is still given by (31) but now the $\mathbf{M}_n$'s are independent for different n.

The transfer matrix which describes the scattering of Bloch waves incident on the disordered region from the leads is derived as follows; For a given energy E the wavefunction in the ordered lead at the left of the disordered section will be a linear combination of the two Bloch waves for this energy, from which we see that for (n<1) we can write

$$a_n = a_+ \exp[ik(n-1)] + a_- \exp[-ik(n-1)] \tag{34}$$

Similarly for the lead at the right

$$a_n = b_+ \exp[ik(n-L-1)] + b_- \exp[-ik(n-L-1)] \tag{35}$$

The coefficients a_+, a_-, b_+ and b_- are related by a momentum space transfer matrix

$$\begin{bmatrix} b_+ \\ b_- \end{bmatrix} = \mathbf{T}(\text{k space}) \cdot \begin{bmatrix} a_+ \\ a_- \end{bmatrix} \tag{36}$$

This obtained from the real space transfer by a similarity transformation

$$\mathbf{T}(\text{k space}) = \mathbf{Q} \cdot \mathbf{T}(\text{r space}) \cdot \mathbf{Q}^{-1} \tag{37}$$

where

$$\mathbf{Q} = \frac{1}{2i\sin(k)} \begin{bmatrix} e^{ik} & -1 \\ -e^{-ik} & 1 \end{bmatrix} \tag{38}$$

and

$$\mathbf{Q}^{-1} = \begin{bmatrix} 1 & , & 1 \\ e^{-ik} & , & e^{ik} \end{bmatrix} \tag{39}$$

and the wave number k is related to the energy E by

$$E = -2\cos(k) \tag{40}$$

The momentum space form of $\mathbf{M}_n$ is obtained by exactly the same transformation

$$\mathbf{M}_n(\text{k space}) = \mathbf{Q} \cdot \mathbf{M}_n(\text{r space}) \cdot \mathbf{Q}^{-1} \tag{41}$$

however we omit it here for reasons of brevity.

We now evaluate <-lnt> by diagonalising <X(**M**,N)> first analytically using perturbation theory in the weak disorder limit and then numerically for strong disorder.

3.2 Weak Disorder Expansion for Off Diagonal Disorder

We restrict our attention in this section to weak off diagonal disorder where only the V's are random and ε_n for all n. We first define our expansion parameter δ

$$\ln(V_n) = \delta_n \tag{42}$$

Then

$$\begin{aligned} \langle\delta^2\rangle &= \text{var}[\ln(V)] \\ &= \langle(\ln V)^2\rangle - \langle\ln V\rangle^2 \end{aligned} \tag{43}$$

In the absence of disorder the eigevalues of <X(M,0)> are

$$\mu_n(0) = \exp[-2ikn] \tag{44}$$

If these are all distinct a simple application of non degenerate perturbation theory to order $\langle\delta^2\rangle$ gives

$$\lim_{L\to\infty} \frac{\langle -\ln t\rangle}{L} = \left[-ik + \frac{2\langle\delta^2\rangle}{(4 - E^2)} \right] \tag{45}$$

Separating out real and imaginary parts we obtain for the localisation length Lc

$$\frac{1}{Lc} = \frac{2var[\ln(V)]}{(4 - E^2)} \qquad (46)$$

and the ensemble average integrated density of states $\sigma(E)$

$$<\sigma(E)> = \frac{L}{\pi} k \qquad (47)$$

These can be compared with the results for diagonal disorder [3-4] which are of the same form

$$\frac{1}{Lc} = \frac{var(\varepsilon)}{2.(4 - E^2)} \qquad (48)$$

$$<\sigma(E)> = \frac{L}{\pi} k$$

It is clear from (43) that degeneracy in the zero order eigenvalues occurs at all rational k values. However there are corrections at order $<\delta^2>$ only when $k=\pi/2$ at the band centre. In the case of diagonal disorder this leads to the same form for Lc and $<\sigma(E)>$ but with an altered numerical factor for Lc [1] and [5]. For off diagonal disorder it is found that Lc [6-8] diverges at the band centre but that the electrons are localised due to fluctuations [9]. We discuss this case further in section 3.4.

3.3 Numerical Diagonalisation for Strong Disorder

When weak disorder expansions are not applicable we proceed by means of numerical calculation. We make an explicit choice of distribution $p(\mathbf{M})$ and evaluate the average in the **X** matrix definition by discrete summation. This allows exact calculation for discrete distributions but only approximate calculation for continuous distributions. In the results given below we use a discrete distribution for both ε and V

$$p(\varepsilon) = \frac{1}{m_\varepsilon} \sum_{n=1,m_\varepsilon} \delta[\varepsilon + W_\varepsilon \left(-\frac{1}{2} + \frac{(n-1)}{(m_\varepsilon - 1)} \right)] \qquad (49)$$

$$= \delta(\varepsilon) \quad \text{if } m_\varepsilon = 1$$

$$p(V) = \frac{1}{m_v} \sum_{n=1,m_v} \delta[\ln V + W_v \left(-\frac{1}{2} + \frac{(n-1)}{(m_v-1)} \right)]$$

$$= \delta(\ln V) \text{ if } m_v = 1$$

Both distributions are each characterised by two parameters W_ε and m_ε for the diagonal distribution and W_v and m_v for the off diagonal distribution. We use large values of both m_ε and m_v to give an approximation for continuous distributions of both variables.

Since the **X** matrix has infinite size we approximate it for numerical purposes by truncating it at a finite size. The eigenvalue μ_o is then obtained by numerical diagonalisation of the truncated matrix. The derivative at N=0 is then evaluated as

$$\frac{d}{dN} \mu_o(N) \Big|_{N=0} = \lim_{N \to 0} \frac{\mu_o(N) - \mu_o(0)}{N} \qquad (50)$$

This procedure requires that we check both for convergence against N and also truncation size.

We also give results below for the energy derivative of the ensemble average density of states (denoted in the figures simply as the density of states). This is estimated from numerical differentiation of $\langle\sigma(E)\rangle$

$$\frac{d \langle\sigma(E)\rangle}{dE} \Big|_{E=E_o} = \lim_{\delta E \to 0} \left[\frac{\langle\sigma(E_o+\delta E)\rangle - \langle\sigma(E_o-\delta E)\rangle}{2\delta E} \right] \qquad (51)$$

Naturally this requires that we check for convergence of the numerical derivative against δE.

Before discussing the results of these numerical calculations we make two further comments concerning the numerical implementation of the method. The first concerns the calculation of the X matrix elements. The most efficient way to do this is to rewrite equation (8)

$$X_{i,j} = \sum_{k=0}^{\min(i,j)} \sqrt{\left({}^{N-i}C_{j-k} \; {}^{N-j}C_{i-k} \; {}^{i}C_{k} \; {}^{j}C_{k} \right)}$$

$$\cdot \; T_{1,1}^{N} \; [T_{1,2}/T_{1,1}]^{j-k} \; [T_{2,1}/T_{1,1}]^{i-k} \; [T_{2,2}/T_{1,1}]^{k} \qquad (52)$$

In this form the largest power of any matrix element or combination of matrix elements which needs to be evaluated is equal the truncation size. This is as opposed to twice the truncation size in the previous form (8). Nevertheless for large truncation sizes (>50) this, together with the summations over k and the disorder distribution, can lead to numerical inaccuracy in the matrix elements and hence in μ_o. Fortunately the truncation sizes which are needed to obtain convergence are in all but exceptional cases smaller than this.

The second point concerns the transformation to the momentum space representation of the transfer matrix (41). This transformation is singular at the band edge (E=+/-2) and again leads to numerical problems near this energy. This is easily overcome however by employing a complex energy shift Ec in the definition of the transformation matrix **Q**

$$\mathbf{M}_n(\mathbf{k}\text{ space}) = \mathbf{Q}(E+iEc)\ .\ \mathbf{M}_n(E|\mathbf{r}\text{ space})\ .\ \mathbf{Q}^{-1}(E+iEc) \qquad (53)$$

It is important to notice here that we retain a real energy in the definition of $\mathbf{M}_n$ and we have found that results for the localisation length and the ensemble averaged integrated density of states are insensitive to this parameter. We now proceed to the discussion of the results of these calculations.

In figures 2.1 and 2.2 we present a calculation of the inverse localisation length 1/Lc and the energy derivative of the ensemble average integrated density of states for diagonal disorder (W_ε=1 m_ε=21 W_v=0 m_v=1), off diagonal disorder (W_ε=0 m_ε=1 W_v=1 m_v=21) and a mixed disorder case (W_ε=1 m_ε=21 W_v=1 m_v=21.) We find qualitatively the same behaviour in all three cases. The localisation length is finite across the band indicating that all states are localised. The exception to this is off diagonal disorder at the band centre where the localisation length diverges. The singularities in the density of states at the band edges (E=+/-2) of the ordered system are removed by disorder and the band width widened in all cases.

In figures 2.3 and 2.4 we compare the disorder dependence of the inverse localisation length for off diagonal disorder

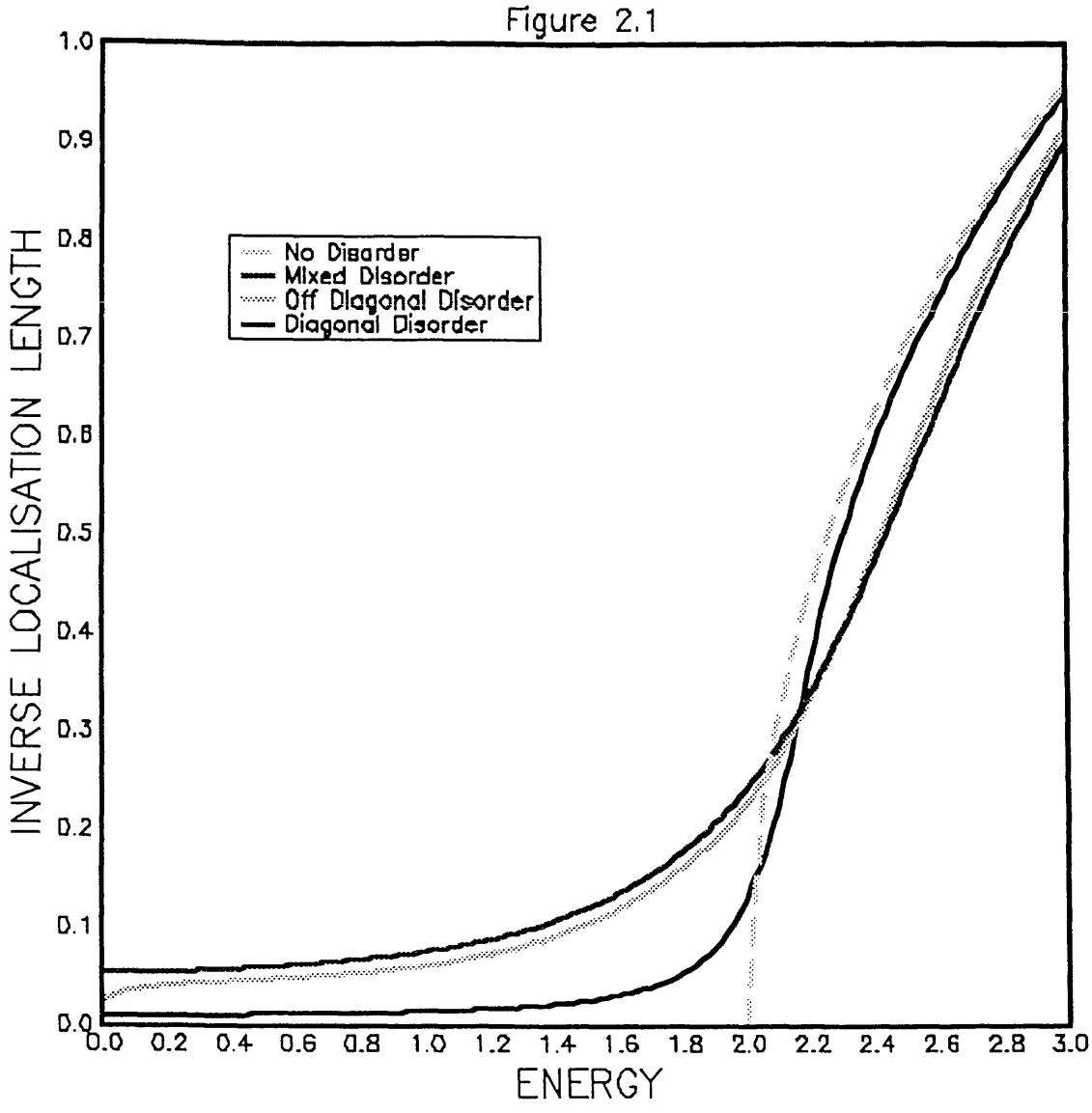


Figure 2.1 - Comparison of the energy dependence of the inverse of the localisation length for different types of disorder: diagonal disorder (W_ε=1 m_ε=21 W_v=0 m_v=0), off diagonal disorder (W_ε=0 m_ε=1 W_v=1 m_v=21) and a mixed disorder case (W_ε=1 m_ε=21 W_v=1 m_v=21.) We also plot the inverse of the localisation length in the absence of disorder.

Figure 2.2

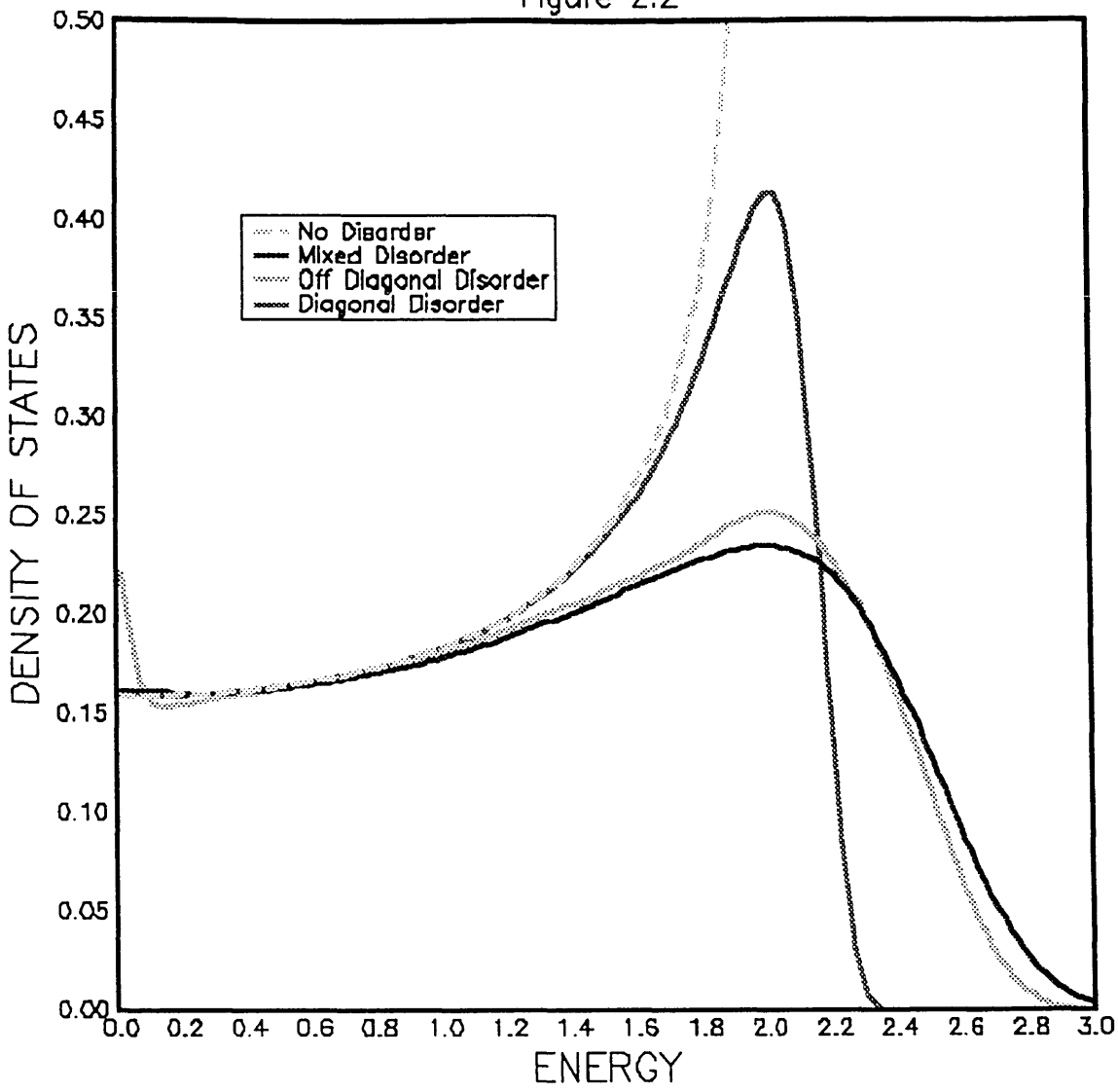


Figure 2.2 - Comparison of the energy dependence of the density of states for different types of disorder: diagonal disorder (W_ε=1 m_ε=21 W_v=0 m_v=0), off diagonal disorder (W_ε=0 m_ε=1 W_v=1 m_v=21) and a mixed disorder case (W_ε=1 m_ε=21 W_v=1 m_v=21.) We also plot the density of states in the absence of disorder.

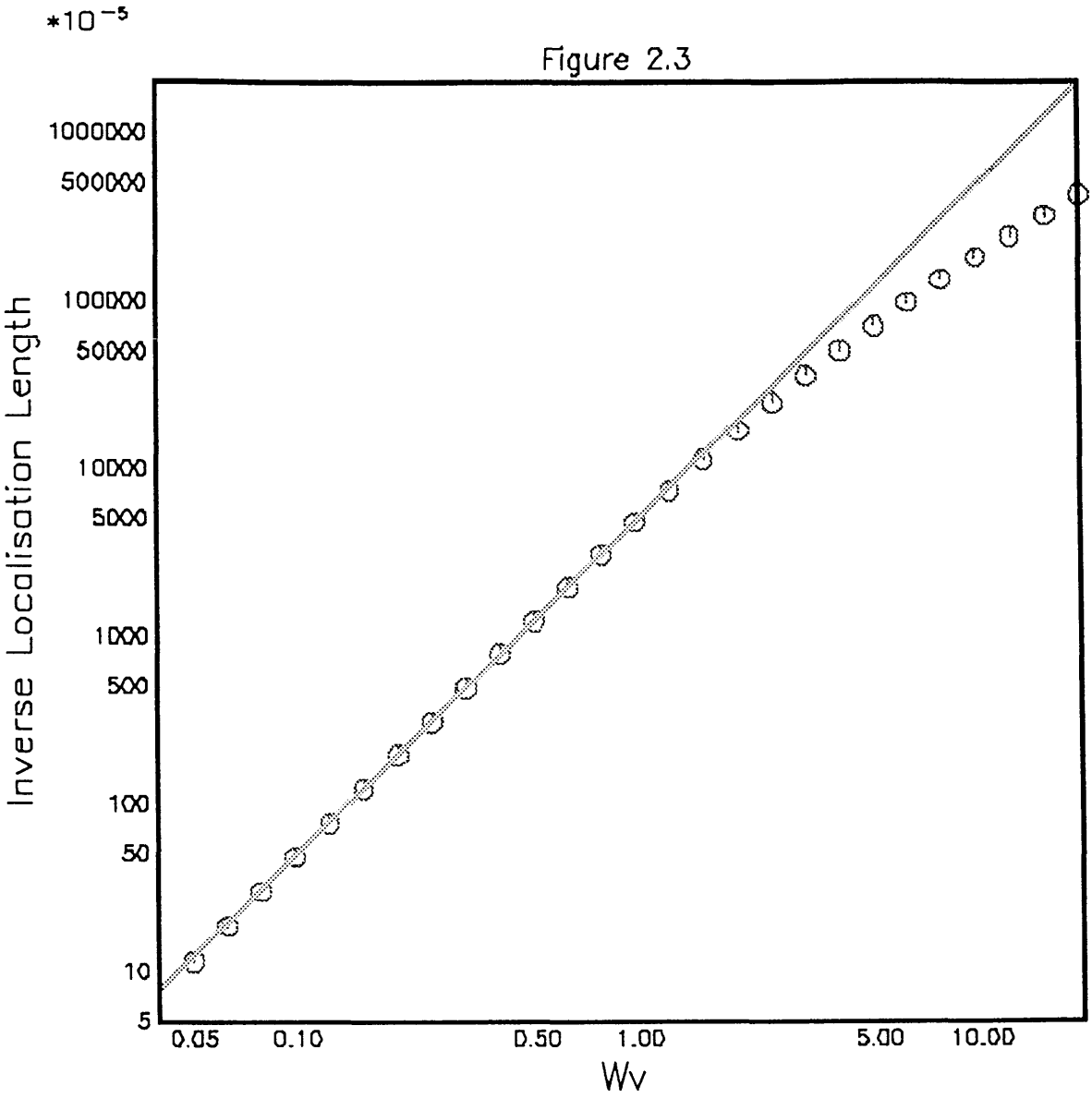


Figure 2.3 - Disorder dependence of the inverse of the localisation length for off diagonal disorder (W_ε=0 m_ε=1 m_v=21) at energy E=0.5. The solid line is the weak disorder expansion result and the symbols are the results of numerical diagonalisation of <**X**>.

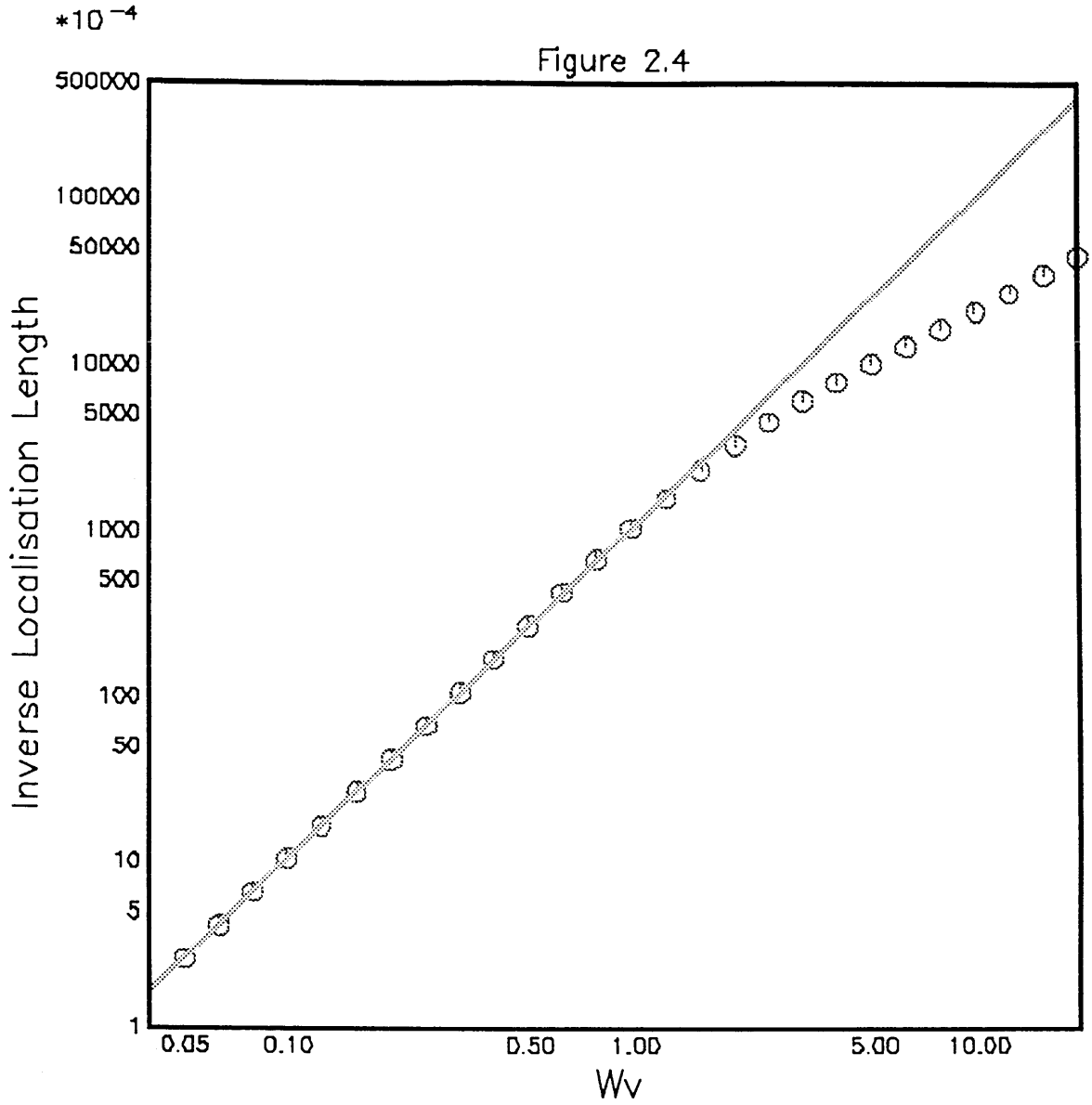


Figure 2.4 - Disorder dependence of the inverse of the localisation length for off diagonal disorder (W_ε=0 m_ε=1 m_v=21) at energy E=1.5. The solid line is the weak disorder expansion result and the symbols are the results of numerical diagonalisation of <**X**>.

obtained using the numerical implementation with that obtained from the weak disorder expansion of section 3.2. The variance of ln(V) for the distribution of p(V) given in (49) is easily shown to be

$$\text{var}[\ln(V)] = W_v^2 \left(\frac{1}{12} + \frac{1}{6(m_v-1)} \right) \qquad (54)$$

For the two energies shown (E=0.5 and E=1.5) we obtain an accurate fit to the perturbation result for $W_v<1$ with deviations at higher disorder as expected.

In figure 2.5 we examine the disorder dependence of the inverse localisation length at the band edge (of the ordered system) where the weak disorder expansion is not applicable. For small W_v we find from the numerical data that

$$\frac{1}{Lc} \approx W_v^{2/3} \qquad W_v \to 0 \qquad (55)$$

This is the same behaviour as found for diagonal disorder at the band edge by Derrida and Gardner [10]

$$\frac{1}{Lc} \approx W_e^{2/3} \qquad W_\varepsilon \to 0 \qquad (56)$$

3.4 Band Centre Anomaly for Off Diagonal Disorder

The divergence of the localisation length and density of states has been discussed by a number of authors [6-9] and the form of the divergences found to be

$$\frac{1}{Lc} = \frac{\text{var}[\ln(V)]}{2|\ln E^2|} \qquad (57)$$

$$\frac{d}{dE}\langle\sigma(E)\rangle = \frac{2\text{var}[\ln(V)]}{|E\ln E^2|}$$

These are generalisations of Dysons results for chains of harmonic oscillators [11]. In figure 2.6 and 2.7 we show that the presence of diagonal disorder destroys the divergence in both quantities

It is interesting to note that despite the fact that $Lc \to \infty$ the state at the band centre is still localised. A simple application of the central limit theorem [9] shows that

$$a_{2L} = a_0 \cdot \exp[\, y\sqrt{(2L)} + i\pi L] \qquad (58)$$

where y is a random variable which fluctuates with L but has an asymptotic distribution in the limit $L \to \infty$ which is independent of L

$$p(y) \to \frac{1}{\sqrt{[2\pi \mathrm{var}(\ln V)]}} \exp[\, -y^2/2\mathrm{var}(\ln V)\,] \qquad (59)$$

From this we deduce that the eigenstates of the disordered system are localised as $\exp[-\sqrt{r}]$ as opposed to $\exp[-r]$ for other energies.

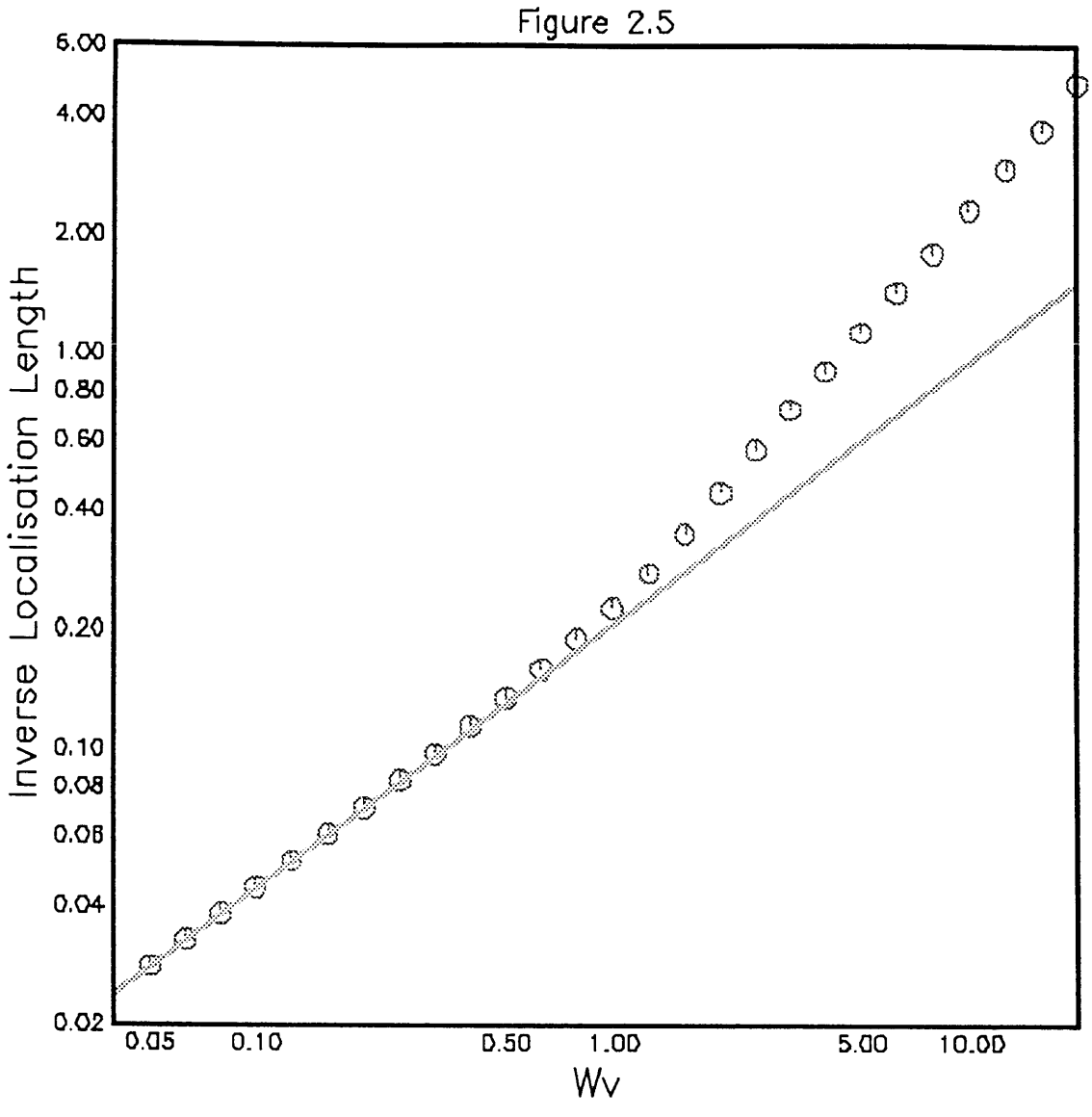


Figure 2.5 - Disorder dependence of the inverse of the localisation length for off diagonal disorder (W_ε=0 m_ε=1 m_v=21) at the band edge of the ordered system E=2.0. The symbols are the results of numerical diagonalisation of **<X>**. The solid line is a fit to the data for small W_v. The exponent of the disorder dependence is 2/3 (see equation 55.)

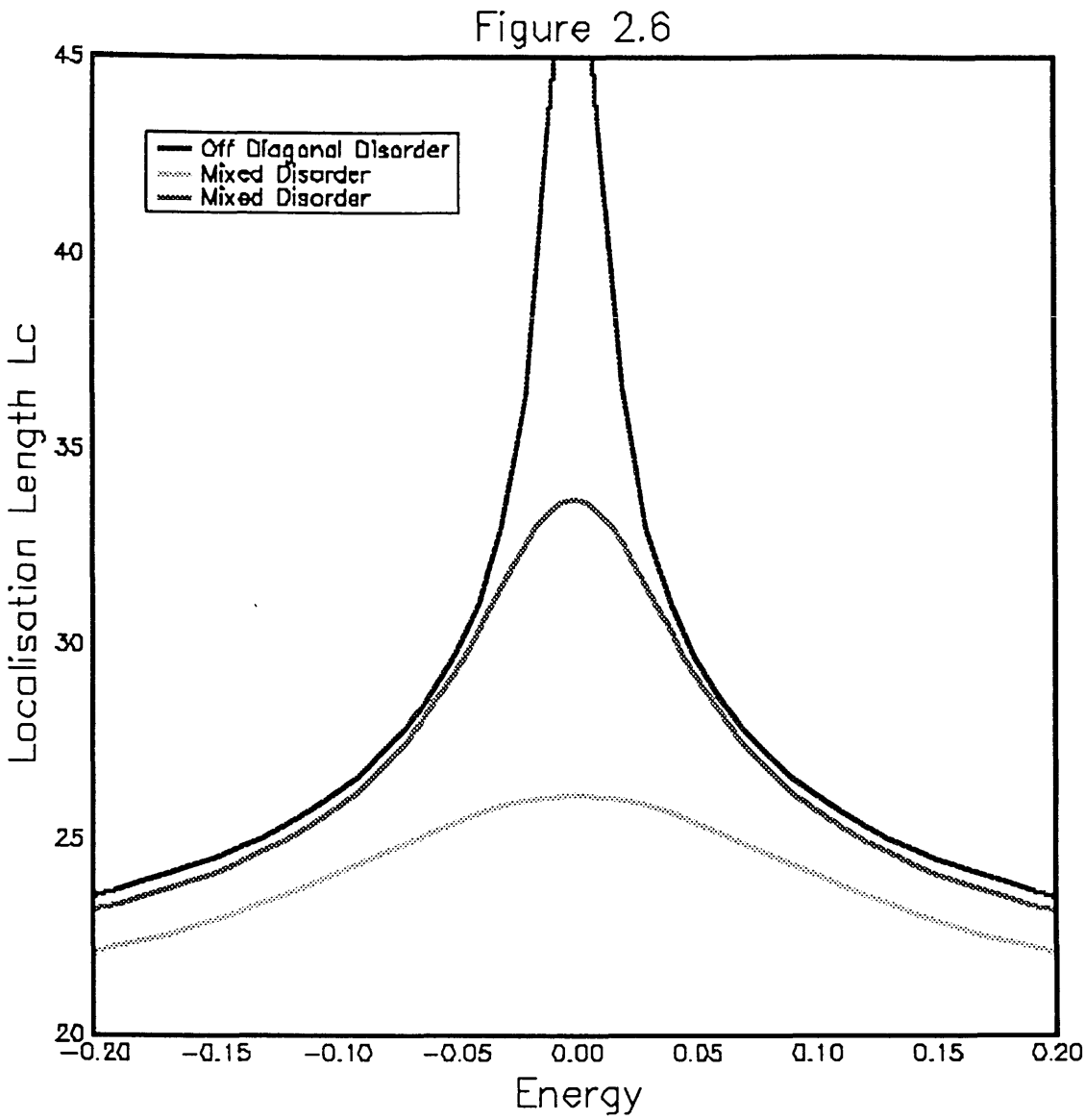


Figure 2.6 - The divergence of the localisation length at the band centre for off diagonal disorder (W_v=1 m_v=21 W_ε=0 m_ε=1.) The divergence disappears as diagonal disorder is introduced (W_ε=0.25 and 0.5 m_ε=21.)

Figure 2.7

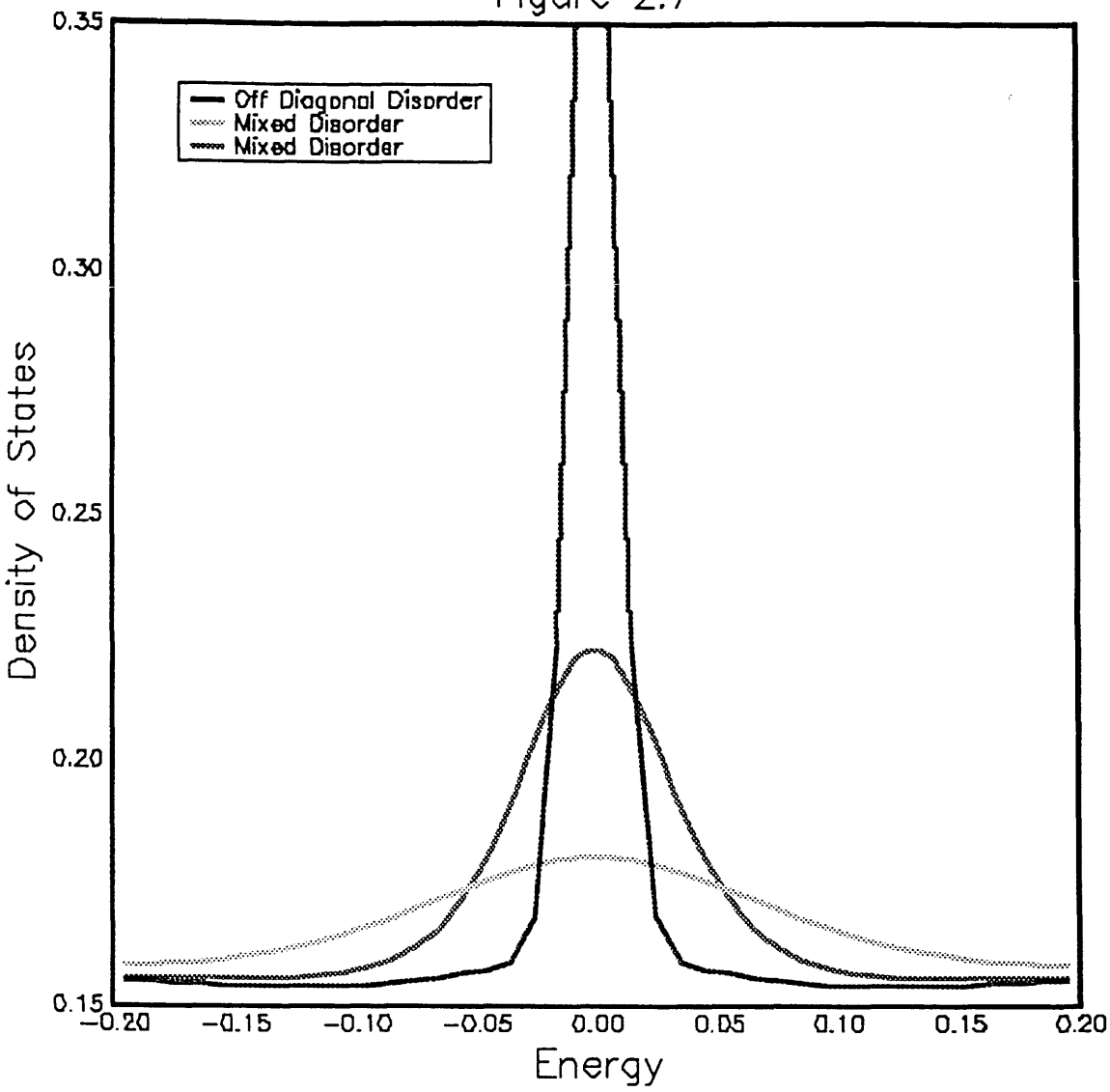


Figure 2.7 - The divergence of the density of states at the band centre for off diagonal disorder (W_v=1 m_v=21 W_ε=0 m_ε=1.) The divergence disappears as diagonal disorder is introduced (W_ε=0.25 and 0.5 m_ε=21.)

Appendix I - The One Dimensional Transfer Matrix

Here we give a brief derivation of the general form of the one dimensional transfer matrix in terms of transmission and reflections coefficients.

We represent a one dimensional scatterer as a rectangular box and we suppose that we have input and output wave amplitudes a_+ and a_- respectively at the left of the scatterer. Similarly at the right we have input and output wave amplitudes b_- and b_+ respectively.

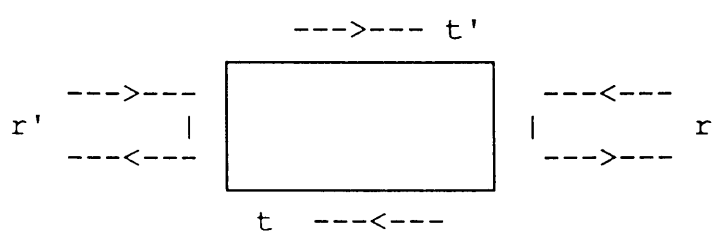
(1)

Here the labels + and - refer to the direction of propagation of the waves. We define the transmission coefficients t and t' and reflection coefficients r and r' by the relations

$$b_+ = t'a_+ + r\,b_- \qquad (2)$$

$$a_- = t\,b_- + r'a_+$$

Diagrammatically we represent these coefficients by



(3)

so as to make their meaning clearer. The transfer matrix **T** for this system is defined by

$$\begin{bmatrix} b_+ \\ b_- \end{bmatrix} = \mathbf{T} \cdot \begin{bmatrix} a_+ \\ a_- \end{bmatrix} \qquad (4)$$

If we rearrange equation (2) we obtain **T** explicitly as

$$\mathbf{T} = \begin{bmatrix} t'-r'r/t & , & r/t \\ -r'/t & , & 1/t \end{bmatrix} \tag{5}$$

This form can be simplified if the system has time reversal symmetry. This symmetry implies that if we have the relation (4) then we must also have the relation[3]

$$\begin{bmatrix} b_-^* \\ b_+^* \end{bmatrix} = \mathbf{T} \begin{bmatrix} a_-^* \\ a_+^* \end{bmatrix} \tag{6}$$

This and (4) imply that

$$\mathbf{T}^* = \mathbf{U}\,\mathbf{T}\,\mathbf{U} \tag{7}$$

where

$$\mathbf{U} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \tag{8}$$

This gives a relation between the elements of the transfer matrix

$$\begin{aligned} T_{1,1} &= T_{2,2}^* \\ T_{1,2} &= T_{2,1}^* \end{aligned} \tag{9}$$

We can now write the transfer matrix as

$$\mathbf{T} = \begin{bmatrix} 1/t^* & r/t \\ [r/t]^* & 1/t \end{bmatrix} \tag{10}$$

---

[3]We are assuming here that the directions of propagation + and - are interchanged by the time reversal operation. This will be true for propagating waves but not for evanescent waves.

The fundamental theorem of scattering theory that the scattering matrix **S** defined by

$$\begin{bmatrix} b_+ \\ a_- \end{bmatrix} = \mathbf{S} \cdot \begin{bmatrix} a_+ \\ b_- \end{bmatrix} = \begin{bmatrix} t' & r \\ r' & t \end{bmatrix} \begin{bmatrix} a_+ \\ b_- \end{bmatrix} \qquad (11)$$

is unitary implies the relation

$$|t^2| + |r^2| = 1 \qquad (12)$$

This is interpreted as a conservation rule for flux and also has the consequence that the determinant of the transfer matrix is unity and hence that it is symplectic.

Appendix II - The Eigenvalue Spectrum of the X Matrix

In the main text we derive the general expression

$$< [t^*]^{-N} > = \sum_{m=0}^{\infty} \mu_m(N)^L <0,0|N,m><m,N|0,0> \qquad (1)$$

The simplification of this expression for large L (equation (17) of the main text) is based on the properties of the eigenvalue spectrum in the interval around N=0 which we now discuss in detail.

On physical grounds we must have

$$0 \leq |t| \leq 1 \qquad (2)$$

which places a strict bound on the average (1) when N<0. This implies that

$$|\mu_m(N)| \leq 1 \qquad (3)$$

when N<0. At N=0 the block diagonal structure ensures that

$$\mu_0 = 1 \qquad (4)$$

regardless of disorder. When N>0 we expect the average to diverge if the system is localised and therefore we expect we will have at least one eigenvalue outside the unit circle.

Stronger conditions on the eigenvalue spectrum than (3) and (4) require a knowledge of the probability distribution $p(\mathbf{M})$. The results presented in the main text concern the Anderson model and we shall confine further discussion to this case. In the absence of disorder at N=0 we have

$$\mu_m = \exp(-2ikm) \qquad (5)$$

When disorder is introduced we can estimate the new eigenvalues using perturbation theory. As a representative example we consider weak diagonal disorder. If the eigenvalues (5) are non degenerate we find

$$\mu_m = \exp(-2ikm)\ [\ 1 - \frac{m^2 var(\varepsilon)}{4 - E^2}\ ] \qquad (6)$$

This should be accurate for small m but clearly breaks down for large m. For the eigenvalues for which (6) is accurate we have

$$|\mu_m| < 1 \qquad m \geq 1 \qquad (7)$$

To see what happens to the higher eigenvalues we diagonalise **X** numerically. This requires that we truncate **X** at a finite size, which provides good estimates of the eigenvalues of the infinite **X** matrix for m less than the truncation size but bad estimates for m close to the truncation size. In figure 2.8 we plot the eigenvalue spectrum at N=0 for a typical case with a truncation size of 40. It is quite clear that condition (7) is satisfied and that at N=0 we have μ_0=1 and

$$\mu_m < 1 \qquad m \geq 1 \qquad (8)$$

These conditions imply that for large L the m=0 term will dominate the sum in equation (1). We can estimate the order of magnitude of the largest correction term (m=1) using the perturbation expression (6), we find

$$[\mu_1/\mu_0]^L \approx \exp(-L/Lc) \qquad (9)$$

where we have used the weak disorder result for the localisation length Lc (equation (48) of the main text.) For L>>Lc and N near zero equation (1) is now easily simplified by neglecting terms above m=0

$$< [t^*]^{-N} > = \mu_0(N)^L \ <0,0|N,0><0,N|0,0> \qquad (10)$$

In figure 2.8 we also check that the spectrum satisfies condition (8) for the range of N necessary to calculate the derivative at N=0 and obtain the localisation length Lc

$$\frac{1}{Lc} = Re\ [\ \frac{d}{dN}\ \mu_0(N)\ |_{N=0}\ ] \qquad (11)$$

In figures 2.9-10 we test expression (11) for a typical case by a comparison with the results of a Monte-Carlo simulation.

Figure 2.8

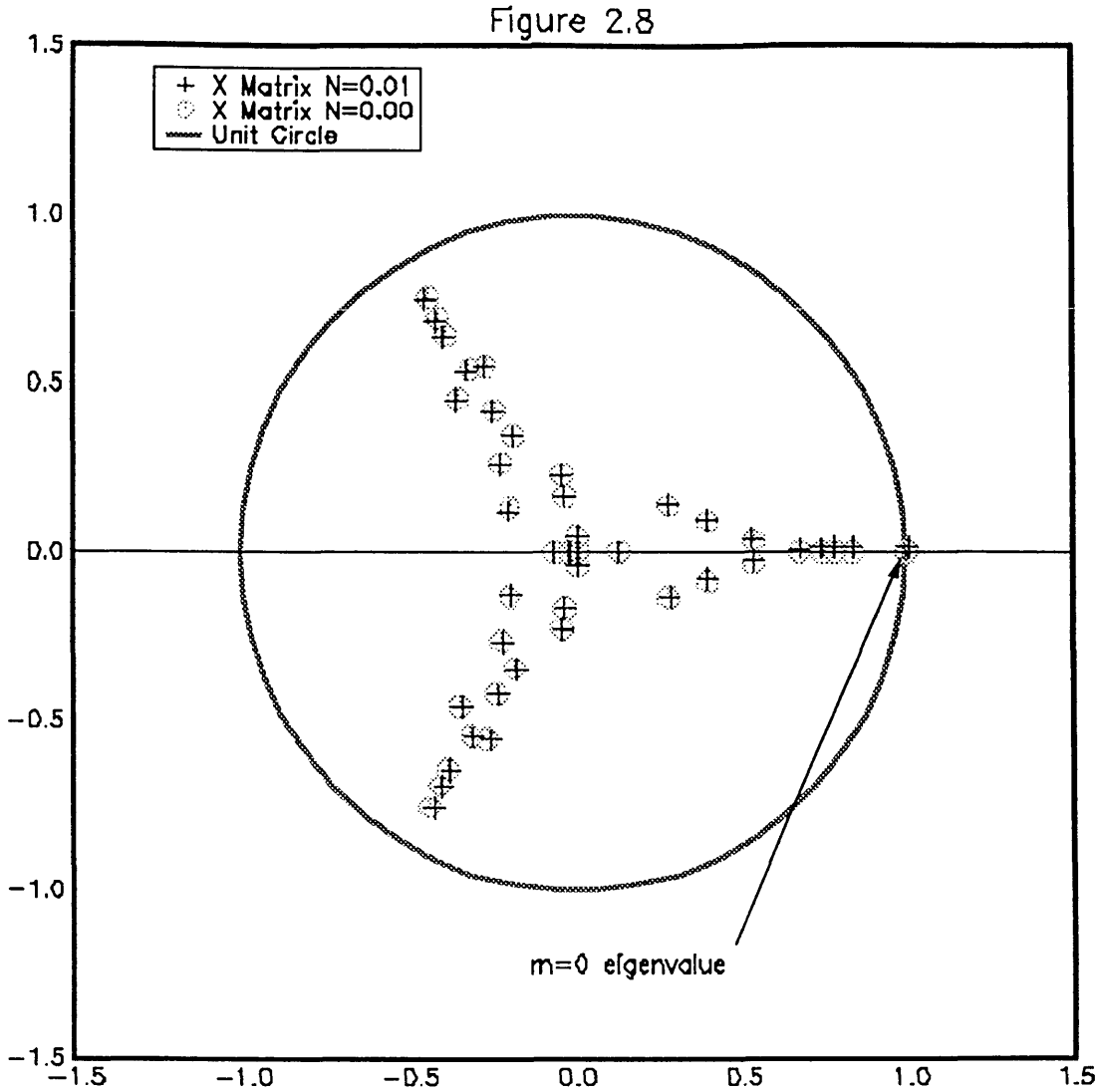


Figure 2.8 - The eigenvalue spectrum of the **X**(N) matrix for the Anderson model with W_ε=2 m_ε=2 W_v=0 m_v=1. The **X** matrix is truncated at size 40.

Figure 2.9

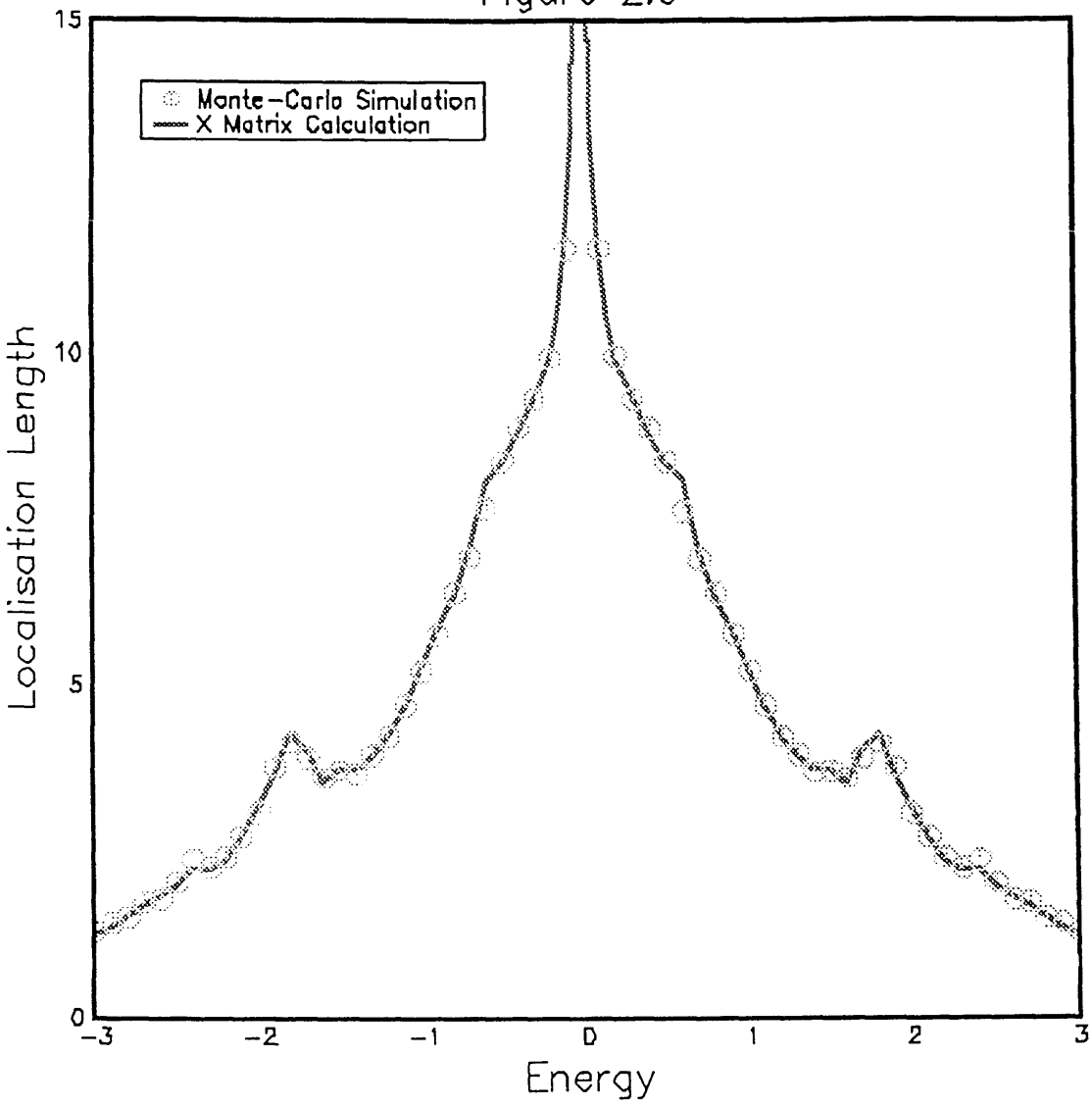


Figure 2.9 - Energy dependence of the localisation length for the Anderson model with $W_\varepsilon=0$ $m_\varepsilon=1$ $W_v=1$ $m_v=2$. The figure compares the results of a Monte-Carlo simulation with the results obtained using expression (11) of Appendix II.

Figure 2.10

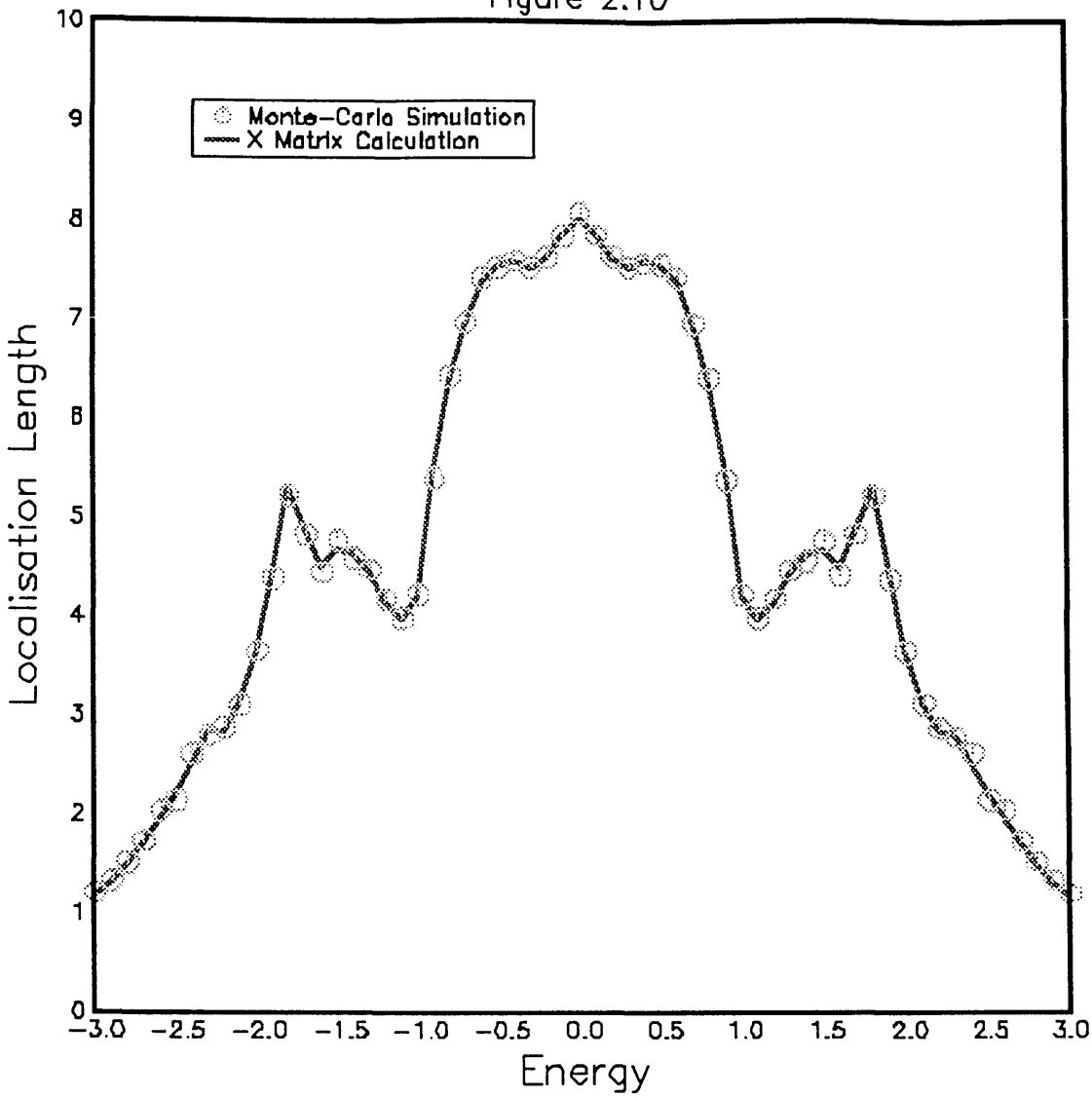


Figure 2.10 - The energy dependence of the localisation length for the Anderson model with $W_\varepsilon=2$ $m_\varepsilon=2$ $W_v=0$ $m_v=1$. The figure compares the results of a Monte-Carlo simulation with the results obtained using expression (11) of Appendix II.

References

[1] Kirkman P D and Pendry J B Journal of Physics:C 17 4327 (1984)

[2] "Group Theory in Physics" Cornwell J F (Academic Press London 1984) Chapt. 16 Vol. 2

[3] Anderson P W Physical Review 109 1492 (1958)

[4] Thouless D J in "Ill Condensed Matter" editor Balian R (1979)

[5] Kappus M and Wegner F Z. Phys. B 45 15 (1981)

[6] Theodorou G and Cohen M H Phys. Rev. B 13 4597 (1976)

[7] Eggarter T P and Riedinger R Phys. Rev. B 18 569 (1978)

[8] Ziman T A L Phys. Rev. Lett. 49 337 (1982)

[9] Fleishman L and Licciardello D C Journal of Physics:C 10 L125 (1977)

[10] Derrida B and Gardener E J. Physique 45 1283 (1984)

[11] Dyson F J Physical Review 92 1331 (1953)

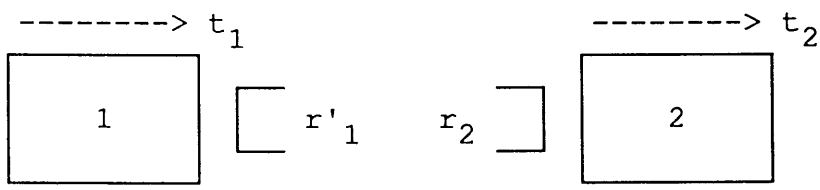
Chapter III - Generalised Transfer Matrices and the Scaling of Distributions in One Dimensional Systems.

1. Introduction

In Chapter II we introduced the generalised transfer matrix method and applied it to obtain a general expression for $<-\ln t>$. In this chapter we are interested in a more comprehensive description of the statistics than is afforded by a knowledge of the mean alone. In particular we are interested here to obtain the asymptotic distributions of $-\ln|t|^2$ and Θ, where Θ is the phase of t, in the large system size limit and to determine whether the distributions can be parameterised by a small number of independent variables.

This problem has been of interest to a number of authors, widespread interest in the problem being aroused after the proposal of the scaling theory of localisation [1]. In an attempt to provide rigorous backing to the scaling theory the scaling of distributions for one dimensional systems have been studied in detail [2-9]. We begin by outlining the approach presented by Anderson, Thouless, Abrahams and Fisher in their influential paper [2].

We consider the composition of two scatterers.



We then ask what the transmission coefficient $t_{[1+2]}$ of the combined system will be in terms of the transmission and reflection coefficients of the the two sub units. By considering the multiple scattering between the units we find easily that

$$t_{[1+2]} = t_1 t_2 + t_1 r_2 r'_1 t_2 + t_1 (r_2 r'_1)^2 t_2 + \ldots.$$

$$= \frac{t_1 t_2}{1 - r_2 r'_1} \qquad (1)$$

This can be rewritten as a resistance composition law

$$R_{[1+2]} = R_1 + R_2 + 2R_1R_2 - 2\sqrt{[R_1R_2(1+R_1)(1+R_2)]}\cos(\phi) \qquad (2)$$

where ϕ is the phase of $r_2 r'_1$ by using the Landauer formula [10] to relate the dimensionless resistance R to the scattering properties

$$R = \frac{|r|^2}{|t|^2} \qquad (3)$$

If we now consider the composition of L scatterers chosen at random from some given distribution, the question arises as to what the distribution of $R_{[L]}$ will be where

$$R_{[L]} = R_{[1+2+ \ldots\ldots +L]} \qquad (4)$$

In particular we can ask whether the distribution of $R_{[L]}$ tends to a well behaved limiting form as $L \to \infty$. Under the assumption that

$$p(\phi) = \frac{1}{2\pi} \qquad \phi \text{ in } [0, 2\pi] \qquad (5)$$

it is shown in reference [2] that the variance of $\ln(1+R_{[L]})$ approaches a linear behaviour as $L \to \infty$ showing that the corresponding distribution is well behaved in that limit. A rigorous and detailed treatment of this "random phase" model has been presented by Mello [3]. In this work the problem is recast in terms of transfer matrices. We have

$$\mathbf{T}_L = \prod_{n=1}^{L} \mathbf{M}_n \qquad (6)$$

where each M_n is parameterised as $\mathbf{M}_n \equiv \mathbf{M}_n(R_n, v_n, \mu_n)$ with the explicit form

$$\mathbf{M}_n \equiv \begin{bmatrix} e^{-iv_n} & 0 \\ 0 & e^{iv_n} \end{bmatrix} \begin{bmatrix} \sqrt{(1+R_n)} & \sqrt{R_n} \\ \sqrt{R_n} & \sqrt{(1+R_n)} \end{bmatrix} \begin{bmatrix} e^{-i\mu_n} & 0 \\ 0 & e^{i\mu_n} \end{bmatrix} \qquad (7)$$

and similarly $\mathbf{T}_L \equiv T(R_{[L]}, v_{[L]}, \mu_{[L]})$. Under the assumption that $p(M) \equiv p(R)$ (which is equivalent to the random phase assumption (5)) Mello is able to prove that

- $p(T_{[L]}) \equiv p(R_{[L]})$
- $\ln(1+R_{[L]})$ is normally distributed in the limit that $L \to \infty$

In reference [3] exact analytic expressions for the both the mean and variance of the asymptotic distribution in terms of the starting distribution $p(R)$ are obtained.

The above results for the random phase model are extremely informative however it is important to examine the random phase assumption carefully. There are two main objections to this assumption, the first is that the phases μ_n and v_n will surely be correlated with R_n. The second objection is that the assumption of a uniform phase distribution implies that the integrated density of states is independent of energy which seems unphysical.

The main purpose of the work in this chapter is to show that the random phase assumption can be abandoned. In particular we study the Anderson model (explained in Chapter II and not to be confused with the random phase model above) which contains explicit correlations between the phases μ and v and the resistance R. We find in the limit that $L \to \infty$ that both the variables $-\ln|t|^2$ and Θ are normally distributed. The basis of our approach is to obtain a general expression for the statistical cumulants of both variables from which the distributions can be deduced.

2. A General Expression for the Cumulants

In this section we obtain a general expression for the statistical cumulants of $-\ln|t|^2$ and Θ where $t=|t|\exp(i\Theta)$ is the transmission coefficient for waves travelling through a one dimensional disordered material and from this deduce the

asymptotic form of the distributions of both quantities. As in Chapter II we characterise the scattering of the system by a transfer matrix **T** which relates incident and reflected wave amplitudes at the left (a_+ and a_- respectively) to those at the right (b_+ and b_-) of the system.

$$\begin{bmatrix} b_+ \\ b_- \end{bmatrix} = \mathbf{T} \cdot \begin{bmatrix} a_+ \\ a_- \end{bmatrix} \tag{8}$$

The transfer matrix **T** is a product of transfer matrices

$$\mathbf{T} = \prod_{n=1}^{L} \mathbf{M}_n \tag{9}$$

where $\mathbf{M}_n$ n=1,..,L are independent random matrices with some probability distribution p(**M**). It was shown in chapter II that if the system is time reversal symmetric then **T** has the explicit form

$$\mathbf{T} = \begin{bmatrix} 1/t^* & (r/t) \\ (r/t)^* & 1/t \end{bmatrix} \tag{10}$$

where t and r are the amplitude transmission and reflection coefficients respectively (see Appendix I of Chapter II for the exact definition of t and r.)

As in chapter II the first step is to write for positive integer N

$$[t^*]^{-N} = [1,0] \otimes .. [1,0]\ \mathbf{T} \otimes .. \mathbf{T} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes .. \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{11}$$

where each direct product is taken N times and

$$\mathbf{T} \otimes .. \mathbf{T} = \prod_{n=1}^{L} \mathbf{M}_n \otimes .. \mathbf{M}_n \tag{12}$$

We recall from chapter II that expressions (11) and (12) can be simplified using the permutation symmetry of the direct product, and after doing so we obtain

$$[t^*]^{-N} = \mathbf{w} \cdot \mathbf{X}(\mathbf{T},N) \cdot \mathbf{w}^T \tag{13}$$

where $\mathbf{X}(\mathbf{T},N)$ is an (N+1)x(N+1) matrix with elements

$$X_{i,j} = \sum_{k=0}^{\min(i,j)} \sqrt{\left({}^{N-i}C_{j-k}\ {}^{N-j}C_{i-k}\ {}^{i}C_{k}\ {}^{j}C_{k} \right)} \cdot T_{1,1}^{N-i-j+k}\ T_{1,2}^{j-k}\ T_{2,1}^{i-k}\ T_{2,2}^{k} \qquad (14)$$

with $0 \leq i,j \leq N$. In equation (13) $\mathbf{w}$ is the N+1 component vector [1,0,...,0] and $\mathbf{w}^T$ is the transpose of $\mathbf{w}$. The $\mathbf{X}$ matrix has the usual multiplicative property of a transfer matrix

$$\mathbf{X}(\mathbf{T},N) = \prod_{n=1}^{L} \mathbf{X}(\mathbf{M}_n,N) \qquad (15)$$

By taking a further direct product and averaging over $p(\mathbf{M})$ we obtain

$$\langle |t|^{-2N} \rangle = [\mathbf{w} \otimes \mathbf{w}] \cdot \langle \mathbf{X}(\mathbf{M},N) \otimes \mathbf{X}(\mathbf{M}^*,N) \rangle^L \cdot [\mathbf{w}^T \otimes \mathbf{w}^T] \qquad (16)$$

where $\mathbf{M}^*$ is the complex conjugate (not the hermitian conjugate) of $\mathbf{M}$.

We analytically continue in N by generalising the definition of the $\mathbf{X}$ matrix as explained in Chapter II, which allows us to obtain the cumulants of the distribution of $-\ln|t|^2$

$$c_n(-\ln|t|^2) = \frac{d^n}{dN^n} \ln \langle |t|^{-2N} \rangle \Big|_{N=0} \qquad (17)$$

where c_n is the nth cumulant and we have made use of the Taylor expansion of the cumulant generating function

$$\ln\langle |t|^{-2N} \rangle = \sum_{n=0}^{\infty} N^n/n!\ c_n(-\ln|t|^2) \qquad (18)$$

In the limit that $L \to \infty$ a more explicit expression for the cumulants can be obtained. We first express $\langle \mathbf{X} \otimes \mathbf{X} \rangle$ in terms of its eigenvalues μ_m and right and left eigenvectors $|m\rangle$ and $\langle m|$ respectively as

$$\langle \mathbf{X}(\mathbf{M},N) \otimes \mathbf{X}(\mathbf{M}^*,N) \rangle = \sum_{m=0}^{\infty} \mu_m(N)^L\ |N,m\rangle\langle m,N| \qquad (19)$$

Then

$$\langle |t|^{-2N} \rangle = \sum_{m=0}^{\infty} \mu_m(N)^L \, g(N,m) \tag{20}$$

with

$$g(N,m) = \mathbf{w} \otimes \mathbf{w} \; |N,m\rangle\langle m,N| \; \mathbf{w}^T \otimes \mathbf{w}^T \tag{21}$$

We need now to consider what form the eigenvalue spectrum takes. For N<0 we have strict bounds on the average

$$0 \leq \langle |t|^{-2N} \rangle \leq 1 \tag{22}$$

this implies that $|\mu_m(N)| \leq 1$ for all m. At N=0 it is easy to show that $\mathbf{w} \otimes \mathbf{w}$ and $\mathbf{w}^T \otimes \mathbf{w}^T$ are eigenvectors of $\langle \mathbf{X} \otimes \mathbf{X} \rangle$ with eigenvalue unity. We label these by m=0

$$\mu_{m=0}(N=0) = 1 \tag{23}$$

$$|N=0,m=0\rangle = \mathbf{w}^T \otimes \mathbf{w}^T$$

$$\langle m=0,N=0| = \mathbf{w} \otimes \mathbf{w}$$

When N>0 we find with some exceptions[1] that for N>0

$$| \mu_0(N) | > 1 \tag{24}$$

and

$$| \mu_m(N) | < 1 \tag{25}$$

With these properties of the eigenvalue spectrum we find to a good approximation in the large L limit that

$$\langle |t|^{-2N} \rangle = \mu_0(N)^L \, g(N,0) \tag{26}$$

With the aid of (17) we can now obtain the cumulants

$$c_n(-\ln|t|^2) = \frac{d^n}{dN^n}[\, L \ln \mu_0(N) + \ln g(N,0) \,] \, \Big|_{N=0} \tag{27}$$

---

[1]The exceptions correspond to Bloch states in the absence of disorder or special cases such as the band centre of a system with pure off-diagonal disorder.

This result should hold provided that the distribution **p(M)** is not such that for example the eigenvalue spectrum of the operator is continuous with a spectrum limit on $\mu_0(N)$.

The most important feature of (27) is that all cumulants depend linearly on L in the limit L->∞. This allows a simple form for the asymptotic distribution of $-\ln|t|^2$ to be deduced. In the interest of brevity we make a small change of notation and set

$$z \equiv -\ln|t|^2 \tag{28}$$

so that

$$\langle |t|^{-2i\alpha} \rangle = \langle \exp(i\alpha z) \rangle \tag{29}$$
$$= \int_{-\infty}^{+\infty} p(z)\, \exp(i\alpha z)\, dz$$

After inversion of the fourier transform and a trivial transformation of integration variable we arrive at

$$p(z) = \frac{1}{2\pi i} \int_{-i\infty}^{+i\infty} \langle \exp(\alpha z) \rangle \exp(-\alpha z)\, d\alpha \tag{30}$$

Using the result for the cumulants of z obtained above we have in the limit that L->∞

$$\ln\langle \exp(\alpha z) \rangle = L\, [\, c'_1 \alpha + c'_2 \alpha^2/2! + \ldots \,] \tag{31}$$

where

$$c'_n = \frac{d^n}{dN^n} \ln \mu_0(N) \Big|_{N=0} \tag{32}$$

The integral (30) can now be written

$$p(z) = \frac{1}{2\pi i} \int_{-i\infty}^{+i\infty} \exp[L f_z(\alpha) - \alpha z]\, d\alpha \tag{33}$$

where we define

$$f_z(\alpha) \equiv c'_1 \alpha + c'_2 \alpha^2/2! + \ldots. \tag{34}$$

In the limit that L->∞ this can be approximated using the saddle point method and we obtain

$$p(z) \rightarrow \frac{1}{\sqrt{(2\pi Lc'_2)}} \exp[\, -(z - Lc'_1)^2/2Lc'_2 \,] \qquad (35)$$

We find that $z \equiv -\ln|t|^2$ has a normal distribution in the limit $L \rightarrow \infty$ and as is obviously the case for any normal distribution is completely determined by the mean $\langle z \rangle = Lc'_1$ and variance $var(z) = Lc'_2$

$$p(z) \equiv p(z, Lc'_1, Lc'_2) \quad \text{as } L \rightarrow \infty \qquad (36)$$

In particular the asymptotic form is not dependent on c'_n $n>2$. Equation (35) is in effect a "central limit theorem" for the variable z. In the language of scaling the limiting distribution of z obeys a two parameter scaling.

The range of z implied by (35) is $[-\infty, +\infty]$ but physically it is clear that

$$0 \leq |t| \leq 1 \qquad (37)$$

which implies that the physical range of z is $[0, +\infty]$. This apparent contradiction is resolved by noting that the integrated probability density over the unphysical interval $[-\infty, 0]$ is zero in the asymptotic limit,

$$\int_{-\infty}^{0} [\, \lim_{L \rightarrow \infty} p(z) \,] \, dz = 0 \qquad (38)$$

At finite L this integral will be approximately zero if $Lc'_1 \gg 1$, which is equivalent to

$$L \gg Lc \qquad (39)$$

where Lc is the localisation length

$$\frac{1}{Lc} = \lim_{L \rightarrow \infty} \frac{\langle z \rangle}{2L} \qquad (40)$$

Even when $L \gg Lc$ the asymptotic form will not give the positive moments correctly. By definition we have

$$\langle |t|^{2n} \rangle = \int_{-\infty}^{+\infty} p(z) \exp(-nz) \, dz \qquad (41)$$

If we substitute the asymptotic from for p(z) into (41) we find that the integrand is maximal for $z<0$ when

$$n > \frac{\langle z \rangle}{\mathrm{var}(z)} \tag{42}$$

Therefore for n satisfying this condition the integral will be dominated by the unphysical part of the asymptotic distribution in $[-\infty,0]$. This leaves open the possibility that when

$$n < \frac{\langle z \rangle}{\mathrm{var}(z)} \tag{43}$$

the moments will be given correctly by the asymptotic form. In general we therefore expect that the positive moments of $|t|^2$ will not be consistent with (35) while the negative moments may be.

To determine whether the negative moments will in fact be given correctly by (35) we examine the saddle point approximation more carefully. The position of the saddle point α_0 is determined by the condition

$$\frac{d}{d\alpha}\left[Lf_z(\alpha) - \alpha z \right] \Big|_{\alpha=\alpha_0} = 0 \tag{44}$$

To find the root of this equation we truncate $f_z(\alpha)$ at order α^2 which gives

$$\alpha_0 = \frac{z - Lc'_1}{Lc'_2} \tag{45}$$

For the truncation of $f_z(\alpha)$ to be valid we must have

$$\alpha_0 \ll 1 \tag{46}$$

unless the higher cumulants of z are zero. For any L, no matter how large, condition (46) is not met for values of z sufficiently far from the mean $\langle z \rangle = Lc'_1$. The asymptotic form (35) will not give the probability of such values of z accurately. We therefore expect that the negative moments of $|t|^2$ will be consistent with (35) only if the higher cumulants of $z \equiv -\ln|t|^2$ are zero.

We should also consider whether the moments, or alternately the cumulants, of z will be consistent with the asymptotic distribution. All but the first two cumulants of a normal

distribution are zero and we have already seen that in the limit of large L that $c_n(z) \approx L\, c'_n$ which may or may not be zero. Therefore the higher cumulants cannot be consistent with the asymptotic distribution unless they are zero.

In figure 3.1 we plot the distribution of the renormalised variable z' where

$$z' = \frac{z - \langle z \rangle}{\sqrt{[\mathrm{var}(z)]}} \tag{47}$$

obtained from a Monte-Carlo simulation of the Anderson model. The simulation results fit very closely with a normal distribution with mean zero and variance unity indicating that the asymptotic distribution of z' is

$$p(z') = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{z'^2}{2} \right) \tag{48}$$

in agreement with the asymptotic form (35) for the distribution of $z \equiv -\ln|t|^2$.

The cumulants of the phase distribution can be calculated from

$$\langle \exp(N\Theta) \rangle \tag{49}$$
$$= [\mathbf{w} \otimes \mathbf{w}] \,.\, \langle \mathbf{X}(\mathbf{M}, iN/2) \otimes \mathbf{X}(\mathbf{M}^*, -iN/2) \rangle^L \,.\, [\mathbf{w}^T \otimes \mathbf{w}^T]$$

using the equivalent of (17), giving a normal distribution in the large L limit

$$p(\Theta) \rightarrow \frac{1}{\sqrt{[2\pi \mathrm{var}(\Theta)]}} \exp[\, -(\Theta - \langle \Theta \rangle)^2 / 2\mathrm{var}(\Theta) \,] \tag{50}$$

with

$$\langle \Theta \rangle = L \left. \frac{d}{dN} \ln \mu_0(N) \right|_{N=0} \tag{51}$$

and

$$\mathrm{var}(\Theta) = L \left. \frac{d^2}{dN^2} \ln \mu_0(N) \right|_{N=0} \tag{52}$$

where $\mu_0(N)$ is the relevant eigenvalue of the operator

$$\langle \mathbf{X}(\mathbf{M}, iN/2) \otimes \mathbf{X}(\mathbf{M}^*, -iN/2) \rangle \tag{53}$$

Figure 3.1

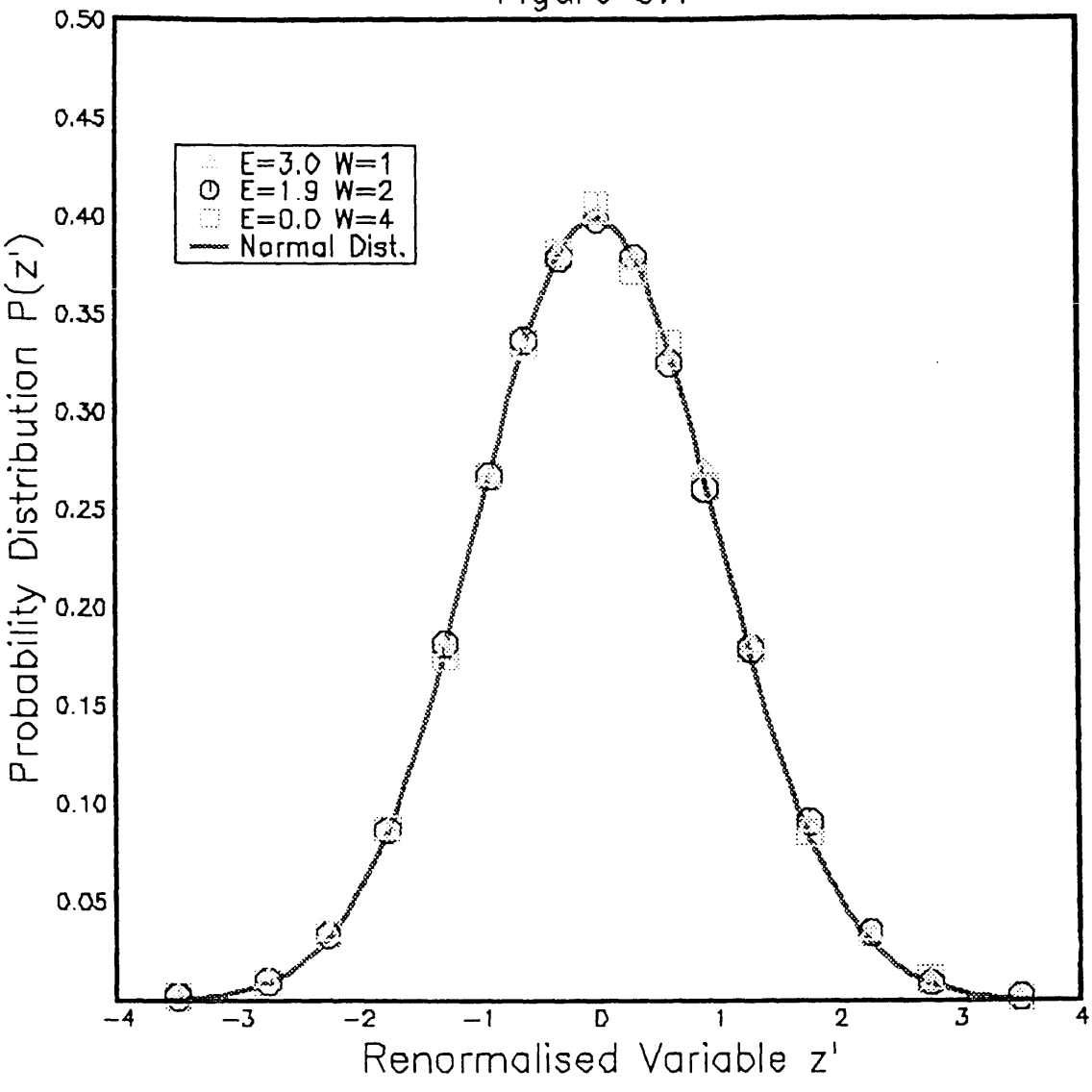


Fig 3.1 - The distribution of the renormalised variable z' for various energies E and disorders W. The symbols are the results of a Monte-Carlo simulation for systems of length L=1000 obtained by sampling over 50000 systems at random. The solid line is the normal distribution (mean zero and variance unity) expected on theoretical grounds.

the phase is related to the integrated density of states $\sigma(E)$ at energy E

$$\sigma(E) = \frac{-1}{\pi}\,\Theta \tag{54}$$

Since σ cannot be negative on physical grounds and the upper bound will be effectively infinite in the limit $L\to\infty$, we have that the physical range for Θ is $[-\infty,0]$. The asymptotic form implies that Θ will be distributed in the range $[-\infty,\infty]$. As before this is resolved by noting that the integrated density over the physical region is zero

$$\int_{0}^{\infty} \left[\lim_{L\to\infty} p(\Theta) \right] d\Theta = 0 \tag{55}$$

In this case since Θ is normally distributed (whereas $|t|^2$ was log normally distributed) we can say immediately that the higher moments of Θ will be consistent with the asymptotic form only if the higher cumulants of Θ are zero.

3. Application to the Anderson Model

3.1 Weak Disorder Limit

In this section we calculate explicit expressions for the distribution of $-\ln|t|^2$ and Θ for the Anderson model (described in section 3 of Chapter II) in the weak disorder limit. Here we recall that the transfer matrix **T** is of the form of equation (8) with

$$\mathbf{M}_n = \mathbf{Q} \begin{bmatrix} \varepsilon_n - E & , & -1 \\ 1 & , & 0 \end{bmatrix} \mathbf{Q}^{-1} \tag{56}$$

$$= \begin{bmatrix} (1-i\delta_n)e^{ik} & , & -i\delta_n e^{ik} \\ i\delta_n e^{-ik} & , & (1+i\delta_n)e^{-ik} \end{bmatrix}$$

where

$$\delta_n = (\varepsilon_n - \langle\varepsilon\rangle) \; / \; 2\sin(k) \tag{57}$$

and

$$E - \langle\varepsilon\rangle = -2\cos(k) \tag{58}$$

As explained in chapter II **T** describes the scattering of Bloch waves incident from the leads by the disordered region. We set $\langle\varepsilon\rangle=0$ as in Chapter II.

In the absence of disorder for $|E|<2$, the energy range for which the Bloch states of the leads are propagating rather than evanescent, we have

$$[\langle X(M,N) \otimes X(M^*,N)\rangle]_{mm',nn'} = \delta_{m,n}\,\delta_{m',n'} \cdot e^{2ik(m'-m)} \tag{59}$$

The zero order eigenvalues are highly degenerate and in particular there is large degeneracy of the eigenvalues on unity (m=m'). The introduction of disorder breaks this degeneracy. The new eigenvalues can be estimated from degenerate perturbation theory and working to first order in var(ε) we obtain a tri-diagonal perturbation matrix **Ω**

$$\mathbf{\Omega}(N) = \mathbf{I} + \frac{var(\varepsilon)}{E^2 - 4}\;\mathbf{\Omega}'(N) \tag{60}$$

where **I** is the identity matrix and **Ω'** has elements $(0\leq j\leq\infty)$

$$\Omega'_{j,j} = N(1+2j) - 2j^2 \tag{61}$$

$$\Omega'_{j,j+1} = (N-j)(j+1)$$

The perturbation matrix is real symmetric and therefore its eigenvalues are real. At N=0 we find as required that $\mu_0=1$ and that

$$\mu_m(N=0) < 1 - \frac{var(\varepsilon)}{4(E^2 - 4)} \tag{62}$$

Recalling the weak disorder result for the localisation length obtained in Chapter II we find that

$$[\,\mu_m/\mu_0\,]^L < \exp(\,-L/2Lc\,) \tag{63}$$

which implies that the central result for the cumulants (27) is accurate provided that L>>Lc. Using (27) and expanding the logarithm to first order in var(ε) we find the explicit expression

$$c_n(-\ln|t|^2) = L \quad \frac{var(\varepsilon)}{E^2 - 4} \quad \frac{d^n}{dN^n} \mu'_o(N) \Big|_{N=0} \tag{64}$$

where $\mu'_o(N)$ is the relevant eigenvalue of $\mathbf{\Omega}'$. The first derivative of μ'_o at N=0 is easily shown to be unity

$$c'_1 = \frac{var(\varepsilon)}{4 - E^2} \tag{65}$$

confirming the perturbation estimate of the localisation length obtained in Chapter II. The higher derivatives are obtained by numerical diagonalisation of $\mathbf{\Omega}'$. We truncate $\mathbf{\Omega}'$ at a finite size and then look for convergence of the derivatives against truncation size. Using this procedure we find that the second derivative is two (Fig 3.2)

$$c'_2 = \frac{2\ var(\varepsilon)}{4 - E^2} \tag{66}$$

and hence that

$$\langle -\ln|t|^2 \rangle = L\ var(\varepsilon) \ / \ (4 - E^2) \tag{67}$$

$$var(-\ln|t|^2) = 2L\ var(\varepsilon) \ / \ (4 - E^2)$$

which implies the direct relation between the mean and variance

$$var(-\ln|t|^2) = 2 \langle \ln|t|^2 \rangle \tag{68}$$

This means that the asymptotic distribution of $-\ln|t|^2$ is determined by a single parameter in the weak disorder regime. In figure 3.3 we examine the range of validity of the perturbation result (68) using a Monte-Carlo simulation of the Anderson model with with a continuous site energy distribution

$$p(\varepsilon) = \frac{1}{W} \qquad |\varepsilon| \leq \frac{W}{2} \tag{69}$$

As expected we find deviations from (69) for strong disorder, however these deviations do not in themselves imply a

Figure 3.2

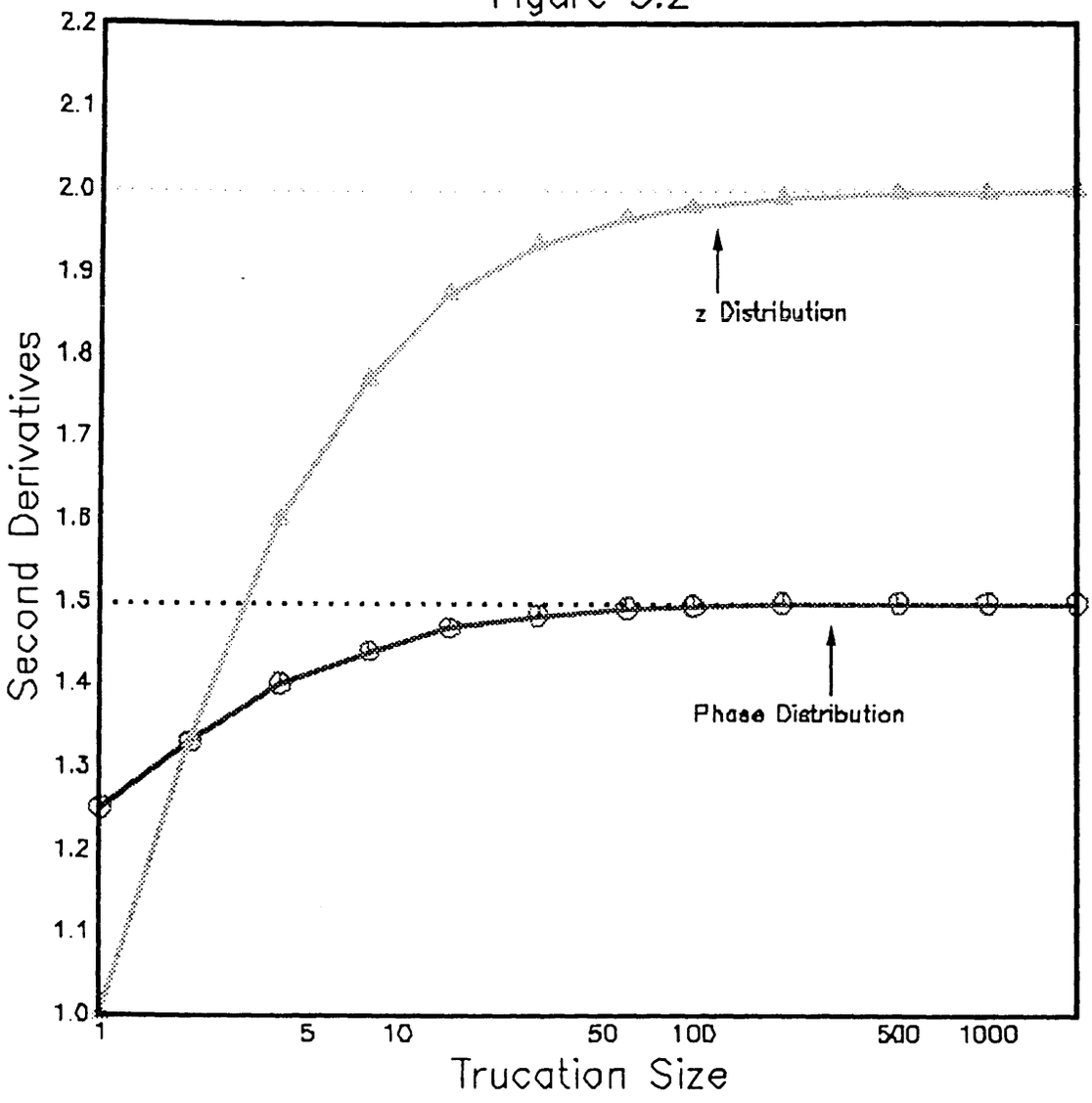


Fig 3.2 - Convergence of the derivatives which yield the variance of the of z and Θ, in the weak disorder limit of the Anderson model, against the truncation size of the perturbation matrix Ω'.

Figure 3.3

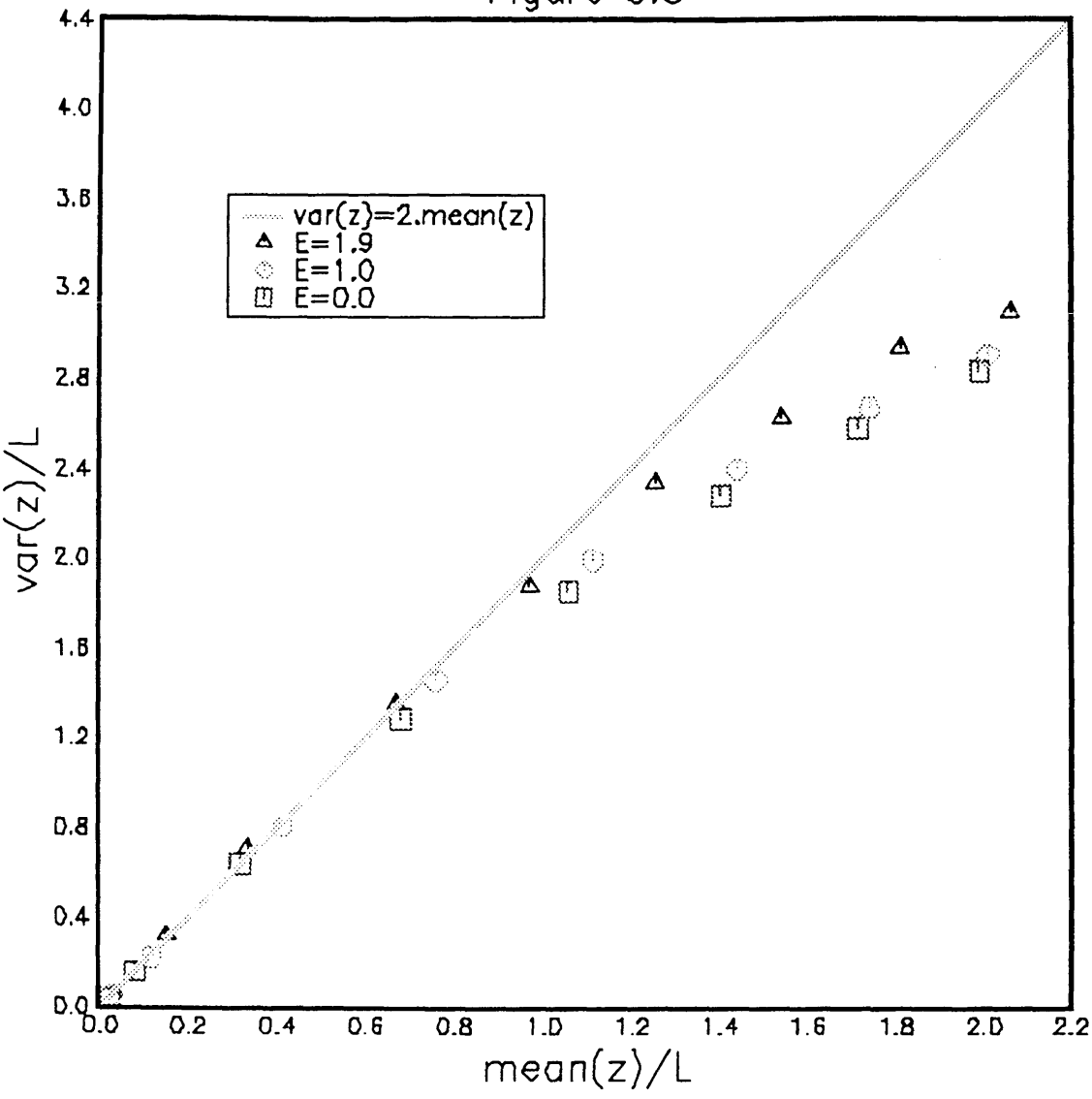


Fig 3.3 - The relationship between the mean and variance of z for various energies E and disorders W (W=1,2,4,6,8,10,12, 14.) The figure shows the breakdown of single parameter scaling for strong disorder. These results are for energies at which the Bloch states of the leads are propagating waves.

crossover to two parameter scaling. For single parameter scaling to be valid it would be sufficient that all the simulation results of Figure 3.3 lay on the same curve. However it is clear from Figure 3.3 that for strong disorder they do not and that there is a crossover to two parameter scaling. It is also apparent from Figure 3.3 that the dependence on the second parameter is however rather weak.

When $|E|>2$ the Bloch states in the leads are not propagating but are evanescent and consideration of their transmission properties is therefore not of great physical relevance. Nevertheless we carry through the weak disorder analysis in the interest of completeness. In the absence of disorder we have

$$[<X(M,N) \otimes X(M^{*},N)>]_{mm',nn'} = \delta_{m,n}\,\delta_{m',n'}\,\exp[2ik(N - m' - m)] \qquad (70)$$

since ik is now real. At N=0 the eigenvalue $\mu_0=1$ is no longer degenerate and we find using non degenerate perturbation theory that

$$c'_1 = 2ik - \frac{var(\varepsilon)}{E^2 - 4} \qquad (71)$$

$$c'_2 = 4\,\frac{var(\varepsilon)}{E^2 - 4} \qquad (72)$$

A surprising feature of the results is that the perturbation correction to the localisation length is negative, the localisation length itself however remains positive. In Figure 3.4 this result is confirmed in a comparison with a Monte-Carlo simulation of the Anderson model. In contrast to the case $|E|<2$ there is no direct relationship between the mean and variance of the distribution in the weak disorder limit and we have a two parameter scaling for arbitrary disorder.

Figure 3.4

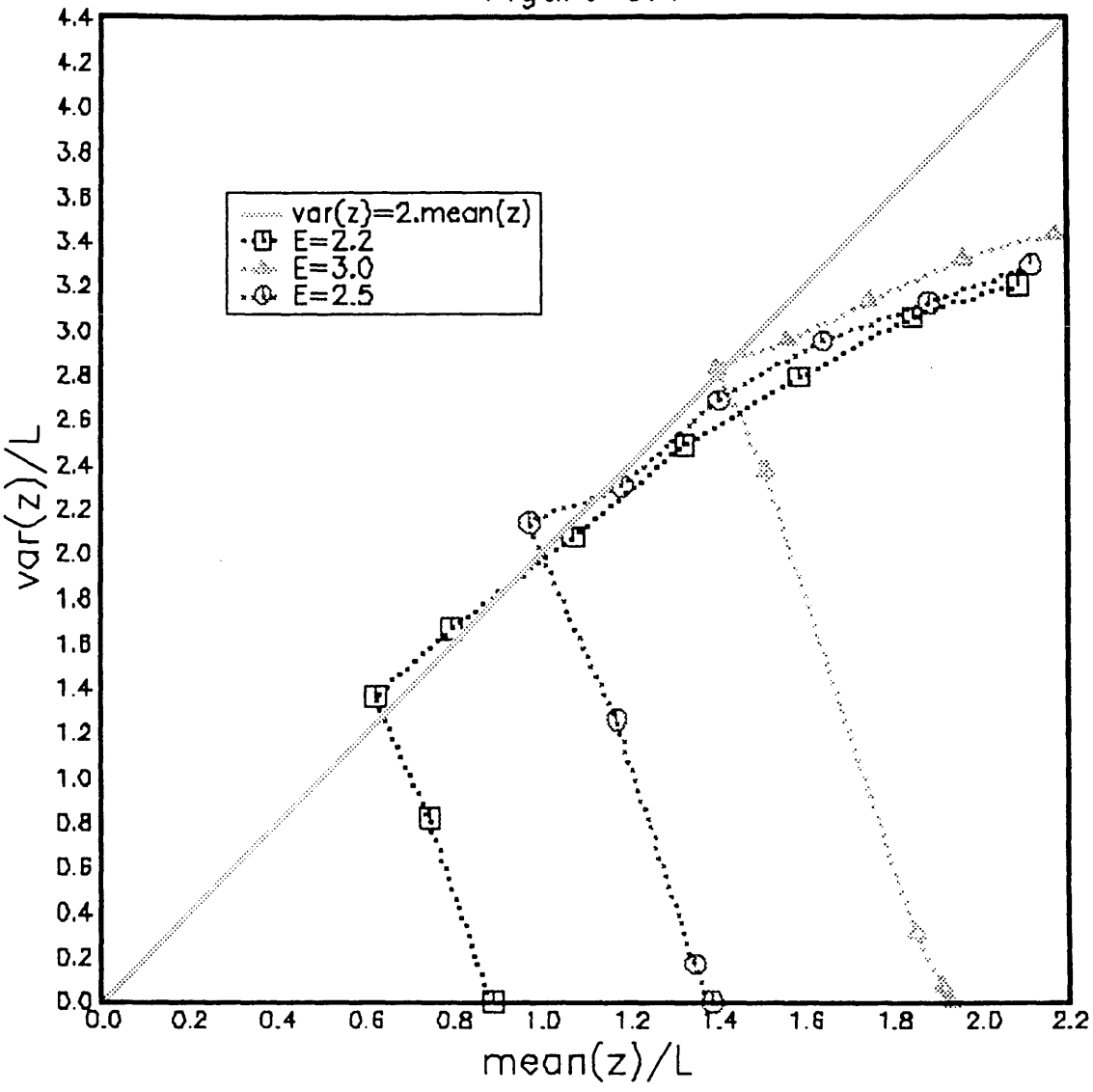


Fig 3.4 - The relationship between the mean and variance of z for energies at which the Bloch states of the leads are evanescent. Here single parameter scaling is not valid even in the weak disorder limit.

The phase distribution can be obtained in the weak disorder limit in a similar way. When $|E|<2$ we again use degenerate perturbation theory. Here the perturbation matrix Ω' is

$$\Omega'_{j,j} = N^2/2 - 2j^2 \tag{73}$$

$$\Omega'_{j,j+1} = (j+1).\sqrt{(j^2 + N^2/4)}$$

with the cumulants given by

$$c_n(\Theta) = -kL\delta_{n,1} + \frac{var(\varepsilon)}{4\sin^2(k)} \frac{d^n}{dN^n} \mu'_o(N) \Big|_{N=0} \tag{74}$$

Perturbation theory for small N gives the first derivative as zero. Using numerical diagonalisation we find that the second derivative is 3/2 (Fig 3.2) and hence that

$$\langle\Theta\rangle = -kL \tag{75}$$

$$var(\Theta) = L\,\frac{3}{2}\,\frac{var(\varepsilon)}{(4 - E^2)}$$

This implies a two parameter scaling of the Θ distribution. When $|E|>2$ non degenerate perturbation theory gives

$$\langle\Theta\rangle = 0 \quad E < -2 \tag{76}$$

$$= \pi \quad E > 2$$

and

$$var(\Theta) = 0 \tag{77}$$

The fluctuations in Θ are quenched since the density of states tends to zero beyond $E=\pm(2+W/2)$ in accordance with the Saxon Hutner [11] theorem and this is reflected in the perturbation estimates (76-77).

3.2. Weak Disorder Results for the Higher Cumulants

We can also calculate the higher cumulants of both $-\ln|t|^2$ and Θ in the weak disorder limit in exactly the same way as the first two cumulants were calculated in the previous section.

For $|E|<2$ we find that $c_3(-\ln|t|^2)$ and $c_4(-\ln|t|^2)$ are both zero (Fig 3.5). For the higher cumulants we are not able to obtain convergence of the necessary derivatives against the truncation size of the perturbation matrix Ω'. Nevertheless we do find that the higher derivatives decrease with increasing truncation size suggesting that they are in fact zero. When $|E|>2$ we find from non degenerate perturbation theory that all higher cumulants are zero. This leads us to conjecture that to first order in the statistical variance

$$c_n(-\ln|t|^2) = 0 \quad n > 2 \tag{78}$$

With reference to the discussion of section 2 this implies that the negative moments of $|t|^2$ will be consistent with the log-normal distribution. The simplest way to obtain explicit expressions for the negative moments is to use the defining expansion for the cumulants

$$\ln\langle|t|^{-2N}\rangle = \sum_{n=0}^{\infty} c_n(-\ln|t|^2)\ \frac{N^n}{n!} \tag{79}$$

which terminates in this case at second order. This gives immediately with reference to equation (26) that

$$\langle|t|^{-2N}\rangle = g(N,0)\ \exp[\ L\ c'_1\ (N + N^2)\ ] \tag{80}$$

in the asymptotic limit. Here $g(N,0)$ is the numerical factor of equation (21) and is independent of L. From equations (42) and (69) find that expression (69) should breakdown below $N\approx -1/2$, implying that the Taylor expansion (79) does not accurately represent the cumulant generating function for values of N below this limit. This is consistent with the behaviour of μ'_0 which is plotted in Figure 3.7 with the its associated Taylor expansion about N=0.

The higher cumulants of the phase distribution are calculated in analogous manner (Fig 3.6) and again would appear to be zero. In this case this indicates that both the negative and positive moments of Θ will be consistent with the asymptotic distribution in the weak disorder limit.

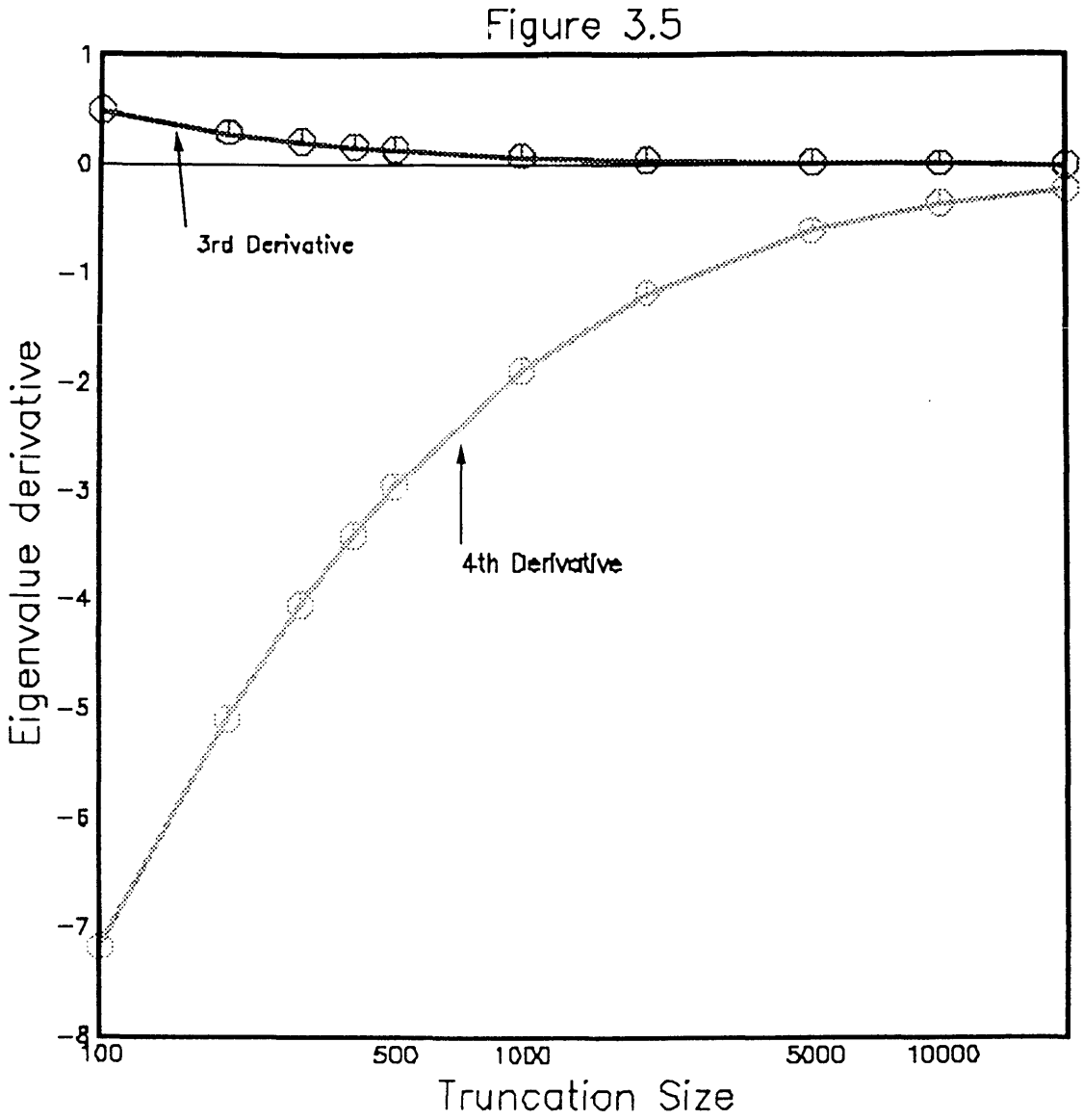


Fig 3.5 - Convergence of the derivatives which yield the 3rd and 4th cumulants of the z distribution against truncation size of the perturbation matrix Ω'.

Figure 3.6

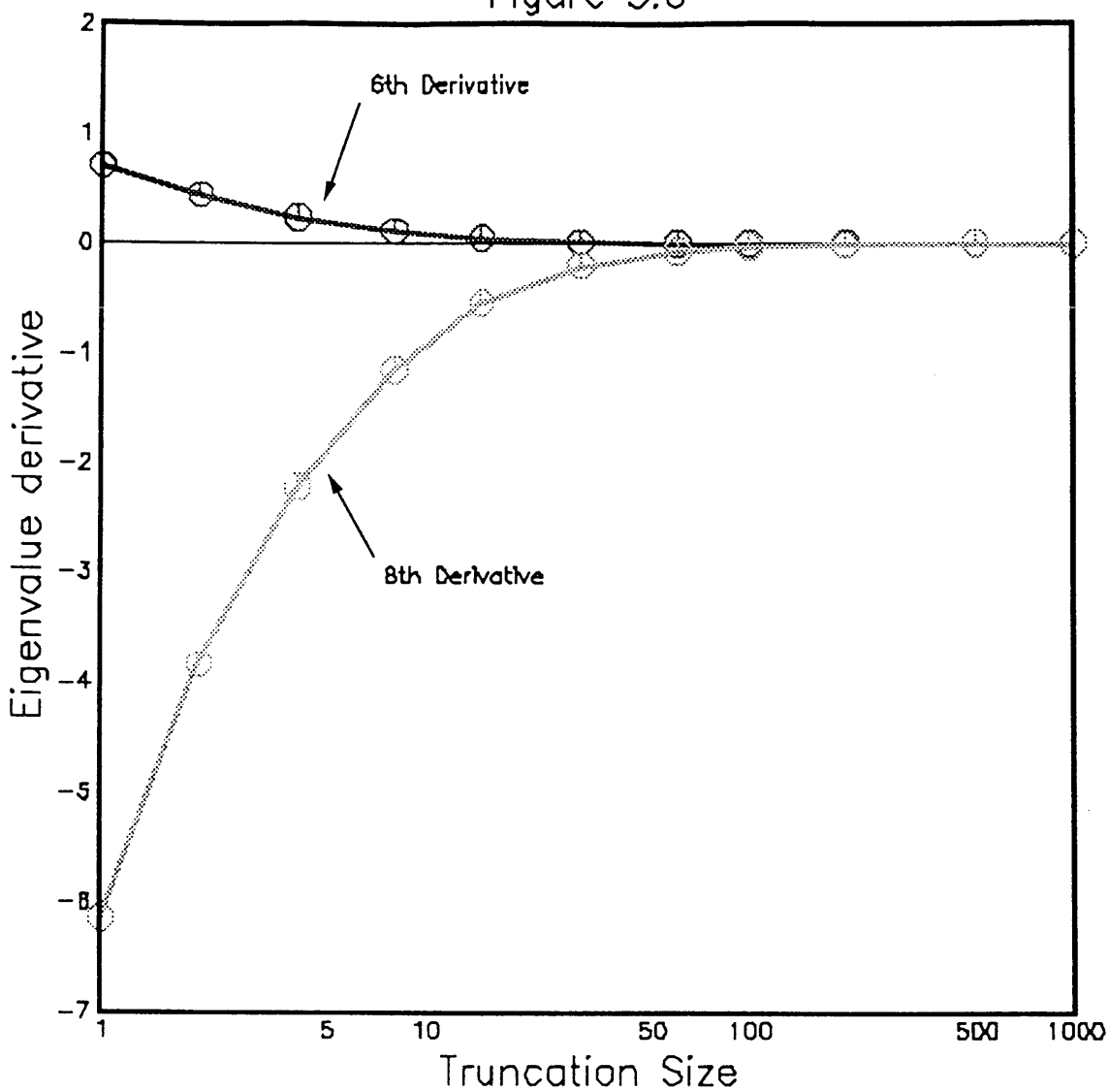


Fig 3.6 - Convergence of the derivatives which yield the 6th and 8th cumulants of the Θ distribution against truncation size of the perturbation matrix $\boldsymbol{\Omega}'$. The odd derivatives are zero at all truncation sizes.

Figure 3.7

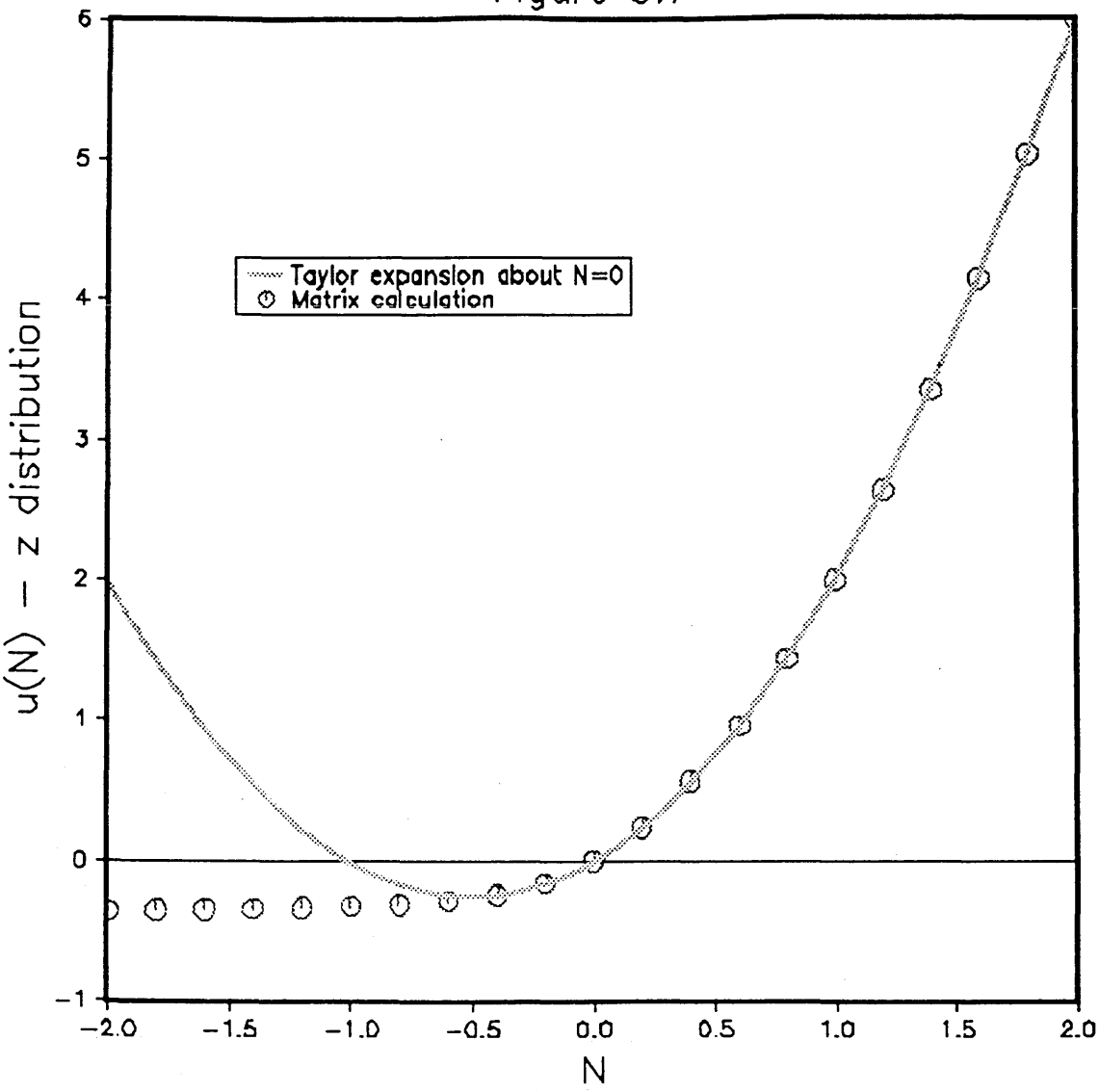


Fig 3.7 - The breakdown of the Taylor expansion of $\mu'_0(N)$ (for the z distribution) at negative N. The solid line is the Taylor expansion about the origin and the symbols are the results obtained by direct diagonalisation of $\boldsymbol{\Omega}'(N)$.

3.3 Strong Disorder

There is no reason to expect that the eigenvalue spectrum of the operators (19) and (49) will be fundamentally different for strong disorder. We expect therefore that $-\ln|t|^2$ and Θ are normally distributed as $L\to\infty$ for arbitrary disorder strength W of the site energy distribution (70). This should also hold for off-diagonal and mixed disorders except for the anomalous case of the band centre of an off-diagonally disordered system (see chapter II).

The result of section 3.2 that all higher cumulants are zero to first order in $\mathrm{var}(\varepsilon)$ will probably be modified at higher orders. For strong disorder we therefore expect that the negative, in addition to the positive moments, of $|t|^2$ and Θ will be inconsistent with the asymptotic distribution. This has been shown explicitly for the resistance moments in the very strong disorder limit by a direct calculation [12].

4. Conclusions

The main conclusion of this chapter is that the both $-\ln|t|^2$ and Θ are normally distributed in the limit that $L\to\infty$, a result should hold quite generally, given the restrictions on the eigenvalue spectrum discussed in section 2. Since the normal distribution is completely defined by its mean and variance this implies a two parameter scaling for the distributions. This will reduce to a single parameter scaling when a relation exists between the mean and variance, as for example in the weak disorder limit of the Anderson model discussed in section 3.

It is clear from section 2 that a knowledge of the asymptotic form for $p(-\ln|t|^2)$ does not permit the evaluation of the positive moments of $|t|^2$. The positive moments can in principle be evaluated using equation (16) directly. It is found in practice however that a more useful approach is to symmetry reduce the equation

$$\langle |t|^{-2N} \rangle = [(1,0) \otimes (0,1)]^{\otimes N} \cdot [\mathbf{T} \otimes \mathbf{T} \,..\, \otimes \mathbf{T}]^{\otimes 2N} \cdot \left[\begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right]^{\otimes N} \tag{81}$$

where we have used the notation that $\mathbf{A}^{\otimes N}$ indicates taking the direct product of **A** with itself N times. This is considerably more complicated than the reduction of (11) but has been achieved by Kirkman and Pendry [13]. They find

$$\langle |t|^{2N} \rangle = \beta(N) \, [\alpha_0 / (\alpha_2 L)^{3/2}] \exp(\alpha_1 L) \tag{82}$$

where $\beta(N)$ is a known numerical factor independent of the disorder and the α's are parameters which depend on the disorder but which cannot in general be found analytically. This result is in agreement with the results of Abrikosov and Ryzhkin [5] for weak disorder for a model with Gaussian random potentials.

References

[1] Abrahams A, Anderson P, Licciardello D and Ramakrishnan T Physical Review Letters 42 673 (1979)

[2] Anderson P, Thouless D, Abrahams E and Fisher D Physical Review B 22 3519 (1980)

[3] Mello P Journal of Mathematical Physics 27 2876 (1986)

[4] Cohen A, Roth Y and Shapiro B Physical Review B 38 125 (1988)

[5] Abrikosov A and Ryzhkin I Advances in Physics 27 147 (1978)

[6] Abrikosov A Solid State Communications 37 997 (1980)

[7] Kumar N Physical Review B 31 5513 (1985)

[8] Soukoulis C and Economou E Solid State Communications 37 409 (1981)

[9] Andereck B and Abrahams E Journal of Physics C L383 (1980)

[10] Landauer R Philosophical Magazine 21 863 (1970)

[11] Hori J and Matsuda H Progress in Theoretical Physics 32 183 (1964)

[12] Pendry J B Journal of Physics C 15 4821 (1982)

[13] Kirkman P and Pendry J B Journal of Physics C 17 5707 (1984)

Chapter IV - Generalised Transfer Matrices for Quasi-One Dimensional Disordered Systems

1. Introduction

In this and the following chapter we deal with quasi-one dimensional disordered systems. These are systems for which the transverse dimensions Lx and Ly are finite but much less than the length Lz. As in the strictly one dimensional case we describe the scattering properties of the system using a transfer matrix formalism and are thus led quite naturally to consider products of random matrices and their associated Lyapunov exponents. We begin in section 2 by recalling the definition of these exponents and discussing their relevance to the electronic properties of quasi-one dimensional systems. In section 3 we show how to calculate the exponents using the generalised transfer matrix method and in section 4 we apply our results to the Anderson model for these systems. In comparisons with Monte Carlo simulations of the model we find disagreements with the generalised transfer matrix expressions under certain conditions. We conjecture that these disagreements are due to some form of symmetry breaking.

2. Transfer Matrix Formalism and Lyapunov Exponents

In the strictly one dimensional case the transfer matrix for the disordered system is a product of transfer matrices

$$\mathbf{T} = \prod_{n=1}^{Lz} \mathbf{M}_n \qquad (1)$$

$\mathbf{M}_n$ describes the scattering at the nth site and is a function of the transmission t_n and reflection r_n for waves incident at this site. The situation for quasi-one dimensional systems is essentially the same except that t_n and r_n

become non-commuting matrices $\mathbf{t}_n$ and $\mathbf{r}_n$ which describe the scattering of waves at the nth layer. The precise form of the transfer matrix in terms of the reflection and transmission matrices is more complicated than the strictly one dimensional case and is discussed in Appendix I.

Each transfer matrix $\mathbf{M}_n$ is assumed to be independent and distributed with a probability distribution $p(\mathbf{M})$ which is independent of n. This allows us to apply the theorem of Oseledec [1] to the random matrix product (1). This theorem proves the existence of a limiting matrix $\boldsymbol{\Omega}$ of the form

$$\boldsymbol{\Omega} = \lim_{Lz\to\infty} [\mathbf{T}^{+}\mathbf{T}]^{1/2Lz} \qquad (2)$$

The logarithms of the eigenvalues of this matrix are defined as the Lyapunov exponents. The existence of this limit implies quite rigorously the inequality

$$\frac{1}{2Lz} |\log|\mathbf{Tu}|| \geq \alpha_{min} \qquad (3)$$

where α_{min} is the smallest positive exponent[1] and $\mathbf{u}$ is any vector. We infer from this that the electron eigenstates of the system are localised at least as

$$\Phi(\mathbf{r}) \approx \exp[\, -(\mathbf{r}-\mathbf{r}_o)/L_{max}\,] \qquad |\mathbf{r}|\to\infty \qquad (4)$$

where

$$L_{max} = 1/\alpha_{min} \qquad (5)$$

and $\mathbf{r}_o$ is the point about which the electron is localised. If $\alpha_{min}=0$ then $Lmax=\infty$ and we can not conclude that the eigenstates are exponentially localised. However Thouless [2] has argued on physical grounds that the eigenstates of disordered one dimensional wires are always exponentially localised. Ishii [3] has applied the theorems of Furstenberg [4] to provide rigorous mathematical backing for this conclusion. We thus expect that in virtually all cases that

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[1] Conservation of current implies that T is symplectic so that the exponents occur in pairs of opposite sign.

$\alpha_{min} \neq 0$. For the precise meaning of "virtually all" the reader is referred to the review by Ishii [3].

The main relevance of calculations for quasi-one dimensional systems is that the results allow deductions to be made concerning the behaviour of two dimensional (d=2) and three dimensional (d=3) systems. It has been found in Monte Carlo simulations [5-9] of two dimensional strips and three dimensional bars (Lx=Ly) that the dependence of L_{max} on the the transverse dimension Lx obeys a scaling form

$$L_{max}(Lx)/Lx = f[\ Lc/Lx\ ] \qquad (6)$$

where f is a function which depends only on the symmetries and the dimension, Lc is a fitting parameter which is determined from the numerical data and Lz is effectively infinite. Three main types of behaviour for L_{max} against Lx can be distinguished;

(i) If L_{max}/Lx decreases for increasing Lx it is found that

$$L_{max}(Lx) \rightarrow Lc \qquad \text{as } Lx \rightarrow \infty \qquad (7)$$

and we identify Lc as the localisation length associated with the eigenstates of the corresponding two or three dimensional system with $Lx=\infty$.

(ii) If L_{max}/Lx increases with Lx then the eigenstates of the two or three dimensional system are expected to be extended. In this case the interpretation of Lc is not as obvious [5].

(iii) Intermediate between cases (i) and (ii) is a linear increase in L_{max} with Lx and $Lc=\infty$. This is associated with a fixed point of the scaling form (6) and signals a transition from localised eigenstates to extended eigenstates in the corresponding two or three dimensional system with $Lx=\infty$.

For two dimensional systems type (i) behaviour is always found (with the exception of systems with spin-orbit

scattering [10] and magnetic fields [11]) and we conclude that the two dimensional systems is always localised in the presence of disorder in agreement with the scaling theory of localisation [12].

In three dimensions all three type of behaviour are found as a function of disorder and fermi energy. At fixed disorder there is in general an energy Ec, called the mobility edge, at which Lc diverges. This energy separates localised from extended eigenstates. However if the disorder is increased a point is reached where type (i) behaviour occurs at all energies and all states are then localised regardless of energy. This point is called the Anderson transition. This again is in general agreement with the scaling picture of Abrahams et al [12].

Under certain conditions the conductance of the quasi-one dimensional system can be expressed in terms of the transmission matrix $\mathbf{t}$ as [13]

$$g = 2.tr[\mathbf{t}^{+}\mathbf{t}] \tag{8}$$

This can be expressed in terms of the eigenvalues α'_j of the matrix Ω' where

$$\Omega' = [\mathbf{T}^{+}\mathbf{T}]^{1/2Lz} \tag{9}$$

(here we do not take the limit Lz->∞) as [14]

$$g = (e^2/\hbar) \sum \frac{4}{\cosh(2Lz\alpha'_j) + 1} \tag{10}$$

The relation to the Lyapunov exponents α_j is obvious

$$\alpha_j = \lim_{Lz\to\infty} \alpha'_j \tag{11}$$

However, an unambiguous statement about the conductance requires a knowledge of the fluctuations in the α'_j at finite Lz not just their limiting value for infinite Lz [15-17].

Having explained the relevance and usefulness of the Lyapunov exponents we attempt in the next section to calculate them without recourse to Mote Carlo methods. The essence of our approach is to use a symmetry analysis and an

analytic continuation to derive a secular equation for each exponent.

3. Calculation of the Lyapunov Exponents Using Generalised Transfer Matrices

In this section we show how to use the theory of the symmetric group to obtain the Lyapunov exponents associated with the product of random matrices

$$\mathbf{T}_L = \prod_{n=1}^{Lz} \mathbf{M}_n \tag{12}$$

where the M's are independent, identically distributed random matrices. We calculate the Lyapunov exponents as follows. Let $\{\mathbf{w}(i): i=1, \ldots, p\}$ be a set of orthogonal vectors. Then consider the determinant of the pxp matrix formed from the elements

$$\mathbf{w}(i)^T \cdot \mathbf{T}_{Lz} \cdot \mathbf{w}(j) \quad (1 \leq [i,j] \leq p) \tag{13}$$

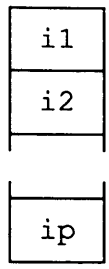
We define $D_p(\mathbf{T}_{Lz})$ as the maximum over the set of determinants obtained by taking all distinct sets of p orthogonal vectors. We then obtain the sum of the p largest Lyapunov exponents Γ_p as [15]

$$\Gamma_p = \lim_{Lz \to \infty} \frac{1}{Lz} < \log|D_p(\mathbf{T}_{Lz})| > \tag{14}$$

We expect our results to be independent of the representation of $\mathbf{T}_{Lz}$. In the following we assume a convenient representation where $w(i)_j = \delta i,j$, $1 \leq [i,j] \leq m$ and m is the dimension of $\mathbf{T}_{Lz}$.

The first step in our symmetry analysis is to note that this set of determinants can be obtained as the diagonal elements of the antisymmetric projection of the direct product of $\mathbf{T}_{Lz}$ with itself p times. To obtain the projection we must first choose a basis for the antisymmetric subspace. A convenient basis for our purposes can be most easily defined by vertical Young tableaux.

Let i1 , ... ,ip a set of strictly increasing integers



$$1 \leq i1 < i2 < \ldots\ldots < ip \leq m \qquad (15)$$

The vector defined by this tableau has components

$$u(i1\ ..\ ip)_{j1\ ..\ jp} = \frac{1}{\sqrt{p!}} \quad j1\ ..\ jp \text{ an even permutation of } i1\ ..\ ip \qquad (16)$$

$$= \frac{-1}{\sqrt{p!}} \quad j1\ ..\ jp \text{ an odd permutation of } i1\ ..\ ip$$

$$= 0 \quad \text{otherwise}$$

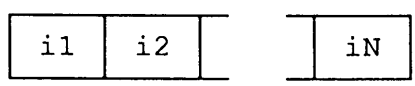
We can write this projection as a matrix $\mathbf{Y_p}(T_{Lz})$, with elements

$$\mathbf{u}(i1\ ..\ ip)^T\ .\ \mathbf{T}_{Lz} \otimes\ ..\ \mathbf{T}_{Lz}\ (p \text{ times})\ .\ \mathbf{u}(j1\ ..\ jp) \qquad (17)$$

$D_p(\mathbf{T}_{Lz})$ is now the maximum over the diagonal elements of $\mathbf{Y_p}$. Noting that $\mathbf{T}_{Lz} \otimes\ ..\ \mathbf{T}_{Lz}$ (p times) maps the antisymmetric subspace onto itself we can immediately write

$$\mathbf{Y_p}(\mathbf{T}_L) = \prod_{n=1}^{Lz} \mathbf{Y_p}(\mathbf{M}_n) \qquad (18)$$

Now consider the direct product of $\mathbf{Y_p}$ with itself N times and its projection onto the symmetric subspace. We define a basis for the symmetric subspace using horizontal tableaux.



$$1 \leq i1\ ..\ \leq iN \leq y \qquad (19)$$

where y is the dimension of $\mathbf{Y_p}$. The vector defined by this tableau has components

$$v(i1\ ..\ iN)_{j1\ ..\ jN} = \frac{\pi \sqrt{l_i!}}{\sqrt{N!}} \quad j1\ ..\ jN \text{ a permutation of } i1\ ..\ iN \qquad (20)$$

$$= 0 \quad \text{otherwise}$$

where l_i (i=1,..,y) is the number of i's in i1,...,iN. We can thus label each vector in this basis by a set of y positive integers $l_1,..,l_y$ which satisfy

$$\sum_{i=1}^{y} l_i = N \tag{21}$$

We can now write the projection onto the symmetric subspace, $\mathbf{X}(N,Y)$, as

$$\begin{aligned} &\mathbf{X}(N,Y)\ (\ l_1\ ..\ l_y\ :\ k_1\ ..\ k_y\ ) \\ &= \mathbf{v}(l_i)^T\ .\ \mathbf{Y} \otimes ..\ \mathbf{Y}\ (N\ \text{times})\ .\ \mathbf{v}(k_i) \\ &= (\prod_i \sqrt{(l_i!\ k_i!)}\ )\ \sum_{\{p_{i,j}\}}\ \prod_{i,j}\ Y_{i,j}^{p_{i,j}}\ 1/p_{i,j}! \end{aligned} \tag{22}$$

where the sum is over the set of y^2 positive integers $p_{i,j}$ satisfying

$$\sum_{j=1}^{y} p_{i,j} = l_i \qquad \sum_{i=1}^{y} p_{i,j} = k_j \tag{23}$$

and

$$\sum_{i,j=1}^{y} p_{i,j} = N$$

The symmetric projection contains D_p^N as the maximum over a subset of diagonal elements, since

$$X(N,\mathbf{Y_p})\ (\ l_j = N\delta j,i\ :\ k_j = N\delta j,i\ ) = [\mathbf{Y_p}]_{i,i}^{N} \tag{24}$$

Again noting that $\mathbf{Y} \otimes ..\ \mathbf{Y}$ (N times) preserves the symmetric subspace, we see that X has the multiplicative property that

$$\mathbf{X}(N,\mathbf{Y_p}(\mathbf{T}_L)) = \prod_{n=1}^{Lz} \mathbf{X}(N,\mathbf{Y_p}(\mathbf{M}_n)) \tag{25}$$

This allows us to think of $\mathbf{X}$ as a generalised transfer matrix.

The value of the symmetry reduction becomes apparent when we average over the disorder or randomness in $\mathbf{M}_n$

$$\langle \mathbf{X}(N,\mathbf{Y_p}(\mathbf{T}_L)) \rangle = \langle \mathbf{X}(N,\mathbf{Y_p}(\mathbf{M})) \rangle^{Lz} \tag{26}$$

making use of the 'statistical symmetry' mentioned earlier. The problem is then reduced to the consideration of a product of Lz identical matrices.

The main problem with the above analysis is that N is restricted to positive integer values or zero. To make progress we need an analytic continuation for N non integer. We can then evaluate Γ_p as

$$\Gamma_p = \lim_{Lz\to\infty} \mathrm{Re}\ \frac{1}{Lz}\frac{d}{dN} \langle D_p(\mathbf{T}_{Lz})^N \rangle \Big|_{N=0} \qquad (27)$$

In making the analytic continuation we follow as closely as possible the procedure for one dimensional systems explained in chapter II.

Suppose that the (1-1) element is the diagonal element of $\mathbf{Y_p}$ with largest modulus (the following is easily generalised to other cases) so that $[\ \mathbf{Y_p}(\mathbf{T}_{Lz})\ ]_{1,1} = D_p(\mathbf{T}_{Lz})$. Let

$$L = l_2 + \ldots + l_y \qquad K = k_2 + \ldots + k_y \qquad (28)$$

then we order $\mathbf{X}$ so that

$$\mathbf{X}(N) = \begin{matrix} \\ L=0 \\ \\ L=N \end{matrix} \begin{matrix} K=0 \qquad\qquad K=N \\ \left[\begin{matrix} \\ X(l_i:k_i) \\ \\ \end{matrix}\right] \end{matrix} \qquad (29)$$

Then

$$D_p(\mathbf{T}_{Lz})^N = \mathbf{s}^T \cdot \mathbf{X}(N, \mathbf{Y_p}(\mathbf{T}_{Lz})) \cdot \mathbf{s} \qquad (30)$$

where $\mathbf{s}$ has components $s_j = \delta_{j,1}$.

So far N is integer and $\mathbf{X}(N)$ is finite in size. In general the size is greater then or equal to N+1 with equality only if $\mathbf{Y}$ is 2x2 (the strictly one dimensional case.) This is because for given values of L and K there are in general multiple solutions of (28) for l_2 .. l_y and k_2 .. k_y, each of which gives a different matrix element of $\mathbf{X}$.

When N is non integer we retain (22) for the matrix elements of our new continued $\mathbf{X}$ matrix but allow l_1 and k_1 non integer

$$l_1 = N - L \qquad k_1 = N - K \qquad (31)$$

and order **X** as before but now allowing L and K to take any values in the range zero to infinity. This makes **X** infinite in size. In performing the summation in (22) we sum over all solutions to (23) with p_{11} non integer but all the other p's positive integer as before so that

$$p_{11} = N - \Sigma' p_{i,j} \tag{32}$$

where Σ' denotes the sum over all p's except p_{11}. The only non integer factorials appear as a ratio and are easily evaluated (using the gamma function continuation of the factorial) as

$$l_1! / p_{11}! = (N-L).(N-L-1) \ldots (N-L-l_1+p_{11}+1) \tag{33}$$
$$= 1 \quad \text{if } l_1 = p_{11}$$

and similarly $k_1!$

So how does the new 'continued' **X** matrix relate to the previous **X** matrix when N is a positive integer? The answer is that it is block diagonal

$$\mathbf{X}(N) = \begin{array}{c} \\ L=0 \\ \\ \\ L=\infty \end{array} \begin{array}{c} \begin{array}{cc} K=0 & \qquad K=\infty \end{array} \\ \left[\begin{array}{c|c} \begin{array}{l} 0\le L\le N \\ 0\le K\le N \end{array} & 0 \\ \hline 0 & L,K>N \end{array}\right] \end{array} \tag{34}$$

the $0\le L,K\le N$ block being identical to the previous X matrix at integer N. This means that (30) is automatically valid for the new **X** matrix. Later in this chapter compare results obtained with the continued **X** matrix with results obtained using Monte Carlo simulation technique.

We can obtain a more explicit expression for Γ_p by writing

$$\langle \mathbf{X}(N,\mathbf{Y}_p(\mathbf{T}_{Lz})) \rangle = \sum_{i=0}^{\infty} \mu_i(N)^{Lz} \, |N,i\rangle\langle i,N| \tag{35}$$

where $\mu_i(N)$ are the eigenvalues and $|N,i\rangle$, $\langle i,N|$ the right and left eigenvectors of $\langle \mathbf{X}(N,\mathbf{Y}_p(\mathbf{M})) \rangle$. We now substitute (35) into (30), differentiate with respect to N and note

that $\mathbf{s}^T$ and $\mathbf{s}$ are eigenvectors of $\mathbf{X}(N=0)$ with eigenvalue unity. If we denote this eigenvalue as $\mu_o(N=0)$ then

$$\Gamma_p = \mathrm{Re}\left[\frac{d}{dN} \mu_o(N) \right] \Big|_{N=0} \tag{36}$$

We can write (36) in a more transparent form by defining a matrix $\mathbf{Z}(N,\mathbf{Y})$

$$\mathbf{X}(N,\mathbf{Y}) = Y_{1,1}{}^N \, \mathbf{Z}(N,\mathbf{Y}) \tag{37}$$

Near N=0 we can then write

$$\langle \mathbf{X}(N,\mathbf{Y}) \rangle = \langle \mathbf{Z}(N,\mathbf{Y}) \rangle + N \langle \ln Y_{11} \, \mathbf{Z}(N,\mathbf{Y}) \rangle + O(N^2) \tag{38}$$

We now use perturbation theory, exact in the limit of small N, to obtain an expansion in powers of N for $\mu_o(N)$, then with reference to (36) we obtain

$$\Gamma_p = \langle \ln Y_{11} \rangle + \frac{d}{dN} \mu'_o(N) \Big|_{N=0} \tag{39}$$

where $\mu'_o(N)$ is the relevant eigenvalue of $\langle \mathbf{Z}(N,\mathbf{Y}) \rangle$. Thus our result is that Γ_p is equal to a 'zero order' estimate plus a correction term.

To generalise to other cases we simply note that if $[\mathbf{Y_p}]_{i,i}$ is the maximal diagonal element of $\mathbf{Y_p}$ we allow only l_i, k_i and p_{ii} non integer and set

$$L = l_1 + .. + l_{i-1} + l_{i+1} + .. l_y \tag{40}$$

similarly K.

4. Application to the Anderson Model

4.1 The Anderson Model for Quasi One Dimensional Systems

The Anderson model for one dimensional systems of finite cross section is exactly analogous to the strictly one dimensional case discussed in chapters II and III. For simplicity we assume a two dimensional geometry. We expand the electronic wave function $\Phi(\mathbf{r})$ for the system as a linear combination of atomic orbitals

$$\Phi(\mathbf{r}) = \sum_{n,m} a_{n,m}\, \Phi_{n,m}(\mathbf{r} - \mathbf{r}_{n,m}) \qquad (41)$$

Here n labels the longitudinal or z direction and m is the transverse label. $\Phi_{n,m}$ is the orbital centred at the site with position $\mathbf{r}_{n,m}$ and $a_{n,m}$ are the coefficients in the expansion. The disordered system is modelled using a tight binding hamiltonian with random site energies $\varepsilon_{n,m}$ and constant nearest neighbour interactions. The Schoedinger equation then gives a relation between the coefficients in the expansion

$$Ea_{n,m} = \varepsilon_{n,m}\, a_{n,m} - a_{n,m+1} - a_{n,m-1} - a_{n-1,m} - a_{n+1,m} \qquad (42)$$

where we have chosen units of energy so that the hopping elements are unity. This can be written in transfer matrix form as

$$\begin{bmatrix} \mathbf{a}_{n+1} \\ \mathbf{a}_n \end{bmatrix} = \mathbf{M}_n \begin{bmatrix} \mathbf{a}_n \\ \mathbf{a}_{n-1} \end{bmatrix} \qquad (43)$$

where

$$\mathbf{a}_n^{\,T} = [\, a_{n,1}, \ \ldots\ , a_{n,Ly} \,] \qquad (44)$$

Here Ly refers to the number of atoms in the transverse direction, that is the number of sites labelled with the same n. The form of $\mathbf{M}_n$ is easily shown to be

$$\mathbf{M}_n = \begin{bmatrix} \mathbf{H}_n & -\mathbf{I} \\ \mathbf{I} & \mathbf{0} \end{bmatrix} \qquad (45)$$

where $\mathbf{H}_n$ is an Ly x Ly matrix with elements

$$[\, \mathbf{H}_n \,]_{i,j} = (\varepsilon_{n,i} - E)\, \delta i,j - \delta i,j\pm 1 \qquad (46)$$

The distribution of site energies is assumed independent of both n and m, $p(\varepsilon_{n,m}) \equiv p(\varepsilon)$. As in the strictly one

dimensional case we first derive a weak disorder expansion for the exponents and then give a numerical implementation for strong disorder.

4.2 Weak Disorder Expansion

Before applying the symmetry analysis we transform from a real space representation to a momentum space representation

$$\mathbf{M}_n \rightarrow \mathbf{Q}\,\mathbf{M}_n\,\mathbf{Q}^{-1} \tag{47}$$

where $\mathbf{Q}$ and $\mathbf{Q}^{-1}$ are the matrices of left and right eigenvectors of $\langle\mathbf{M}\rangle$. In the limit of zero disorder this transformation diagonalises $\mathbf{Z}$ (and also $\mathbf{X}$)

$$Z(N,\mathbf{Y})\ (l_i : k_i) = Y_{11}^{-L} \prod_{i=2}^{y} Y_{ii}^{\,l_i}\ \delta l_i,k_i \tag{48}$$

and L is given by (28).

We now apply perturbation theory to obtain Γ_p for weak disorder. If we have

$$Y_{11}^{\,L} \neq \prod_{i=2}^{y} Y_{ii}^{\,l_i} \tag{49}$$

for any l_2 .. l_y satisfying (28), we may apply non- degenerate perturbation theory to order var(ε) to obtain $\mu'_o(N)=1$. So under this condition we have

$$\Gamma_p = \mathrm{Re}\ \langle \ln\ (D_p(\mathbf{M}))\rangle \tag{50}$$

When condition (49) is not satisfied we must use degenerate perturbation theory which is a considerable complication. We discuss weak disorder expansions in more detail in chapter V.

4.3 Numerical Implementation

To go beyond perturbation theory we diagonalise the $\mathbf{X}$, or equivalently the $\mathbf{Z}$ matrix, numerically. The simplest non-trivial case to which we can apply the theory is that of a

quasi one dimensional system with two atoms per layer. For such a system $\mathbf{M}_n$ is a 4x4 matrix and $\mathbf{H}_n$ has the form

$$\mathbf{H}_n = \begin{bmatrix} E-\varepsilon_{n,1} & -2 \\ -2 & E-\varepsilon_{n,2} \end{bmatrix} \tag{51}$$

and we assume periodic boundary conditions in the transverse direction. We use a binary alloy distribution for the ε's

$$p(\varepsilon) = \frac{1}{2}\,\delta(\varepsilon-\frac{W}{2}) + \frac{1}{2}\,\delta(\varepsilon+\frac{W}{2}) \tag{52}$$

and we transform to a momentum representation using

$$\mathbf{Q}^{-1}[E + iEc] = \begin{bmatrix} 1 & , & 1 & , & 1 & , & 1 \\ 1 & , & -1 & , & -1 & , & 1 \\ \exp(-i\phi_1), & & \exp(-i\phi_2), & & \exp(i\phi_2), & & \exp(i\phi_1) \\ \exp(-i\phi_1), & & -\exp(-i\phi_2), & & -\exp(i\phi_2), & & \exp(i\phi_1) \end{bmatrix} \tag{53}$$

where

$$E - E_c + 2\cos q_i + 2\cos \phi_i = 0 \tag{54}$$

with $q_1 = 0$ and $q_2 = \pi$. E_c is set non-zero to avoid $\mathbf{Q}$ becoming singular at the sub-band edges of the pure system. We retain a real energy in the definition of $\mathbf{M}_n$ so that the exponents are unchanged. After analytic continuation $\mathbf{X}$ is infinite in size. To proceed with numerical calculations we must make an approximation by truncating $\mathbf{X}$ to a finite size. To do this we set a maximum value for L and K, which we call the order of the X matrix. We can then diagonalise the matrix numerically and see how μ_o changes with order. In table I we show how the truncation size increases with order for the case where the M_n are 4 x 4 matrices and we are calculating Γ_p with p=1,2,3.

Table I

order X	size $X(Y_p)$ p=1,3		size $X(Y_p)$ p=2	
0	1	(1)	1	(1)
1	4	(2)	6	(4)
2	10	(6)	21	(13)
3	20	(10)	56	(32)
4	35	(19)	111	(70)
5	56	(28)	-	-
6	84	(44)	-	-
7	120	(60)	-	-

We are able to make a reduction in the truncation size by noticing that after averaging the **X** matrix is block diagonal. It can be shown that when p=1 or 3 it is only necessary to include elements of $\mathbf{X}(\mathbf{Y}_p)$ for which

$$l_2 + l_3 = k_2 + k_3 \tag{55}$$

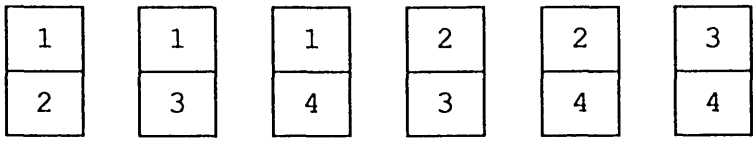
When p=2 we need only include elements of $\mathbf{X}(\mathbf{Y}_2)$ for which

$$l_3 + l_4 = k_3 + k_4 \tag{56}$$

This corresponds to the figures in brackets in Table I. In general we find that μ_o converges quickly and in the following calculations we used a maximum order of 4 for Γ_2 and order 5 for Γ_1 and Γ_3. Convergence is slowest near E=0.

To obtain the maximum exponent, equal to Γ_1 , we need only carry out the symmetric projection as Y_1 is the usual transfer matrix. For E > 0 we allow p_{11} non integer and for E < 0 we allow p_{22} non integer.

To obtain Γ_2, the sum of the two largest exponents we take the antisymmetric projection of $\mathbf{M} \otimes \mathbf{M}$ with respect to the basis vectors defined by the tableaux



(57)

Y_2 is a 6 x 6 matrix and we continue p_{11} at all energies. The smallest positive exponent is found as $\Gamma_2-\Gamma_1$. This gives the longest localisation length, the length relevant to

transport properties. In this case Γ_2 is also the sum of all positive Lyapunov exponents and so the ensemble average integrated density of states $\langle\sigma(E)\rangle$ can be found from its imaginary part [19-20].

Our results for various values of the disorder parameter **W** are plotted against results from a Monte Carlo simulation [5] in figures 1 - 3. The comparisons show good agreement except near E=0. The error arises in the most part from the calculation of the largest exponent as can be seen by reference to fig. 4 where good agreement is obtained for Γ_2 at all energies.

So what is going wrong near E=0? One possibility is a breakdown in the validity of expression (14) for Γ_p. We have been able to rule this out by direct evaluation of (14) using a Monte Carlo simulation. To further check our theory, and also equation (14), we note that because T_L is symplectic, Γ_3 is also equal to the largest exponent. We take the antisymmetric projection of **M** ⊗ **M** ⊗ **M** with respect to the basis

1	1	1	2
2	2	3	3
3	4	4	4

(58)

so Y_3 is a 4 x 4 matrix and we allow p_{11} non integer for E > 0 and p_{22} for E < 0. This give the same results as obtained by calculating Γ_1, with the same problem near E=0.

We conjecture that the source of the disagreement is a breaking of symmetry that is made in the continuation in N. We recall from section 3 that in making the continuation we must know which of the diagonal elements of **Y** has the largest modulus. After the continuation not all the diagonal elements of **Y** remain "equivalent" since **X** contains negative powers of the largest element only and positive powers of all the other diagonal elements. At E=0 there is no unambiguous choice for this largest element and this may be the cause of the disagreement. No such ambiguity arises in the case of Γ_2 and we obtain good agreement at all energies.

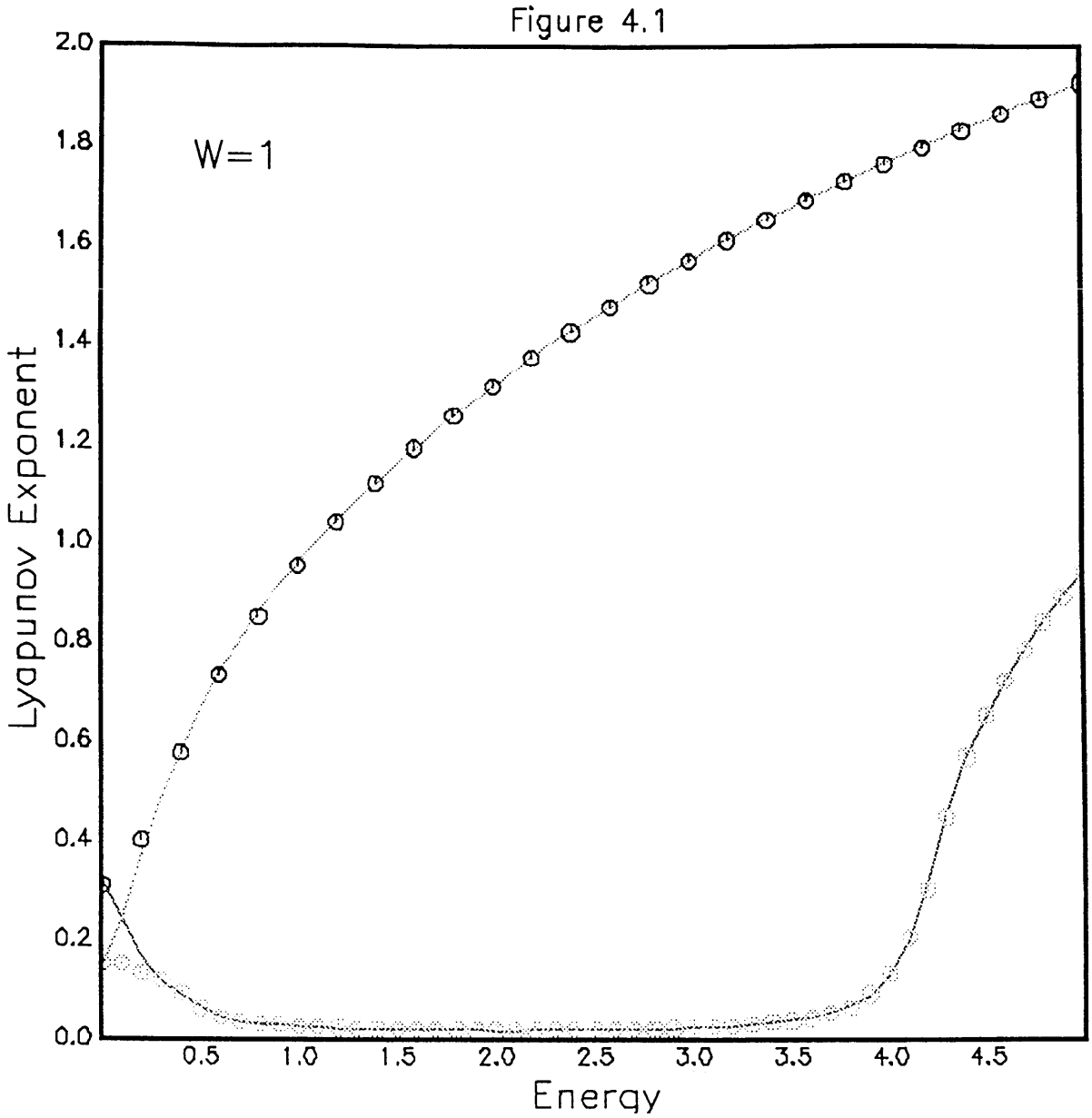


Figure 4.1 - Comparison of Lyapunov exponents obtained from the symmetry reduction (solid line) and numerical simulation (symbols) for disorder W=1. The disagreement near E=0 is discussed in section 4.3.

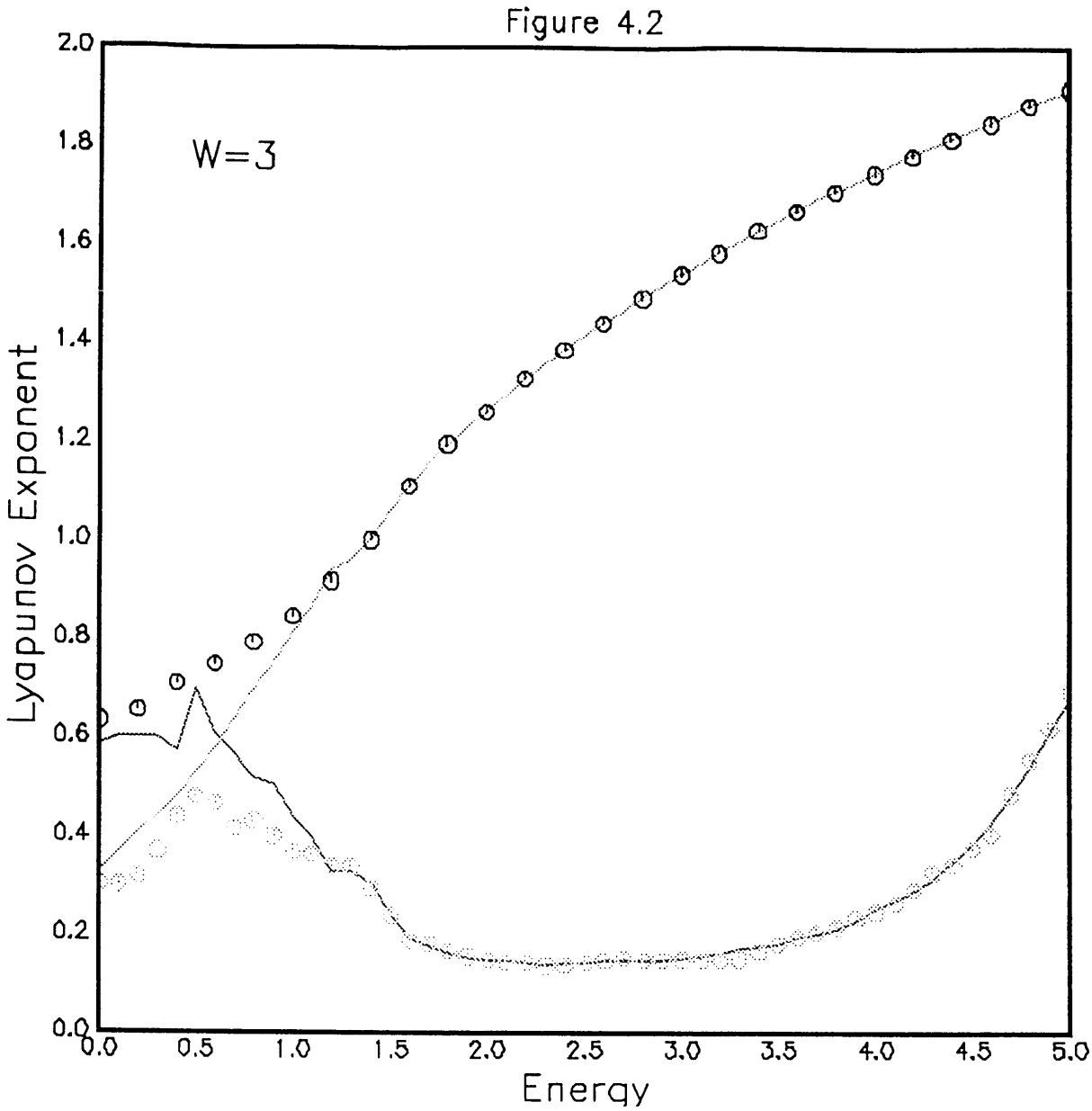


Figure 4.2 - Comparison of Lyapunov exponents obtained from the symmetry reduction (solid line) and numerical simulation (symbols) for disorder W=3

Figure 4.3

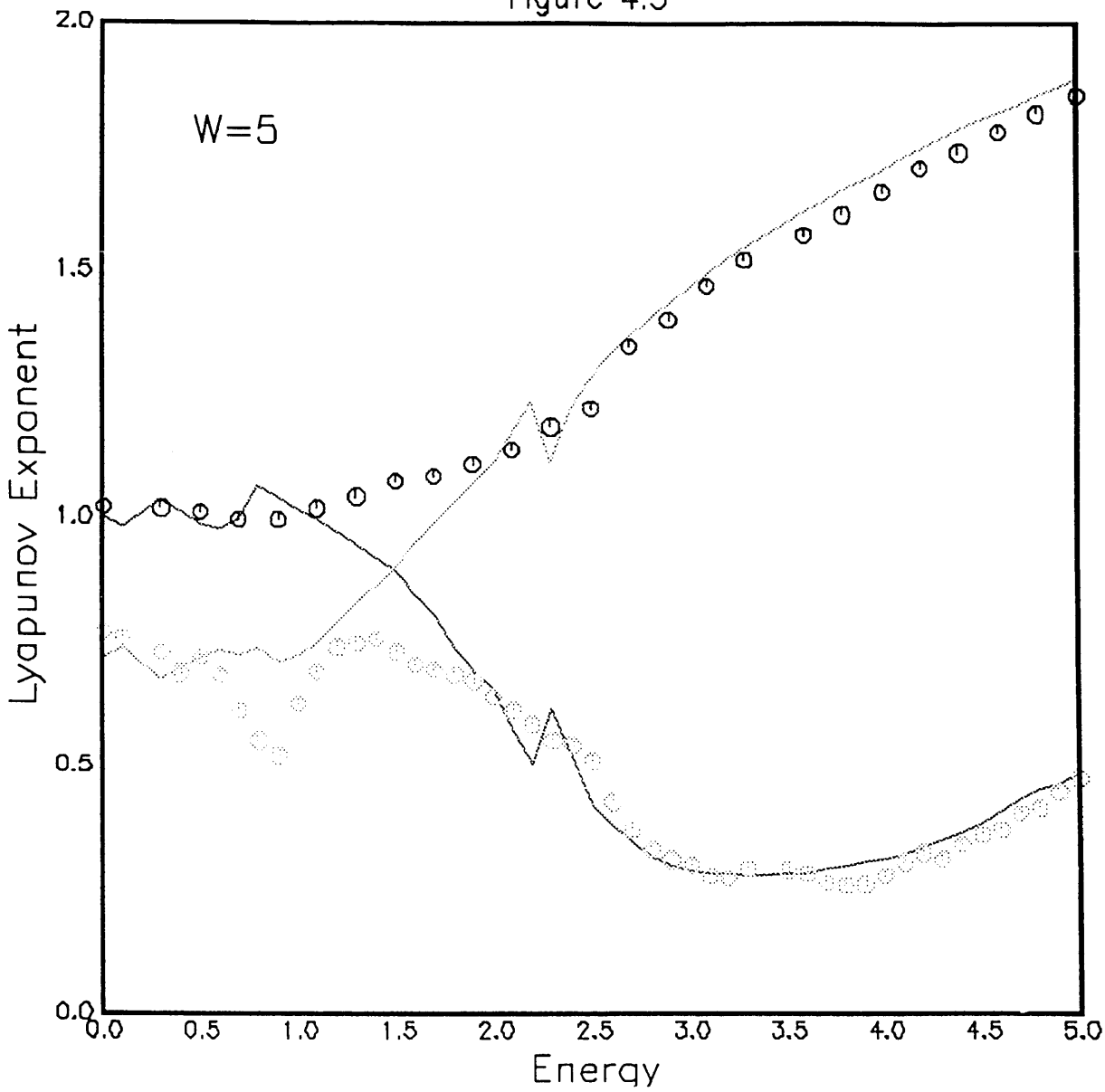


Figure 4.3 - Comparison of Lyapunov Exponents obtained from the symmetry reduction (solid line) and numerical simulation (symbols) for disorder W=5.

Figure 4.4

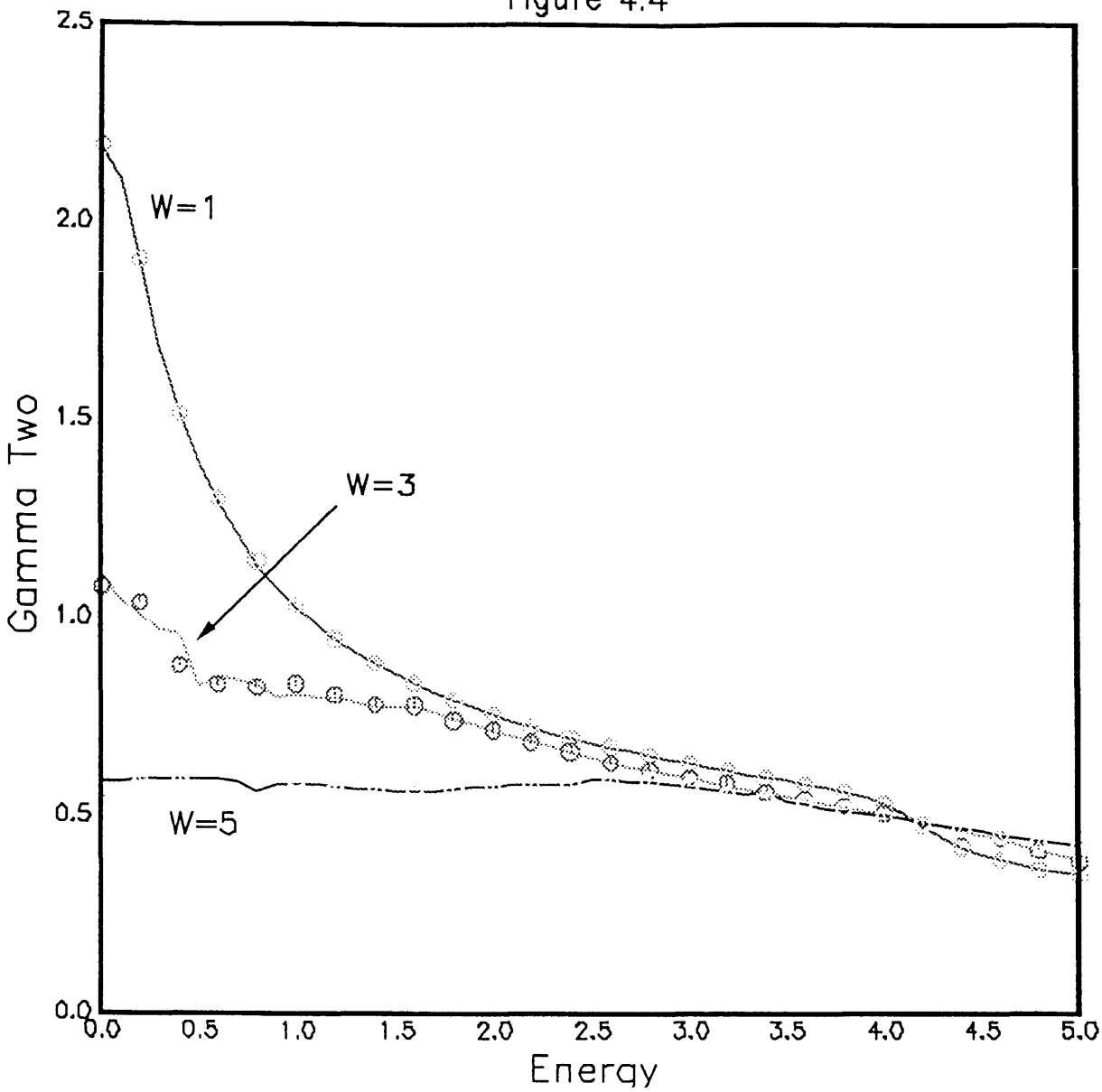


Figure 4.4 - Γ_2 is given correctly at all energies showing that error in the localisation lengths near E=0 arises for the most part in Γ_1.

Appendix I

Here we derive the form of the transfer matrix for a quasi-one dimensional system in terms of its transmission and reflection matrices.

The wave amplitudes on the left of the system $\mathbf{a}(+)$ and $\mathbf{a}(-)$ are related to those on the right $\mathbf{b}(+)$ and $\mathbf{b}(-)$ by transfer matrix $\mathbf{T}$

$$\begin{bmatrix} \mathbf{b}(+) \\ \mathbf{b}(-) \end{bmatrix} = \mathbf{T} \begin{bmatrix} \mathbf{a}(+) \\ \mathbf{a}(-) \end{bmatrix} \tag{1}$$

where + and - refer to the direction of propagation in the z or longitudinal direction. The main difference with the strictly one dimensional system is that $\mathbf{a}(+)$, $\mathbf{a}(-)$, $\mathbf{b}(+)$ and $\mathbf{b}(-)$ are now vectors, the components corresponding to the different transverse modes present in systems with finite transverse dimension.

The transmission and reflection matrices of the system are defined by the relations

$$\begin{aligned} \mathbf{b}(+) &= \mathbf{t}'\,\mathbf{a}(+) + \mathbf{r}\,\mathbf{b}(-) \\ \mathbf{a}(-) &= \mathbf{t}\,\mathbf{b}(-) + \mathbf{r}'\,\mathbf{a}(+) \end{aligned} \tag{2}$$

which are easily re-arranged to give the form of $\mathbf{T}$

$$\mathbf{T} = \begin{bmatrix} \mathbf{t}' - \mathbf{r}\,\mathbf{t}^{-1}\,\mathbf{r}' & , \mathbf{r}\,\mathbf{t}^{-1} \\ -\mathbf{t}^{-1}\,\mathbf{r}' & , \mathbf{t}^{-1} \end{bmatrix} \tag{3}$$

As in the strictly one-dimensional case we simplify (3) by by assuming the system has time reversal symmetry. This symmetry and equation (1) imply that[2]

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[2] We assume that under the time reversal operation the longitudinal wave number k_z maps to $-k_z$ and we describe the transformation of the transverse momenta by a matrix $\mathbf{U}$.

$$\begin{bmatrix} \mathbf{U}\,\mathbf{b}(-)^{*} \\ \mathbf{U}\,\mathbf{b}(+)^{*} \end{bmatrix} = \mathbf{T} \begin{bmatrix} \mathbf{U}\,\mathbf{a}(-)^{*} \\ \mathbf{U}\,\mathbf{a}(+)^{*} \end{bmatrix} \tag{4}$$

where $\mathbf{U}$ represents the operation of time reversal in the representation of the transverse channels. A repetition of the time reversal operation will map the system back onto itself and so we must have $\mathbf{U}^2=\mathbf{I}$. Equation (4) yields the following symmetry relation for $\mathbf{T}$

$$\begin{bmatrix} 0 & \mathbf{U} \\ \mathbf{U} & 0 \end{bmatrix} \mathbf{T} \begin{bmatrix} 0 & \mathbf{U} \\ \mathbf{U} & 0 \end{bmatrix} = \mathbf{T}^{*} \tag{5}$$

Using this relation we can now simplify $\mathbf{T}$

$$\mathbf{T} = \begin{bmatrix} \mathbf{U}\,[t^{-1}]^{*}\,\mathbf{U} & , & \mathbf{r}\,t^{-1} \\ \mathbf{U}\,[\mathbf{r}\,t^{-1}]^{*}\,\mathbf{U} & , & t^{-1} \end{bmatrix} \tag{6}$$

As in the strictly one dimensional case unitarity of the scattering matrix implies the flux conservation rule

$$t^{+}t + r^{+}r = I \tag{7}$$

References

[1] Oseledec V I Trans. Moscow Math. Soc. 19 197 (1968)

[2] Thouless D J Phys. Rev. Lett. 39 1167 (1977)

[3] Ishii K Prog. Theor. Phys. Supp. 53 77 (1973)

[4] Furstenberg H Trans. Amer. Math. Soc. 108 377 (1963)

[5] Mac Kinnon A and Kramer B Z. Phys. B 53 1 (1983)

[6] Pichard J L and Sarma G J. Phys. C 14 L127 (1981)

[7] Pichard J L and Sarma G J. Phys. C 14 L617 (1981)

[8] Bulka B R and Kramer B Z. Phys. B 60 13 (1985)

[9] Schreiber M, Kramer B and Mac Kinnon A Physica Scripta T25 67 (1989)

[10] Liebert A D Phd Thesis University of Cambridge (1989)

[11] Schweitzer L, Kramer B and Mac Kinnon A J. Phys. C 17 4111 (1984)

[12] Abrahams E, Anderson P W, Licciardello D C and Ramakrishnan T V Phys. Rev. Lett. 42 673 (1979)

[13] Imry Y Europhysics Lett. 1 5 (1986)

[14] Pichard J L and Andre G Europhysics Lett. 2 477 (1986)

[15] Muttalib K A, Pichard J L and Stone A D 59 2475 (1987)

[16] Zanon N and Pichard J L J. Phys. France 49 907 (1988)

[17] Mello P Phys. Rev. Lett. 60 1089 (1988)

[18] Derrida, Mecheri and Pichard J L Journal de Physique 48 733 (1987)

[19] Pendry J B and Castano E Physical Review Lett. 60 20 2093 (1988)

[20] Pendry J B and Castano E Journal of Physics C 21 4333-4355 (1988)

Chapter V - Weak Disorder Expansions for the Lyapunov Exponents of Disordered Quasi-One Dimensional Systems

1. Introduction

This chapter is concerned with the development of weak disorder expansions for the Lyapunov exponents associated with a product of random matrices.

It has been shown in the previous chapters that the scattering properties of a disordered system can be described by a transfer matrix **T** and that this matrix is in general given by a product of random matrices

$$\mathbf{T} = \prod_n \mathbf{M}_n \qquad (1)$$

where each M_n is independently and identically distributed according to some distribution $p(\mathbf{M})$. It is usually possible by grouping terms appropriately to write (1) in the form

$$\mathbf{T} = \prod_n (\mathbf{A} + \mu \mathbf{B}_n) \qquad (2)$$

where **A** is fixed non-random matrix, the $\mathbf{B}_n$'s are a set of independent and identically distributed random matrices and μ is a small parameter. In general this parameter describes the strength of the disorder. It is then legitimate to ask what is the expansion in terms of μ for the Lyapunov exponents[1] associated with the matrix product.

In strictly one dimensional systems there is a single positive exponent.[2] The reciprocal of this exponent is the mean localisation length for electrons in the system and a

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[1] These exponents are defined in section 2 of chapter IV.

[2] As mentioned in chapter IV the exponents occur in pairs of opposite sign.

number of authors [1-6] have calculated the weak disorder expansion of this quantity. The situation for one dimensional systems of finite cross section is not as satisfactory. In general there will be as many positive exponents as there are atoms in the cross section of the system or equivalently as many as there are transverse normal modes. Derrida et al [7] have developed an expansion for these exponents which is valid provided that all the eigenvalues of the fixed matrix **A** have different modulli. Their derivation is based on an expansion in powers of μ of the determinant in equation (14) of chapter IV. In section 2 we rederive their result using a more direct method. We then consider the difficulties that arise in application of the expansion to the Anderson model (section 3.) We show that to a certain extent these difficulties may be overcome by the introduction of a complex energy. In section 4 we generalise the approach by introducing a set of complex energy parameters. We then propose a set of self consistent conditions on this set of parameters and in this way we are able to apply the expansion without the need for arbitrary parameters.

In addition to the work presented in this chapter the interested reader is referred to the work of Zanon et al. [8] which attempts to treat degeneracies in the eigenvalues of **A** in a more fundamental manner.

2. Weak Disorder Expansion

In this section we develop a weak disorder expansion for the Lyapunov exponents of a product of random matrices $\mathbf{T}_L$ where

$$\mathbf{T}_L = \prod_{n=1}^{L} (\mathbf{A} + \mu \mathbf{B}_n) \tag{3}$$

Matrix **A** is a fixed diagonal matrix of the form

$$A_{ij} = w_i \, \delta_{ij} \tag{4}$$

and $\{\mathbf{B}_n : n=1,L\}$ are random matrices. These are assumed independently and identically distributed with probability

distribution p(**M**). The expansion we develop here will be valid provided that

$$|w_i| \neq |w_j| \text{ if } i \neq j \tag{5}$$

In the limit that L tends to infinity a limiting matrix Γ exists [9]

$$\Gamma = \lim_{L\to\infty} [\, \mathbf{T}_L^{+}\, \mathbf{T}_L \,]^{1/2L} \tag{6}$$

The Lyapunov exponents are defined as the logarithms of the eigenvalues of the matrix Γ. Here we will estimate the jth exponent α_j as

$$\alpha_j = \lim_{L\to\infty} (1/L) \;\; \mathrm{Re} \langle \log w'_j \rangle \tag{7}$$

where w'_j is the jth eigenvalue of $\mathbf{T}_L$. The reciprocals of the exponents are referred to as the localisation lengths.

We expand the product in (3) as series in powers of μ

$$\mathbf{T}_L = \mathbf{A}^L + \mu\mathbf{C} + \mu^2\mathbf{D} + O(\mu^3) \tag{8}$$

where

$$\mathbf{C} = \sum_{n=1}^{L} \mathbf{A}^{L-n}\, \mathbf{B}_n\, \mathbf{A}^{n-1} \tag{9}$$

$$\mathbf{D} = \sum_{n>m}^{L} \mathbf{A}^{L-n}\, \mathbf{B}_n\, \mathbf{A}^{n-m-1}\, \mathbf{B}_m\, \mathbf{A}^{m-1} \tag{10}$$

Using standard non-degenerate perturbation theory we obtain the ith eigenvalue w'_j of $\mathbf{T}_L$ as

$$w'_i = w_i^L + \mu C_{ii} + \mu^2 D_{ii} + \mu^2 \sum_{j\neq i} \frac{C_{ij}C_{ji}}{w_i^L - w_j^L} + O(\mu^3) \tag{11}$$

If we expand the logarithm of (11), substitute for matrices **C** and **D**, and average over the distribution p(**M**) we obtain in the limit as L->∞

$$\alpha_i = \mathrm{Re}\Big[\log w_i - \frac{\mu^2 \langle B_{ii}^2 \rangle}{2w_i^2} - \sum_{|w_j|>|w_i|} \mu^2 \frac{\langle B_{ij}B_{ji} \rangle}{w_i w_j} \Big] \tag{12}$$

and we have assumed here that

$$\langle \mathbf{B} \rangle = 0 \tag{13}$$

In taking the L->∞ limit we have evaluated

$$\lim_{L\to\infty} \frac{w_j^L}{w_i^L - w_j^L} = \begin{cases} 0 & |w_i| > |w_j| \\ -1 & |w_i| < |w_j| \end{cases} \tag{14}$$

This requires that w_j and w_i have different moduli and this is the origin of the condition (5) on **A**.

If condition (5) is not satisfied the it is still possible to make some progress using this method. Suppose that two eigenvalues w_i and w_j have the same modulus but are not actually equal, and that all other eigenvalues have distinct modulli. Then we can find the sum of the related exponents

$$\alpha_i + \alpha_j = \mathrm{Re}\Big[\log w_i - \frac{\mu^2 \langle B_{ii}^2 \rangle}{2w_i^2} - \sum_{|w_k|>|w_i|} \mu^2 \frac{\langle B_{ik} B_{ki} \rangle}{w_i w_k}$$

$$+ \log w_j - \frac{\mu^2 \langle B_{jj}^2 \rangle}{2w_j^2} - \sum_{|w_k|>|w_j|} \mu^2 \frac{\langle B_{jk} B_{kj} \rangle}{w_j w_k}$$

$$- \mu^2 \frac{\langle B_{ij} B_{ji} \rangle}{w_i w_j} \Big] \tag{15}$$

There is no ambiguity here in the L->∞ limit because of a fortuitous summing of terms

$$\frac{w_j^L}{w_i^L - w_j^L} + \frac{w_i^L}{w_j^L - w_i^L} = -1 \tag{16}$$

The results are easily generalised when

$$\langle \mathbf{B} \rangle \neq 0 \tag{17}$$

in which case the expansion (12) becomes

$$\alpha_i = \mathrm{Re}\Big[\log w_i + \frac{\mu\langle B_{ii}\rangle}{w_i} - \frac{\mu^2\langle B_{ii}^2\rangle}{2w_i^2} \tag{18}$$

$$- \sum_{|w_j|>|w_i|} \frac{\mu^2\langle B_{ij}\rangle\langle B_{ij}\rangle}{w_i w_j} \frac{w_j}{w_i - w_j}$$

$$- \sum_{|w_j|<|w_i|} \frac{\mu^2\langle B_{ij}\rangle\langle B_{ji}\rangle}{w_i w_j} \frac{w_i}{w_j - w_i}$$

$$- \sum_{|w_j|>|w_i|} \frac{\mu^2\langle B_{ij}B_{ji}\rangle}{w_i w_j}$$

3. Application of the Expansion to the Anderson Model

The Anderson model for disordered quasi-one dimensional systems was described in section 4.1 of Chapter IV. We recall that the electronic wave function $\Phi(\mathbf{r})$ of the system is expanded as linear combination of atomic wavefunctions $\Phi_{n,m}(\mathbf{r})$

$$\Phi(\mathbf{r}) = \sum_{n=-\infty}^{n=+\infty} \sum_{m=1}^{Ly} a_{n,m}\, \Phi_{n,m}(\mathbf{r} - \mathbf{r}_{n,m}) \tag{19}$$

and that the coefficients in the expansion obey the relation

$$E\, a_{n,m} = \varepsilon_{n,m}\, a_{n,m} - \beta_t\, a_{n,m-1} - \beta_t\, a_{n,m+1} \tag{20}$$
$$- a_{n-1,m} - a_{n+1,m}$$

Here we have introduced β_t, the ratio of the longitudinal and transverse hopping integrals. The ε's are distributed according to

$$p(\varepsilon_{n,m}) = p(\varepsilon) \quad \text{for } 1 \le n \le Lz \text{ and all } m \tag{21}$$
$$= \delta(\varepsilon - \langle\varepsilon\rangle) \quad \text{for all other n and m}$$

This corresponds to a disordered region of width Ly and length Lz embedded between two semi-infinite ordered sections. The relation for the expansion coefficients is

conveniently re-written in terms of a real space transfer matrix as

$$\begin{bmatrix} \mathbf{a}_{n+1} \\ \mathbf{a}_n \end{bmatrix} = \mathbf{M}_n \begin{bmatrix} \mathbf{a}_n \\ \mathbf{a}_{n-1} \end{bmatrix} \tag{22}$$

where $\mathbf{a}_n^T = [\, a_{n,1}, \ldots\ldots, a_{n,Ly} \,]$ and

$$\mathbf{M}_n = \begin{bmatrix} \mathbf{H}_n & -\mathbf{I} \\ \mathbf{I} & \mathbf{0} \end{bmatrix} \tag{23}$$

Here $\mathbf{H}_n$ is an Ly x Ly matrix with elements[3]

$$[\mathbf{H}_n]_{i,j} = (\varepsilon_{n,i} - E)\, \delta_{i,j} - \delta_{i,j\pm1} \tag{24}$$

The transfer matrix which describes the scattering of Bloch wave states incident form the semi-infinite ordered sections or leads is given by transforming to momentum space

$$\mathbf{T}_{Lz} \;\rightarrow\; \mathbf{Q}\, \mathbf{T}_{Lz}\, \mathbf{Q}^{-1} = \prod_{n=1}^{Lz} [\, \mathbf{Q}\, \mathbf{M}_n\, \mathbf{Q}^{-1} \,] \tag{25}$$

The transformation matrices $\mathbf{Q}$ and $\mathbf{Q}^{-1}$ are respectively the matrices of left and right eigenvectors of $\langle \mathbf{M} \rangle$,

$$\mathbf{Q}^{-1} = \begin{bmatrix} \mathbf{x}_q & , \mathbf{x}_q \\ \mathbf{x}_q\, e^{-i\Theta q} & , \mathbf{x}_q\, e^{+i\Theta q} \end{bmatrix} \tag{26}$$

where x_q (q=1,..,Ly) is a column vector with components

$$[\mathbf{x}_q]_j = \sin(\, k_q j \,) \qquad j = 1,..,Ly \tag{27}$$

and

$$k_q = \frac{q\pi}{Ly+1} \qquad q = 1,..,Ly \tag{28}$$

---

[3] We set $H_{1,Ly} = H_{Ly,1} = 0$ corresponding to fixed boundary conditions.

and also

$$E - \langle\varepsilon\rangle + 2\cos k_q + 2\cos\Theta_q = 0 \qquad q = 1,..,Ly \qquad (29)$$

The form of (29) implies that we can set $\langle\varepsilon\rangle=0$ without loss of generality, this defines the zero of energy E. We now set

$$\mathbf{A} \equiv \mathbf{Q} \langle\mathbf{M}\rangle \mathbf{Q}^{-1} \qquad (30)$$

so that **A** is immediately diagonal

$$A_{p,q} = w_q \delta_{p,q} \qquad (31)$$

with

$$w_q = \exp(+i\Theta_q) \qquad q = 1, \ldots\ldots, Ly$$
$$= \exp(-i\Theta_{q-Ly}) \qquad q = Ly+1, \ldots, 2Ly$$

(The reader should note that equation (29) only defines Θ_q up to an arbitrary sign $\pm\Theta_q$. We shall assume that the Θ's are chosen so that $|w_q| \geq 1$ for $q=1,\ldots,Ly$.) The random elements are collected in matrix $\mathbf{B}_n$

$$\mu\mathbf{B}_n \equiv \mathbf{Q} [\mathbf{M}_n - \langle\mathbf{M}\rangle] \mathbf{Q}^{-1} \qquad (32)$$

or more explicitly

$$\mu\mathbf{B}_n = \begin{bmatrix} \boldsymbol{\Omega}_n & \boldsymbol{\Omega}_n \\ \boldsymbol{\Omega}'_n & \boldsymbol{\Omega}'_n \end{bmatrix} \qquad (33)$$

Here $\boldsymbol{\Omega}_n$ and $\boldsymbol{\Omega}'$ are Ly x Ly matrices with elements

$$[\boldsymbol{\Omega}_n]_{p,q} = \frac{2\beta_p w_p}{Ly+1} \sum_{j=1}^{Ly} \varepsilon_{j,n} \sin(k_p j) \sin(k_q j) \qquad (34)$$

$$[\boldsymbol{\Omega}'_n]_{p,q} = \frac{-2\beta_p w_{p+Ly}}{Ly+1} \sum_{j=1}^{Ly} \varepsilon_{j,n} \sin(k_p j) \sin(k_q j) \qquad (35)$$

and

$$\beta_q = \frac{-1}{2i\sin(\Theta_q)} \qquad q = 1, \ldots, Ly$$

If we now apply the weak disorder expansion we obtain for the positive exponents (p=1, .. ,Ly)

$$\alpha_p = \mathrm{Re}\ [\ i\Theta_p \ - \ \beta_p^{\,2}\ g_{p,p}\ \frac{<\varepsilon^2>}{2} \qquad (36)$$

$$- \sum_{|w_q| > |w_p|} \beta_p\ \beta_q\ g_{p,q}\ \frac{<\varepsilon^2>}{2}\ ]$$

where

$$g_{p,q} = \sum_{j=1}^{Ly} \sin^2(k_p j)\ \sin^2(k_q j) \qquad (37)$$

The expansion is valid provided that **A** satisfies condition (5). This condition is in fact very restrictive since for any energy E such that

$$|\ E + 2\cos k_q\ |\ \leq 2 \qquad (38)$$

we have

$$|w_q| = |w_{q+Ly}| \qquad (39)$$

for that particular q so that condition (5) is not satisfied. This degeneracy can be broken by introducing an imaginary part to the energy Ec. We set

$$\mathbf{A} \equiv \mathbf{Q}(E+iEc)\ <\mathbf{M}(E+iEc)>\ \mathbf{Q}(E+iEc)^{-1} \qquad (40)$$

and

$$\mu\mathbf{B}_n \equiv \mathbf{Q}(E+iEc)\ [\mathbf{M}_n(E+iEc) - <\mathbf{M}(E+iEc)>]\ \mathbf{Q}(E+iEc)^{-1} \qquad (41)$$

In this case the formal expressions for the expansion are unchanged except that we now replace Θ_q with ϕ_q where

$$E + iEc + 2\cos k_q + 2\cos\phi_q = 0 \qquad q=1,..,Ly \qquad (42)$$

There will also be other accidental degeneracies which will make the expansion inapplicable at specific energies even with the use of a complex energy. In figure 5.1 we consider the simplest non-trivial case; Ly=2, β_t=2 and Ec=-0.01. We use a continuous distribution of site energies

$$p(\varepsilon) = \frac{1}{W} \qquad |\varepsilon| \leq \frac{W}{2} \qquad (43)$$

$$= 0 \qquad \text{otherwise}$$

Figure 5.1

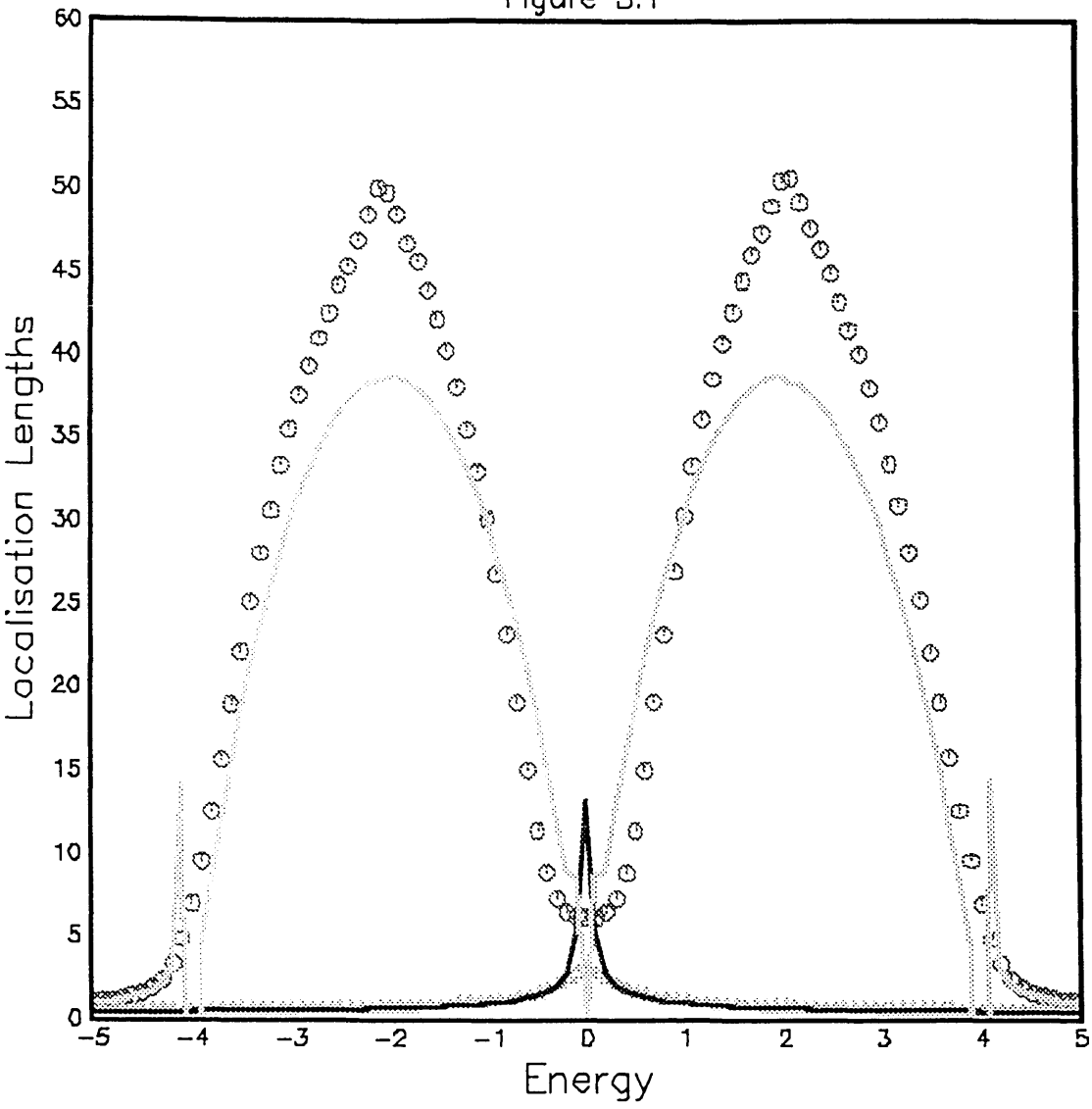

Figure 5.1 - Energy dependence of the localisation lengths for the case Ly=2, β_t=2 with a continuous site energy distribution of width W=2. We compare the results of a Monte-Carlo simulation (symbols) with the perturbation expansion (line) based around equations (36) and (40-42) of the text, with Ec=-0.01.

with W=2 and compare the results of a numerical simulation[4] with the perturbation expansion. We see that the expansion is badly behaved at energies E=+4 and -4 and E=0. These correspond to subband edges of the pure system (W=0) where

$$| E + 2\beta_t \cos k_q | = 2 \qquad (44)$$

A careful analysis shows that near such energies the terms in the expansion (36) of the longer length become almost purely imaginary leading to a divergence in the estimate of the localisation length. This does not occur in the estimate for the shorter length. At E=0 a further problem arises since

$$|w_1| = |w_2| \qquad (45)$$

Here the perturbation estimates for both lengths are badly behaved since condition (5) is violated. This is an example of an accidental degeneracy.

It has been seen above that the application of the perturbation expansion necessitates the introduction of an arbitrary parameter Ec. This has the problematic effect that we no longer obtain the correct zero disorder limit when $<\varepsilon^2>=0$. In fact we obtain the correct zero disorder limit for the Schroedinger equation

$$H \Phi = (E + iEc) \Phi \qquad (46)$$

but not for the case we are actually interested in

$$H \Phi = E \Phi \qquad (47)$$

This difficulty can be overcome by setting

$$\mathbf{A} \equiv \mathbf{Q}(E+iEc) \, <\mathbf{M}(E+iEc)> \, \mathbf{Q}(E+iEc)^{-1} \qquad (48)$$

as before but

$$\mu\mathbf{B}_n \equiv \mathbf{Q}(E+iEc) \, [\mathbf{M}_n(E) - <\mathbf{M}(E+iEc)>] \, \mathbf{Q}(E+iEc)^{-1} \qquad (49)$$

---

[4] The simulation technique is described in appendix I of this chapter.

This alters the form of $\mathbf{B}_n$ through a change in the form of the matrices $\mathbf{\Omega}_n$ and $\mathbf{\Omega'}_n$

$$[\mathbf{\Omega}_n]_{p,q} \rightarrow [\mathbf{\Omega}_n]_{p,q} - \beta_q w_q Ec \delta_{p,q} \qquad (50)$$

$$[\mathbf{\Omega'}_n]_{p,q} \rightarrow [\mathbf{\Omega'}_n]_{p,q} + \beta_q w_{q+Ly} Ec \delta_{p,q}$$

It is clear from these expressions that after this transformation $\langle \mathbf{B} \rangle \neq 0$ if $Ec \neq 0$. We can avoid many of the complications that this implies by making the simple observation that in the limit of zero disorder we have

$$\alpha_p = Re [i\Theta_p] \quad p = 1, .. , Ly \qquad (51)$$

This follows since the transformation (48-49) cannot alter the eigenvalues of $\mathbf{T}_L$. We therefore know that all terms in the expansion which do not go to zero in the zero disorder limit must resum at all orders to give (51). With this in mind it is now clear that we can write

$$\alpha_p = Re [i\Theta_p - \beta_p^2 g_{p,p} \frac{\langle \varepsilon^2 \rangle}{2} \qquad (52)$$

$$- \sum_{|w_q| > |w_p|} \beta_p \beta_q g_{p,q} \frac{\langle \varepsilon^2 \rangle}{2}]$$

where

$$w_q = \exp(+i\phi_q) \qquad q = 1, ... , Ly \qquad (53)$$

$$= \exp(-i\phi_{q-Ly}) \qquad q = Ly+1, .. , 2Ly$$

and

$$\beta_q = \frac{-1}{2i\sin(\phi_q)} \qquad q = 1, ... , Ly \qquad (54)$$

This gives the correct zero disorder limit for (47). In Figure 5.2 we plot the results of this perturbation expansion against those of the numerical simulation. We use the same parameters W=2, β_t=2, Ec=-0.01 and W=2. The agreement is considerably improved at nearly all energies but problems still occur at the sub-band edges of the pure system, corresponding to the zero disorder limit (W=0) of (47).

Figure 5.2

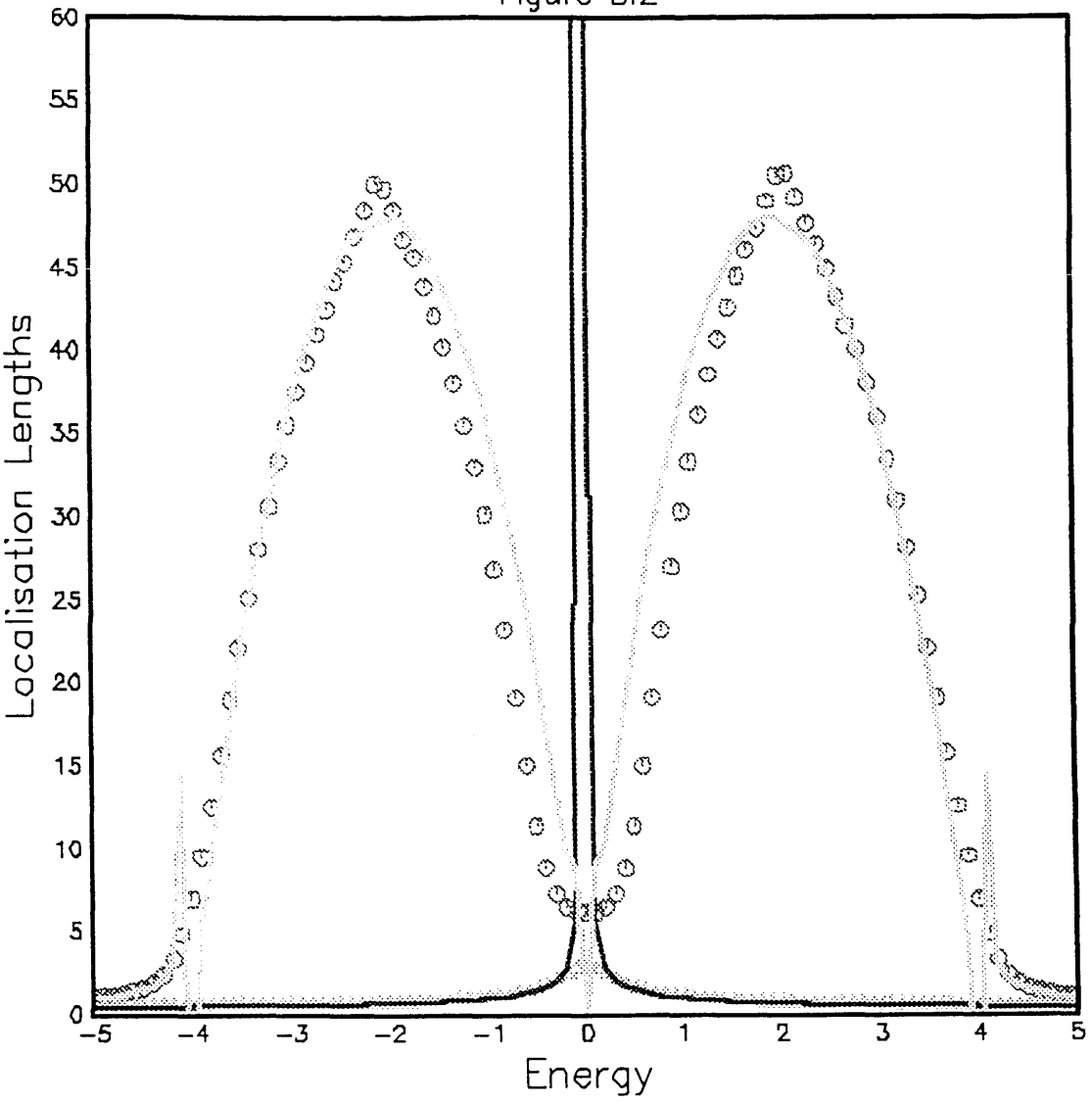

Figure 5.2 - Energy dependence of the localisation lengths for the case Ly=2, $ß_t$=2 with a continuous site energy distribution of width W=2. We compare the results of a Monte-Carlo simulation (symbols) with the perturbation expansion (line) based around equations (52), with Ec=-0.01.

4. A Self Consistent Approximation

In the last section we discussed how the application of the weak disorder expansion of section 5.2 to the Anderson model requires the introduction of an arbitrary complex energy parameter Ec. In this section we show how by making a generalisation to a set of complex parameters Ec^q q=1,..,Ly it is possible to obtain self consistent approximations for the values of these parameters and hence eliminate the necessity for arbitrary parameters.

Consider set of values Ec^q q=1,..,Ly. By generalising equation (42) we can define a set of parameters ϕ_q q=1,..,Ly

$$E + iEc^q + 2\cos k_q + 2\cos\phi_q = 0 \qquad q=1,..,Ly \tag{55}$$

It will be convenient in what follows to consider the ϕ_q as the set of free parameters which define the Ec^q rather than vice versa. In the context of the section 3 the parameters ϕ_q define the basis in which the perturbation expansion is carried out. We now use the perturbation expression (52) to define a set of variables ϕ'_p p=1,..,Ly

$$i\phi'_p = i\Theta_p - \beta_p^2 g_{p,p} \frac{\langle\varepsilon^2\rangle}{2} - \sum_{|w_q| > |w_p|} \beta_p \beta_q g_{p,q} \frac{\langle\varepsilon^2\rangle}{2} \tag{56}$$

where

$$\beta_p = \frac{-1}{2i\sin(\phi_p)} \qquad p=1,..,Ly \tag{57}$$

The self consistency condition is now rather obvious

$$\phi'_p = \phi_p \qquad p=1,..,Ly \tag{58}$$

If this condition can be met we identify the Lyapunov exponents as

$$\alpha_p = \mathrm{Re}[\, i\phi_p \,] \qquad p=1, \ldots ,Ly \tag{59}$$

The basic idea behind the set of self consistent equations (56) is straight forward. In estimating the localisation lengths from the perturbation expansion we have a large

degree of freedom as to the basis in which we make the expansion, the only restriction being the condition (5) on **A**. Here we choose a set of decaying plane waves with decay lengths equal to the perturbation estimates of the localisation lengths. Equation (56) is a sufficient condition for this equality but not a necessary condition. In fact only equality of the real parts of both sides of (56) is required. We introduce the extra restriction on the imaginary parts so as to obtain a unique solution. The most reliable way to solve the set of simultaneous non-linear equations implied by (56) is through the use of the NAG routine C05NBF. This is a general purpose routine for the solution of non linear equations.

In Figure 5.3 we compare the results of the self consistent approximation with those of the numerical simulation for the parameters Ly=2, $ß_t$=2, Ec=-0.01 and W=2 used in section 3. We have excellent agreement at virtually all energies including near two of the sub-band edges E=4 and -4. At E=0 the more fundamental problem of degeneracy in the modulli of eigenvalues corresponding to different transverse momenta k_q remains a problem and cannot be dealt with using this self consistent technique. A more careful treatment of this type of degeneracy has been given by Zanon and Derrida [8].

The results for Ly=2 above are quite reasonable but the limitations of the method quickly become apparent when considering wider chains. In Figures 5.4 to 5.6 we present results for the case Ly=5, $ß_t$=1 with a binary site energy distribution

$$p(\varepsilon) = \frac{1}{2}\left[\, \delta(\varepsilon-\frac{W}{2}) + \delta(\varepsilon+\frac{W}{2}) \,\right] \qquad (60)$$

with W=1. Here we have used a simulation program provided by A. MacKinnon. We find that it is not possible to find a solution at all energies to the equations (56) in this case. A solution for the entire set of equations (p=1,..,5) is only possible for energies above E≈3.0 and below E≈-3.0.

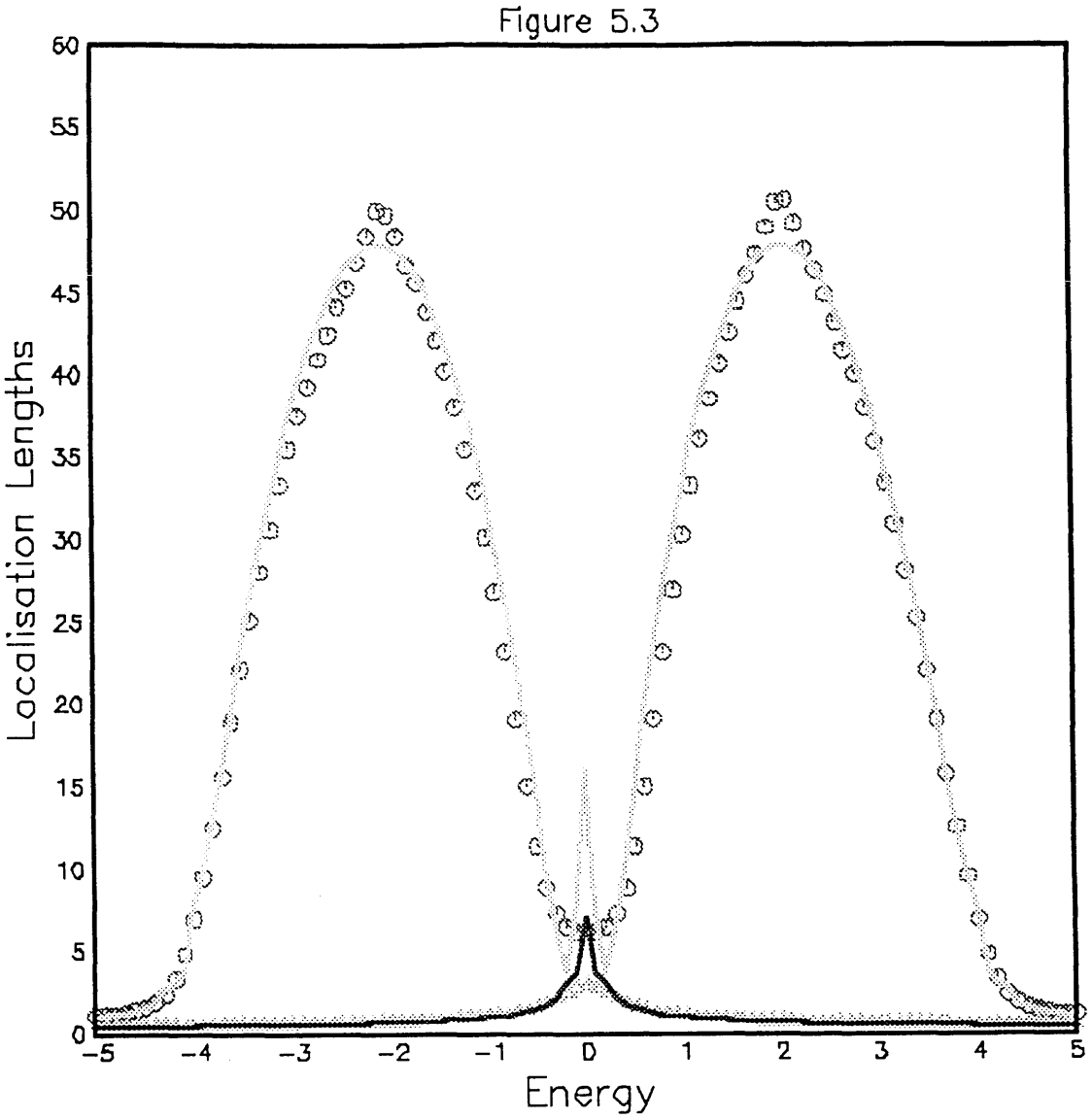

Figure 5.3 - Energy dependence of the localisation lengths for the case Ly=2, β_t=2 with a continuous site energy distribution of width W=2. We compare the results of the self consistent approximation (line) with a Monte-Carlo simulation (symbols).

Figure 5.4

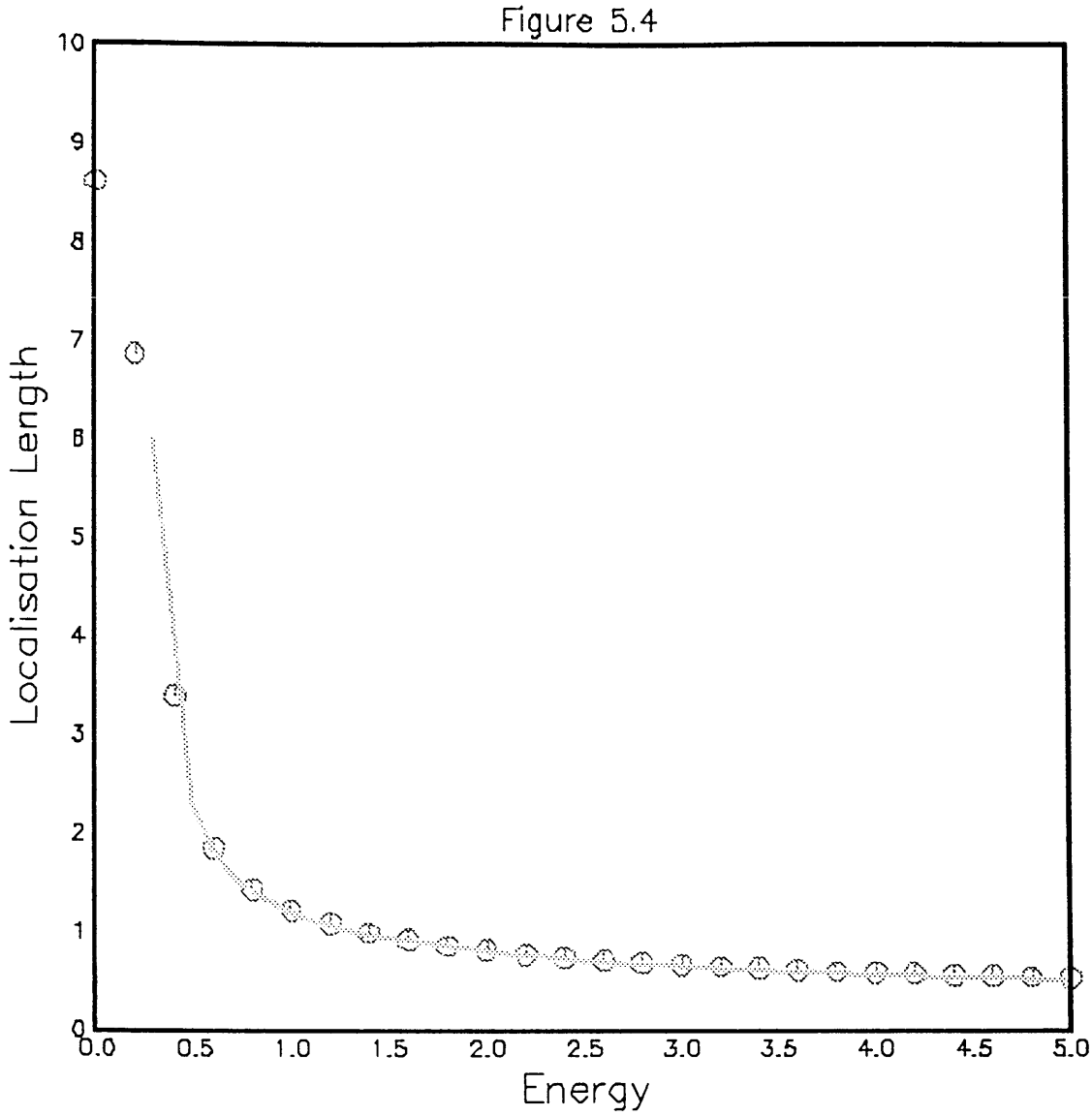

Figure 5.4 - Energy dependence of the shortest localisation length for the case Ly=5, $ß_t$=1 with a binary site energy distribution of width W=1. We compare the results of the self consistent approximation (line) with a Monte-Carlo simulation (symbols), below E≈0.3 we are unable to find a solution to the self consistent equation.

Figure 5.5

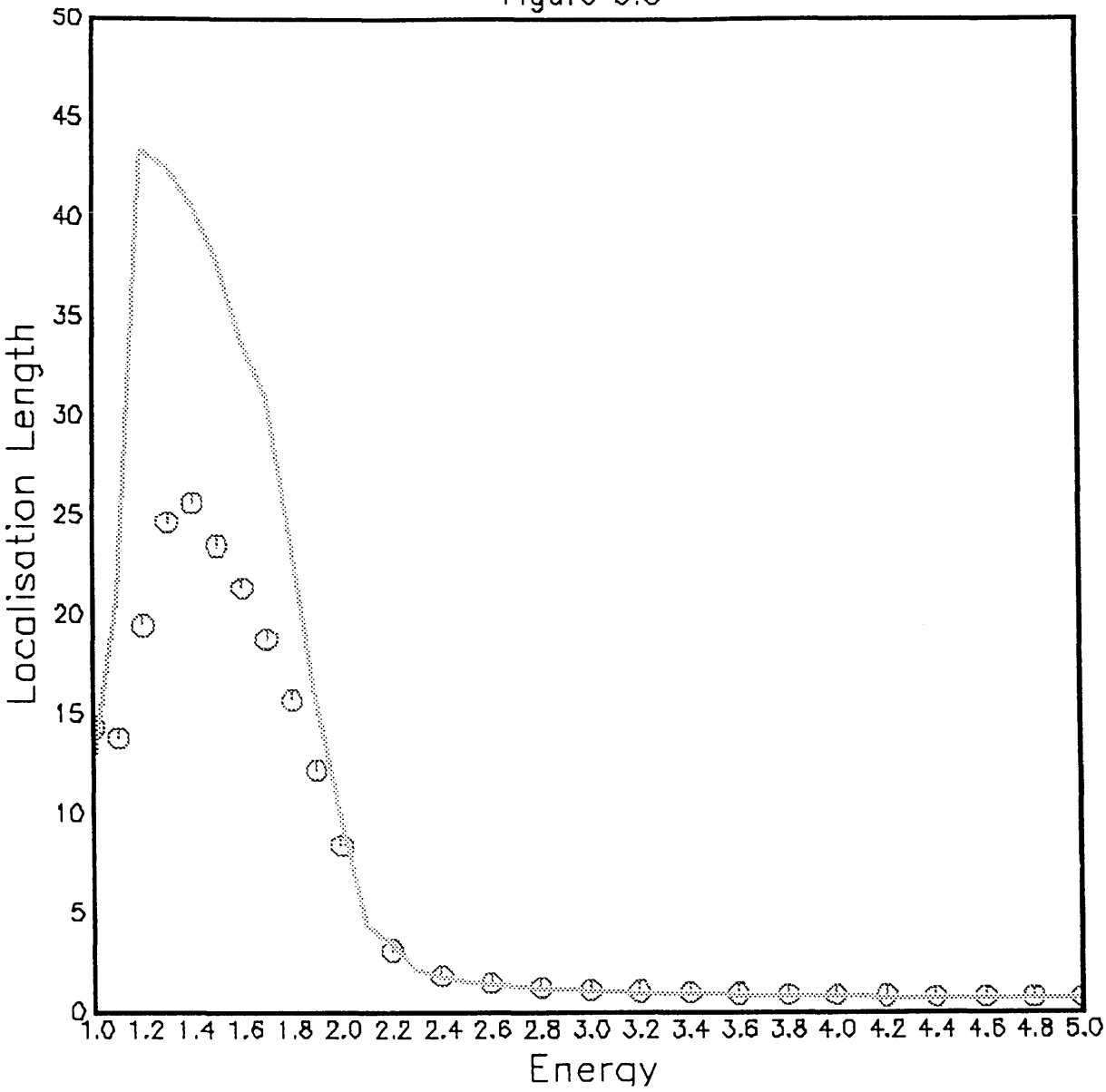

Figure 5.5 - Energy dependence of the third or median localisation length for the case Ly=5, $ß_t$=1 with a binary site energy distribution of width W=1. We compare the results of the self consistent approximation (line) with a Monte-Carlo simulation (symbols), below E≈1.0 we are unable to find a solution to the self consistent equation.

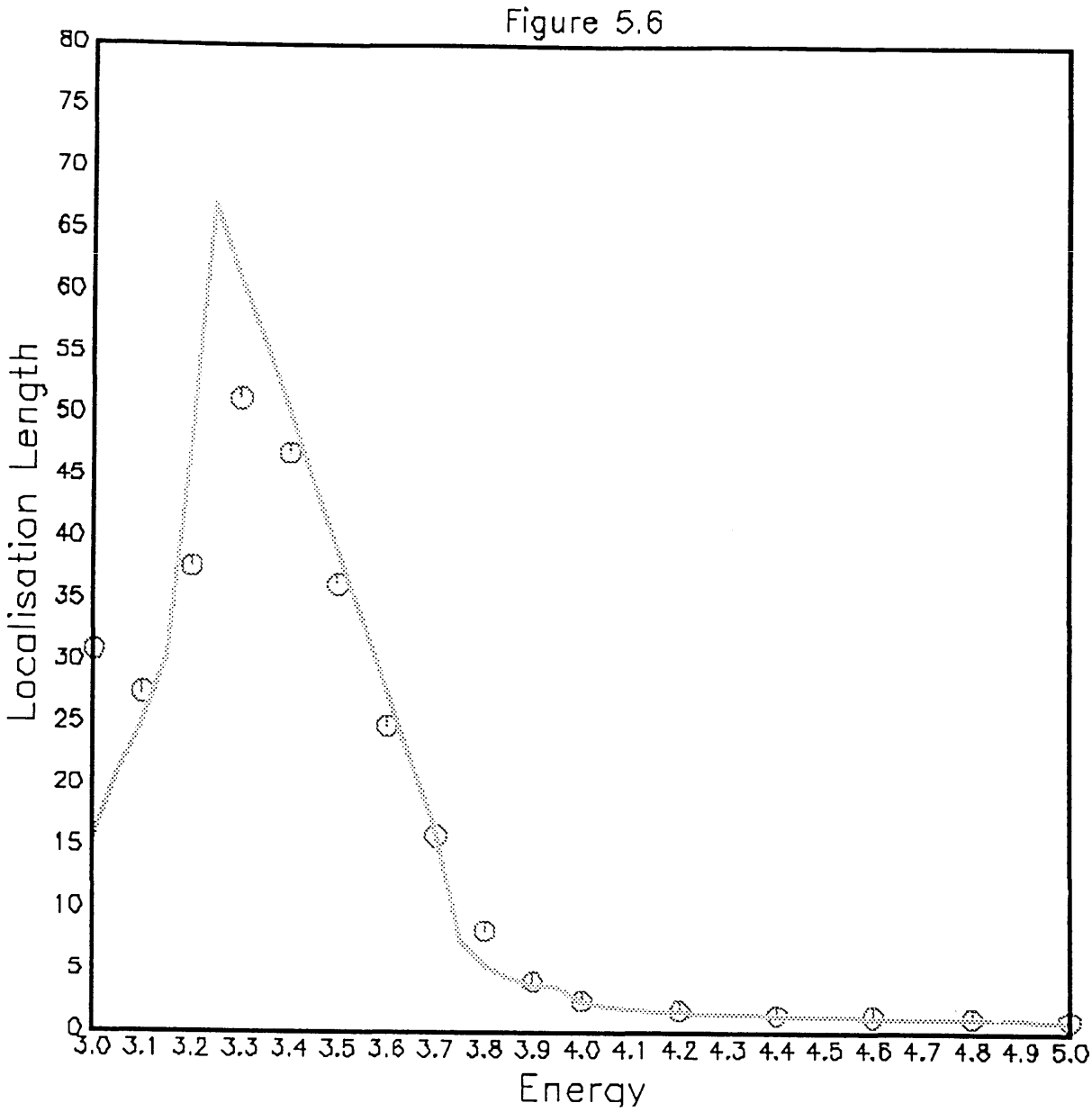

Figure 5.6 - Energy dependence of the longest localisation length for the case Ly=5, $ß_t$=1 with a binary site energy distribution of width W=1. We compare the results of the self consistent approximation (line) with a Monte-Carlo simulation (symbols), below E≈3.0 we are unable to find a solution to the self consistent equation.

For energies closer to the band centre we can obtain solutions for the shorter lengths by noticing that for instance the expansion for the shortest length is independent of the precise values of the longer lengths (because of the condition on the summation in equation 56.) In this way we can build up solutions by starting with the shortest length first. In this case we can obtain a solution for the shortest length above $E\approx 0.3$ and below $E\approx -0.3$. For the median length we can find a solution for energies above $E\approx 1.0$ and below $E\approx -1.0$. In the table below we list the energies of the sub-band edges of the pure system (W=0).

k_q	sub-band edges	
$\pi/6$	-3.73	+0.27
$\pi/3$	-3.0	+1.0
$\pi/2$	-2.0	+2.0
$2\pi/3$	-1.0	+3.0
$5\pi/6$	-0.27	+3.73

We find that the energies at which we become unable to find solutions to equations (56) are clearly correlated with these sub-band edges. However the precise reason for this is unclear. It does seem clear that a solution to the problems encountered near E=0 for the case Ly=2 is needed before progress can be made for wider chains.

To complete the discussion of the self consistent approximation we consider its application to strictly one dimensional systems. The self consistent equation is easily obtained from the expansion of the localisation length for a strictly one dimensional system [Chapter II]

$$i\phi = i\Theta + \frac{<\varepsilon^2>}{8\sin^2\phi} \qquad (61)$$

where

$$0 = E + 2\cos\Theta \qquad (62)$$

Again this equation is solved using the NAG routine and in Figure 5.7 we compare the results of the self consistent approximation with the results of a Monte-Carlo simulation. We find good agreement except at the band centre E=0. Here it is known that the perturbation expansion which implies (61) is altered [2-5 and chapter II].

Figure 5.7

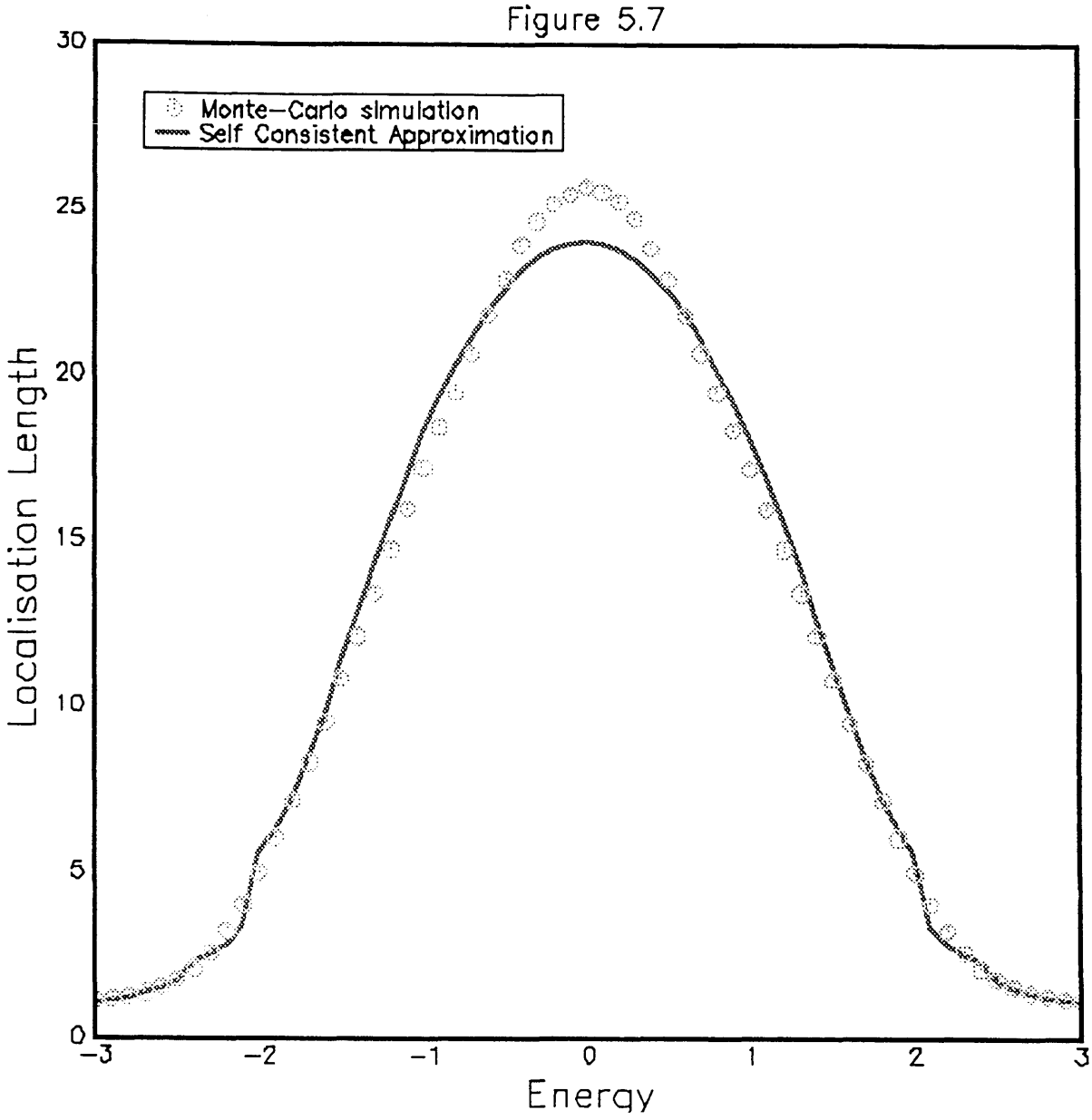

Figure 5.7 - Energy dependence of the localisation length for a strictly one dimensional system (Ly=1) with a continuous site energy distribution of width W=1. We compare the results of the self consistent approximation (solid line) with those of a Monte-Carlo simulation (symbols.)

Appendix I

Here we describe the numerical simulation technique used for the comparison with the perturbation expansions in Figures 5.1 to 5.3. We consider explicitly the case Ly=2 since this is the case relevant to the figures mentioned.

The basis of the technique is an evaluation of equation (14) of Chapter IV using a Monte-Carlo simulation. The largest exponent is evaluated easily as

$$\alpha_{max} = \lim_{L\to\infty} \frac{\log|Tu|}{L} \tag{1}$$

where u is an arbitrary staring vector and T_L is

$$T = \prod_{n=1}^{L} M_n \tag{2}$$

and M_n has the form

$$\begin{bmatrix} D_{n,1}, & -\beta_t, & -1, & 0 \\ -\beta_t, & D_{n,2}, & 0, & -1 \\ 1, & 0, & 0, & 0 \\ 0, & 1, & 0, & 0 \end{bmatrix} \tag{3}$$

with $D_{n,1} = \varepsilon_{n,1} - E$ and similarly $D_{n,2}$. The sum of the two positive exponents is evaluated as

$$\alpha_{max} + \alpha_{min} = \lim_{L\to\infty} \frac{\log|Yu|}{L} \tag{4}$$

Here Y is the antisymmetric projection of T ⊗ T. Below we give the explicit form in the basis of the tableaux (53) of chapter IV.

In Figure 5.8 we compare the results obtained using this technique with results obtained using the previously published technique of MacKinnon and Kramer [10]. We have chosen a binary distribution of site energies

$$p(\varepsilon) = \frac{1}{2}\left[\, \delta\left(\varepsilon-\frac{W}{2}\right) + \delta\left(\varepsilon+\frac{W}{2}\right) \,\right] \tag{7}$$

fore the comparison since this gives more structured localisation lengths. The localisation lengths are as usual simply defined as the inverse of the exponents. Agreement is excellent.

$$Y = \begin{bmatrix} D_{n,1}D_{n,2} - \beta_t^2, & -\beta_t, & -D_{n,1}, & D_{n,2}, & \beta_t, & 1 \\ \beta_t, & 1, & 0, & 0, & 0, & 0 \\ D_{n,1}, & 0, & 0, & 1, & 0, & 0 \\ -D_{n,2}, & 0, & 1, & 0, & 0, & 0 \\ -\beta_t, & 0, & 0, & 0, & 1, & 0 \\ 1, & 0, & 0, & 0, & 0, & 0 \end{bmatrix}$$

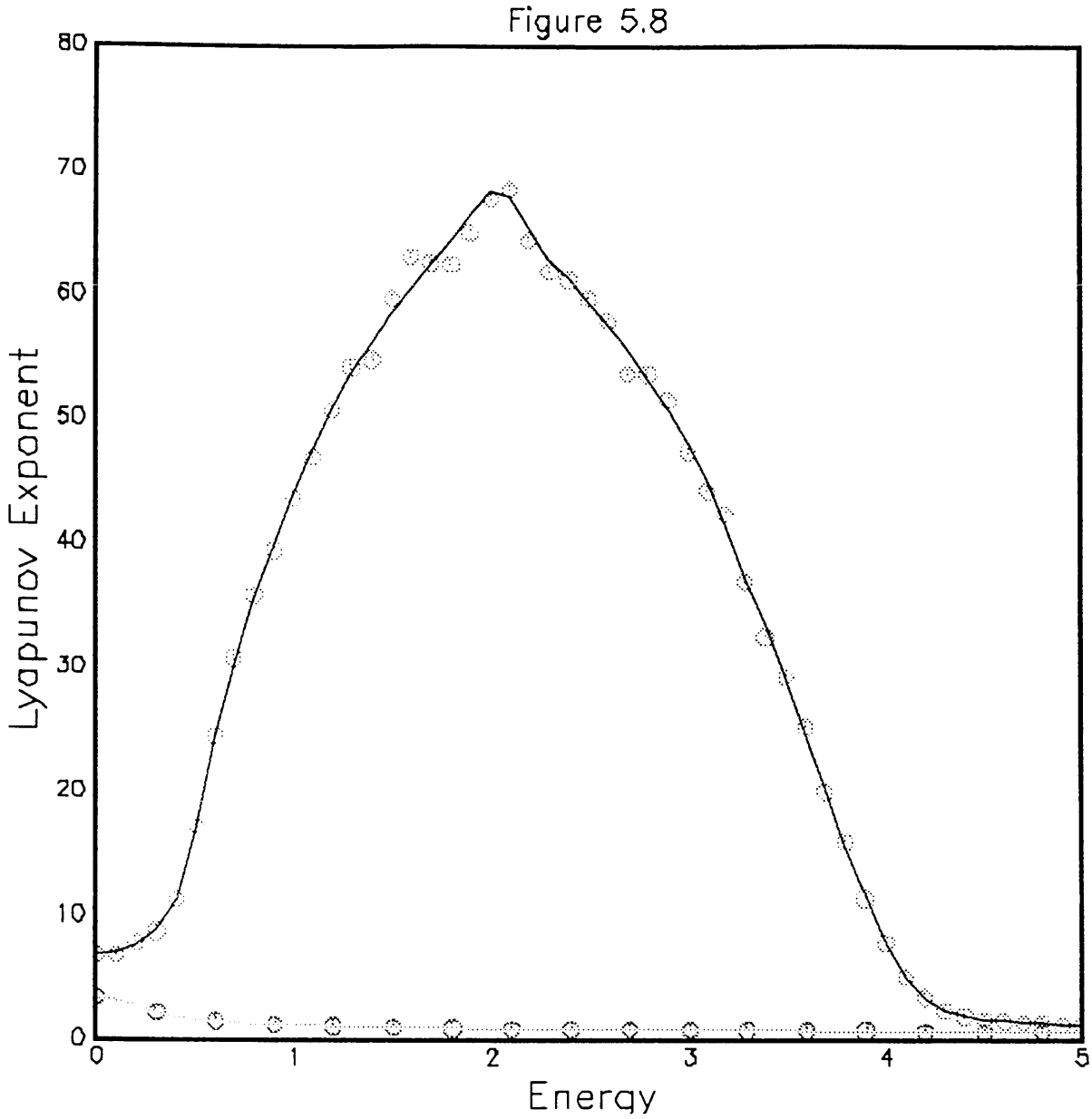

Figure 5.8 - Energy dependence of the localisation lengths for the case Ly=2, β_t=2 with a binary site energy distribution of width W=2. We compare the results of the Monte-Carlo simulation described in Appendix II (solid line) with that of an alternative program provided by A. MacKinnon (symbols)

References

[1] Thouless D J in "Ill Condensed Matter" edited by Balian R (North-Holland 1979)

[2] Kappus M. and Wegner F. Z. Phys. B **45** 15 (1981)

[3] Derrida B. and Gardner E. J. Physique **45** 1283 (1984)

[4] Lambert C. Phys. Rev. B **29** 1091 (1984)

[5] Kirkman P D and Pendry J B J. Phys. C **17** 4327 (1984)

[6] Slevin K and Pendry J B J Phys. C **21** 141 (1988)

[7] Derrida B.,Mecheri K. and Pichard J. J. Physique **48** 733-740 (1987)

[8] Zanon N and Derrida B Journal of Statistical Physics **50** No 3/4 509 (1988)

[9] Oseledec V. Trans. Mosc. Math. Soc. **19** 197 (1968)

[10] MacKinnon A and Kramer B Z. Phys. B **53** 1 (1983)

Chapter VI - Conclusions

Here I discuss briefly the main conclusions arising out of the work presented in this thesis and offer some suggestions for further development.

In Chapter IIIa calculation of the asymptotic distribution of $z \equiv -\ln|t|^2$ was presented. The asymptotic form was found to be parameterised by just two variables

$$p_L(z) \rightarrow p(z, Lc'_1, Lc'_2) \qquad (1)$$

where p(z) is the normal distribution with mean and variance

$$z = Lc'_1 \qquad (2)$$

$$var(z) = Lc'_2$$

The distribution obeys a two parameter scaling in general.

In the weak disorder limit of the Anderson model it was possible to obtain explicit expressions for both parameters and in this way to demonstrate a simple relation between them. On this basis it was concluded that the distribution obeys a single parameter scaling in the weak disorder limit. This result was confirmed in a Monte-Carlo simulation and it was verified that for strong disorder a cross over to two parameter scaling occurs.

To make a connection between the above results and the scaling theory in terms of conductance or resistance [1] we can use the Landauer formula to relate the transmission t to the dimensionless resistance R

$$R = \frac{1}{|t|^2} - 1 \qquad (3)$$

and hence obtain the relation

$$z = \ln(1+R) \qquad (4)$$

In reference [2] the scaling hypothesis is recast in terms of a scale resistance R_s where

$$R_s \equiv \exp[2L/Lc] - 1 \qquad (5)$$

The scale conductance g_s is defined simply as

$$g_s = \frac{1}{R_s} \tag{6}$$

Using the asymptotic form for the distribution of z we can now identify

$$R_s \equiv R_m \tag{7}$$

where R_m is the median resistance defined as

$$\frac{1}{2} = \int_0^{R_m} p(R)\, dR \tag{8}$$

Alternately we may identify R_s as

$$R_s = \exp[<z>] - 1 \tag{9}$$

From (3) we can see that when $|t|^2 \ll 1$, which is the case for nearly the whole of the distribution when $L \gg Lc$, we have

$$g \approx |t|^2 \tag{10}$$

We recall from Chapter III that the moments $<|t|^n>$ $n=1,2,..\infty$ are not consistent with the asymptotic distribution for z. This calls in to question the relevance of the scale conductance to a measurement of the average conductance eg a measurement on many one dimensional chains in parallel.

The the scale resistance would not in general seem to be particularly relevant either. When $|t|^2 \ll 1$ we have

$$R \approx \frac{1}{|t|^2} \tag{11}$$

While for the weak disorder limit of the Anderson model the moments $<|t|^{-n}>$ $n=1,2,..\infty$ are consistent with the asymptotic distribution there is no reason to suppose that this will be so in general. It therefore seems that the scale resistance will not be relevant to a measurement of the average resistance eg a measurement on many 1D systems in series.

In Chapter IV a start was made in applying the concept of generalised transfer matrices to quasi-1D systems. I believe the results are encouraging but some points remain to be dealt with. In particular the disagreement in the calculation of the largest exponent at the band centre for the case $L_y=2$ must be resolved before application to wider systems

can proceed. The number of energies at which such disagreements occur will become more numerous as the width of the system is increased and the number of underlying degeneracies in the problem increases.

The development of the perturbation expansions presented in Chapter V to higher orders in μ can be greatly simplified using the symmetry reduction developed in Chapter IV as a basis for the generalised transfer matrix approach. The key is to recast the problem in terms of an expansion for Γ_p the sum of the largest p exponents. It is clear from Chapter IV that Γ_p will be the largest exponent associated with the random matrix product

$$\prod_{n=1}^{L} \mathbf{Y_p}(\mathbf{M}_n) \qquad (12)$$

where Y_p is the anti-symmetric projection of the direct product

$$\mathbf{T} \otimes \ldots . \mathbf{T} \qquad \text{p times} \qquad (13)$$

defined in section 3 of Chapter IV. It is important to remember here that at this stage of the symmetry reduction no analytic continuation has been made and the analysis is completely rigorous. The simplification arises in that the expansion for the largest exponent contains a much smaller number of "interaction" terms with other exponents. The algebraic manipulations are thus considerably simpler and it should be possible to develop the expansion to much higher order.

[1] Abrahams E, Anderson P, Licciardello D and Ramakrishnan T Physical review Letters 42 673 (1979)

[2] Anderson P, Thouless D, Abrahams E and Fisher D Physical Review B 22 3519 (1980)