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## The resonance structure in a random dimer model

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**Abstract.** We have studied a random dimer model using the transfer matrix method and used the Landauer formula to compute conductances of large dimer chains as a function of the Fermi energy of the incident electron. We find very interesting resonance structures in this system around two special energies, namely the site energies (taken from a binary distribution). The localization length around these energies is found to diverge quadratically as a function of the energy difference as one approaches one of these energies from either side. It is also found that the conductance vanishes for this random dimer chain at almost all the allowable energies, just as it does in the case of a random 'monomer' chain. Thus a localization–delocalization transition (and more certainly a mobility edge) is absent in this system as opposed to what is claimed in some recent articles.

### 1. Introduction

It is quite well known from rigorous results that almost all the electronic states in a one-dimensional disordered system are exponentially localized (see e.g. Mott and Twose 1961). For systems with a tight-binding Hamiltonian the results are usually proved in the case of nearest neighbour hopping. The randomness in the site energy or the hopping integral induces a new length scale in the system, namely the localization length, and for almost all the available energies finiteness of this length leads to exponential localization. There is a random set of discrete energies (of total measure zero in the infinite length limit, see Pendry 1987) for each realization of the sample for which the system is perfectly transmitting and these are stochastic resonance states called Azbel resonances (Azbel 1983). Since isolated resonances cannot contribute to transport at zero temperature, there is no metal transition at zero temperature. While the tight-binding Hamiltonian in one dimension with constant or periodic site energies (i.e. no impurity) gives rise to Bloch states which have zero resistance (ballistic electrons) and the slightest impurity gives rise to exponentially localized states, the search is on to find situations where states of intermediate nature (e.g. diffusive with ohmic resistance behaviour) are possible. This search has prompted works on Fibonacci lattices (see e.g. Kohmoto and Banavar 1986) where all the states are critical, and Aubry or generalized Harper models for site energies (potentials) where a metal–insulator transition has been observed in one dimension (Das Sarma *et al* 1990, Basu *et al* 1991a). The site potentials for all the three cases mentioned in the last sentence follow a certain deterministic pattern and hence have long range correlation in their form. Thus a natural question to ask is whether it is possible to

drive the insulator to metal transition simply by changing the range of correlation in the randomly varying site potential. This question has been addressed recently in several works (see e.g. Varriale and Theumann 1990, Kolomeiskii 1991) within the framework of field theory and renormalization group.

In a recent paper Dunlap, Wu and Phillips (1990), referred to as DWP from now on, made a rather intriguing claim that there is an absence of localization in a random dimer chain. In a later paper (Wu *et al* 1992), there is a further astounding claim that the model 'possesses a mobility edge separating localized from delocalized states'. Their model uses a tight-binding Hamiltonian with each site being occupied by either an A- or a B-type atom with site energies  $\epsilon_A$  and  $\epsilon_B$  in such a way that there are always two A- or two B-type atoms on adjoining lattice sites. The hopping term is of nearest neighbour type and there is no disorder in the hopping term (i.e. the off-diagonal term). Thus this system has the shortest possible range of correlation, namely that of a lattice constant, in the randomness of the site energy. They studied the dynamics of an electron initially localized at a certain site in the random dimer chain by numerically integrating the equation of motion:

$$i \, dc_n/dt = \epsilon_n c_n + V(c_{n+1} + c_{n-1}) \quad (1)$$

for the site amplitudes  $c_n(t)$ . Studying the mean square displacement (MSD),  $\overline{m^2(t)} = \sum m^2 |c_m(t)|^2$ , they claimed that the MSD grows as  $t^{3/2}$  (i.e. a super-diffusive behaviour) provided  $|\epsilon_A - \epsilon_B| < 2V$  and that it grows as  $t$  (diffusive) if  $|\epsilon_A - \epsilon_B| = 2V$ . For all other cases the MSD will be bounded (i.e. the particle remains localized). Since their claim does not involve energy eigenstates of the electron it seems that there is a global metal-insulator transition, i.e. either all the states are localized (if  $|\epsilon_A - \epsilon_B| > 2V$ ) or all the states are extended (if  $|\epsilon_A - \epsilon_B| \leq 2V$ ). According to DWP, the initially localized particle becomes delocalized because  $\sqrt{N}$  of the electronic states remain extended over the entire sample and they are responsible for the transport in this system. This result is very surprising because the system is mappable to a random binary alloy with two atoms per unit cell and according to rigorous results in one dimension (Ishii 1973) almost all states, except for some isolated stochastic resonances (Azbel 1983), are localized for a purely random (i.e. random 'monomer' as opposed to random dimer) infinite chain. Since isolated resonances do not contribute to transport, one observes a vanishing of the diffusion constant (proportional to conductance by the Einstein relation) for any amount of disorder in one dimension. One may look at the problem from another point of view. The scaling theory (Abrahams *et al* 1979) of metal-insulator transitions in a random system predicts a continuous phase transition only for dimensions greater than two. At the transition point in a second-order phase transition, the correlation length (which is the localization length here) becomes infinite. It is surprising that a short range correlation on the atomic scale would give rise to a diverging correlation length and hence change the qualitative nature of the transition in one dimension.

To resolve this perplexing problem we undertook a transfer matrix study of the above system and calculated the transmittance which is also equal to the two-probe conductance according to the Landauer formula (Landauer 1970). The advantage of using the transfer matrix method is that we can go to a very large chain size and, since this method solves for the amplitudes at each site only once as one keeps on expanding the lattice it is much less time consuming (while solving for the time dependent equation (1), one has to update the amplitude at each site for all the time

steps). As will be discussed in the sequel, we find that except for some very special resonance structure near the two site energies, there is nothing unexpected occurring in this model. Just as in the case of a random ‘monomer’ chain, we find an absence of quantum diffusion in this model.

The rest of the paper is organized as follows. In section 2 we discuss the transfer matrix formalism for the sake of completeness. Then in section 3 we give our results and discussions on the transport properties in the random dimer model. Finally in section 4 we present our conclusions along with a short summary of the results.

## 2. Formalism

We shall focus on the simple tight-binding Hamiltonian with nearest neighbour hopping

$$H = \sum_n \epsilon_n \phi_n^+ \phi_n + V \sum_n (\phi_{n+1}^+ \phi_n + \phi_{n-1}^+ \phi_n) \quad (2)$$

where  $\{\phi_n^+\}$  and  $\{\phi_n\}$  are the sets of creation and annihilation operators for the tight-binding basis orbitals,  $\epsilon_n$  is the site energy and  $V$  is the nearest neighbour electron hopping integral. If one writes the eigenfunctions of the above Hamiltonian as linear combinations of the site orbitals, then the site amplitude  $c_n$ -values at three consecutive sites may be related by

$$\begin{bmatrix} c_{n+1} \\ c_n \end{bmatrix} = \mathbf{P}_n(E) \begin{bmatrix} c_n \\ c_{n-1} \end{bmatrix} \quad (3)$$

where  $\mathbf{P}_n(E)$  is the transfer matrix at the site  $n$ , i.e.

$$\mathbf{P}_n(E) = \begin{pmatrix} (E - \epsilon_n)/V & -1 \\ 1 & 0 \end{pmatrix}. \quad (4)$$

The off-diagonal term in the Hamiltonian, i.e. the hopping energy  $V$ , is a non-random quantity and is taken to be 1 to set the energy scale. The diagonal terms, i.e. the  $\epsilon_n$ 's, are taken from a binary distribution in such a way that the site energies on pairs of consecutive lattice sites are assigned the same random value (to create the random dimer chain). The energy  $E$  is the Fermi energy of the incident electron.

To the two ends  $n = 1$  and  $n = N + 1$ , we attach two elementary, perfectly conducting, semi-infinite leads. The purpose of these leads is to bear the incoming, the reflected and the transmitted waves.

$$H_{\text{in}} = \sum_{n=-\infty}^1 [\epsilon_{\text{in}} \phi_n^+ \phi_n + V_{\text{in}} (\phi_{n+1}^+ \phi_n + \phi_n^+ \phi_{n+1})] \quad (5)$$

$$H_{\text{out}} = \sum_{n=N+1}^{\infty} [\epsilon_{\text{out}} \phi_n^+ \phi_n + V_{\text{out}} (\phi_{n+1}^+ \phi_n + \phi_n^+ \phi_{n+1})]. \quad (6)$$

For simplicity we shall take  $\epsilon_{\text{in}} = \epsilon_{\text{out}} = 0$  and  $V_{\text{in}} = V_{\text{out}} = V_{\text{lead}}$ . The solution of the tight-binding Hamiltonian in the two perfect leads is of the Bloch form. We shall

assume that the transport is ideal just up to the contact of the leads with the sample (in this case the random dimer chain), i.e. we assume the eigenstates on the two sides of the sample to be

$$c_n(E) = A \exp(ikn) + B \exp(-ikn) \quad -\infty < n \leq 1 \quad (7)$$

$$c_n(E) = C \exp(ikn) + D \exp(-ikn) \quad N + 1 \leq n < \infty. \quad (8)$$

We have neglected the boundary effects, which is reasonably justified as we are dealing with really very large samples. Finally the wave functions on the RHS of the sample will be connected to those on the LHS using the transfer matrix by the simple relation

$$\begin{bmatrix} D \\ C \end{bmatrix} = \mathbf{T}_N \begin{bmatrix} B \\ A \end{bmatrix} \quad (9)$$

where the transfer matrix  $\mathbf{T}_N$  is given by

$$\mathbf{T}_N = \mathbf{e} \mathbf{s}^{-1} \mathbf{M}_N(E) \mathbf{s} \quad (10)$$

such that

$$\mathbf{M}_N(E) = \mathbf{P}_N(E) \mathbf{P}_{N-1}(E) \dots \mathbf{P}_2(E) \mathbf{P}_1(E) \quad (11)$$

$$\mathbf{s} = \begin{bmatrix} \exp(-ik) & \exp(ik) \\ 1 & 1 \end{bmatrix} \quad (12)$$

$$\mathbf{e} = \begin{bmatrix} \exp[ik(N+1)] & 0 \\ 0 & \exp[-ik(N+1)] \end{bmatrix}. \quad (13)$$

The elements of the transfer matrix are related to the physical quantities reflectance  $r(E, N)$  and transmittance  $t(E, N)$  by the following simple relation

$$r(E, N) = |T_N^{12}/T_N^{11}|^2 \quad (14)$$

$$t(E, N) = |1/T_N^{11}|^2. \quad (15)$$

The Landauer formula relates the energy-dependent, dimensionless, four-probe resistance to the transmission coefficient by

$$R(E, N) = r(E, N)/t(E, N) = |T_N^{12}|^2. \quad (16)$$

(15) is the basic equation that we have used to calculate the transmittance, which is also the two-probe conductance given by

$$G(E, N) = t(E, N) = 1/|T_N^{11}|^2. \quad (17)$$

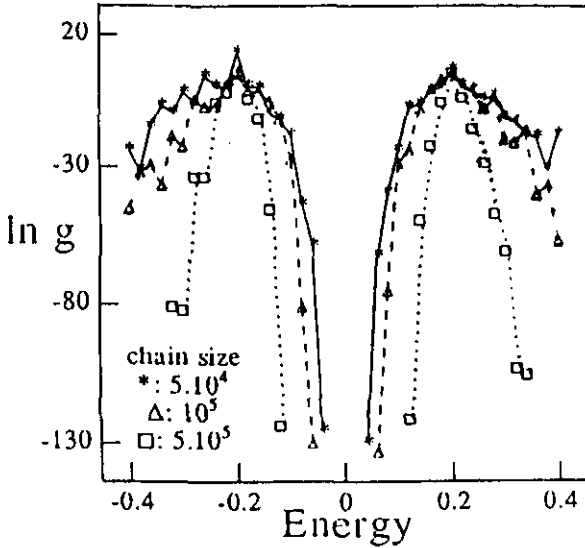
One should note that the concept of semi-infinite geometry is inherent in both the transfer matrix method and the Landauer formula. The special importance of the semi-infinite chain is that all transport experiments in one dimension are essentially performed in semi-infinite geometry in which two perfect current carrying leads are attached at the two ends of the chain so that the current in the form of a plane wave

enters at one end and emerges from the other end in an undistorted form, i.e. there is no momentum transfer so that the  $k$ -value remains unchanged. All information regarding the scattering of the electron in the disordered sample is contained in the transfer matrix, which supplies us with the reflection coefficient, i.e. the amount of backscattering involved in the multiple scatterings inside the disordered sample. We mention in passing the advantage of using such open quantum systems as considered here. The system is open because it is connected to two reservoirs at slightly different electrochemical potentials through the semi-infinite perfect leads. In one sense the system may be compared to a grand canonical ensemble. Thus we do not need to know the 'allowed eigen-energies' of the finite, isolated chain (by diagonalization) before we proceed. In fact, we have shown elsewhere (Kar Gupta and Sen 1992) that any energy here is an allowed energy for the finite version of the semi-infinite, open chain; but the localization characteristic due to disorder is not changed whether we use an isolated chain or an open chain.

### 3. Results and discussion

We start this section by pointing out that in all our work described below for these one-dimensional random dimer chains, we set the length scale by fixing the lattice constant to a value of unity and the energy scale by choosing the hopping energy in the sample to be  $V = 1$ . The hopping energy in the perfect leads  $V_{\text{lead}} = V$ . It is well known that in a quantum fermionic system at  $T = 0$ , transport is mediated by the fermions at the Fermi energy (or energies very close to it, if the distribution function is assumed to deviate slightly from the step function even at  $T = 0$  due to the presence of some interaction). So we have looked at the transmittance (which is related to the conductance by the Landauer formula) as a function of the Fermi energy. Our transfer matrix results show that for a finite chain length there is a close clustering of resonance states of a new type near each of the two site energies of this random dimer chain. Except for energies very close to these two special site energies, the conductance falls drastically to zero at all other energies as one increases the chain length. This is shown in figure 1, which shows the four-probe conductances at three different chain lengths using a coarse energy mesh for  $\epsilon_A = -\epsilon_B = -0.2$ . By using much finer energy meshes (the larger the chain length, the higher the resolution required), we discover a novel and complicated resonance structure around the site energies as we describe below.

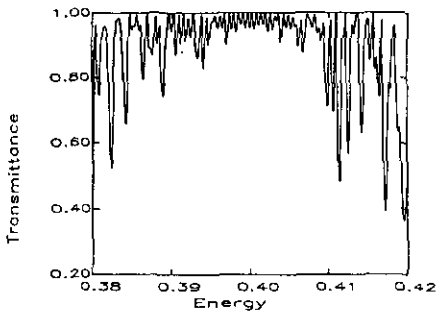
One knows from rigorous results (Ishii 1973) that the transmittance  $t(E, L)$  of a purely random one-dimensional system of length  $L$  decreases exponentially with the length of the system, consistent with an exponential decay of almost all the eigenstates (in a large isolated system) on both sides of their maxima. For a given configuration of the random system,  $t(E, L)$  exhibits maxima corresponding to transmission resonances at some of the eigen-energies which are also random, i.e. they are specific to each particular random sequence of scatterers. The width of these Azbel resonances as a function of the energy of the incoming electron becomes exponentially small as the length of the system or the strength of disorder increases. This width is of the order of  $\exp(-aL/L_0)$  where  $a$  is of the order of unity and  $L_0$  is the localization length. The presence of these Azbel resonance states in a random 'monomer' chain has been known for a long time (Azbel and Soven 1983, Azbel 1983). However, the resonances for the random dimer chain seem to belong to a different category.



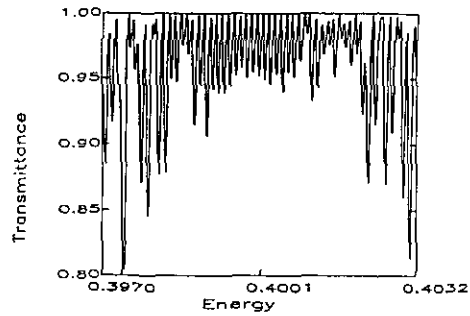
**Figure 1.** Four-probe conductance for three random dimer chains with  $\epsilon_B = -\epsilon_A = 0.2$ , and  $V = 1$ , using a coarse energy mesh. Two very broad resonance structures around the site energies are visible, but when length increases the conductance falls off by tens of orders of magnitude if the Fermi energy is not close to  $\epsilon_A$  or  $\epsilon_B$ .

In contrast to random 'monomers', if we study the resonance structure for the random dimer chain with a very fine energy resolution we find that there is a close bunching of the resonance states around the two site energies. In figure 2 we show this around  $\epsilon_B$  for a system with  $N = 10000$  and  $\epsilon_B = -\epsilon_A = 0.4$ . In figure 3 we draw the resonance structures for the same values of  $\epsilon_A$  and  $\epsilon_B$  as those of figure 2 but for a larger system size ( $N = 50000$ ). It is evident from these figures that as we increase the system size, the basic resonance structure remains similar but the energy domain in which this clustering of the resonances occurs shrinks. The dense resonance clusters around the site energies seem to have two different types of regions. There is a central core region in the middle of a cluster where the transmittances as a function of energy seem to be more or less oscillatory (with peaks very close to one) and the minima of the transmittances do not seem to fall below a certain value (about 0.94 for  $-\epsilon_A = \epsilon_B = 0.4$  as seen from figures 2 and 3) when the length of the chain is increased. On both sides of the energy domain where the cluster core appears, there is a fragmentation region (as one can see) where the decay of the width of the individual resonances is found to be consistent with an exponential law like that in a purely random system (or a power law decay with a large exponent  $\geq 3$ ). That the width of the central cluster core decreases is shown in figure 4 with the same values of  $\epsilon_A$  and  $\epsilon_B$  as before. We have plotted the cluster core width for different system sizes extending up to three decades in length. The power law fitting of this result shows that this cluster core width decays algebraically as  $N^{-2/3}$  where  $N$  is the chain size. From a very basic viewpoint, it would have been highly surprising if the cluster width of the central core (peaks of which are almost perfectly transmitting) had not decayed with length, because in that case, this non-decaying cluster would have formed a stable band of almost extended states for this 'random' dimer chain. Furthermore we have studied the width of some individual resonances inside the cluster core as a function of the chain length. In contrast to the Azbel states whose widths fall off exponentially, the widths of the resonance states inside this cluster core decay algebraically as  $N^{-1}$ . This is shown in figure 5 for  $\epsilon_B = -\epsilon_A = 0.4$ . This fact is consistent with the observation that the number of resonance states inside the

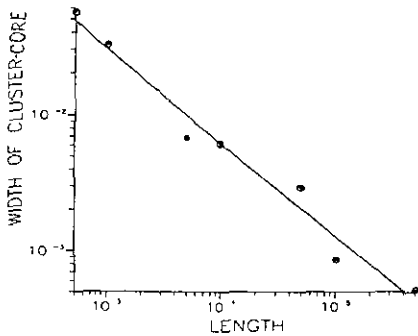
cluster core increases as  $N^{1/3}$  (see figure 6). In table 1 we have shown the actual numbers for the resonance cluster cores for different chain sizes keeping the disorder characteristic the same. Incidentally this exponent of  $1/3$  seems to be different from that  $(1/2)$  reported by DWP who claimed that  $c\sqrt{N}$  ( $c =$  proportionality constant  $= 1$ ) states will remain extended over the length of the system and that they are responsible for transport in this system.



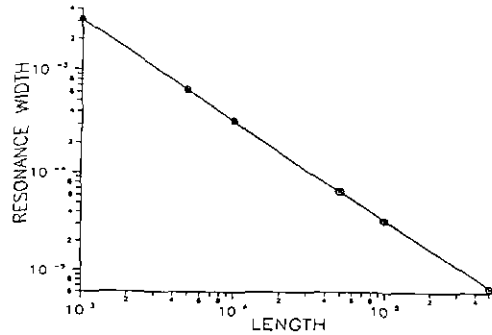
**Figure 2.** Transmittance as a function of the Fermi energy for a random dimer chain with  $\epsilon_B = -\epsilon_A = 0.4$ , and  $N = 10\,000$  using a very fine energy mesh around one of the site energies only. There is a similar structure (not shown here) around the other side energy.



**Figure 3.** The same as figure 2 but for  $N = 50\,000$ .



**Figure 4.** Graph showing the decay of the width of the cluster core with chain length for random dimers with the same disorder parameters as in figure 2 (data given in table 1). The best fitting line shown here indicates an algebraic decay with an exponent close to  $2/3$ .



**Figure 5.** Graph showing how the width of an individual resonance deep inside the cluster core scales with chain length. The best fitting line indicates very clearly an inverse proportionality.

We have also diagonalized numerically the Hamiltonian for several chain lengths and computed the transmittance at these 'exact' eigenstates. For different chain lengths, we counted the number of states whose transmittances were greater than or equal to  $\exp(-2)$  (i.e. whose localization lengths were greater than or equal to the



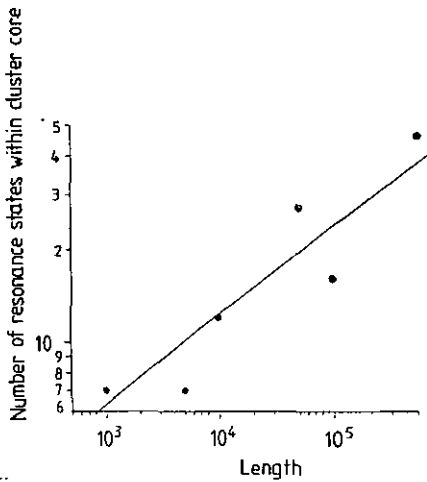


Figure 6. Scaling plot for the estimated number of resonance states inside the cluster core for different chain lengths. The best fit line indicates that this number increases algebraically with an exponent close to  $1/3$ .

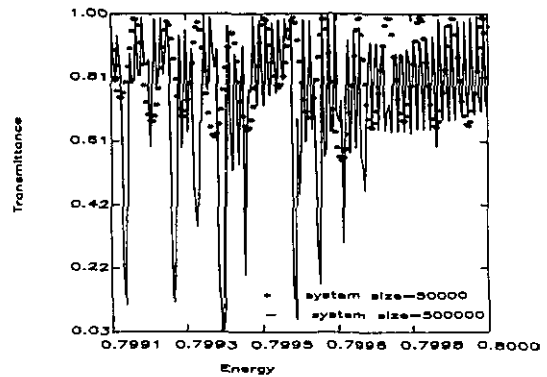


Figure 7. Transmittance versus energy for two random dimer chains of lengths 50 000 and 500 000 but the same  $\epsilon_B = -\epsilon_A = 0.8$  on one side of the cluster core around  $\epsilon_B$ . One can see very clearly the effect of disorder at a higher length scale because the core region shrinks. The effect of disorder at the same length scale (more 'fragmentation') becomes clear on comparison with figure 3.

Table 1. A random dimer chain with  $V = 1$ ,  $\epsilon_B = -\epsilon_A = 0.4$ .

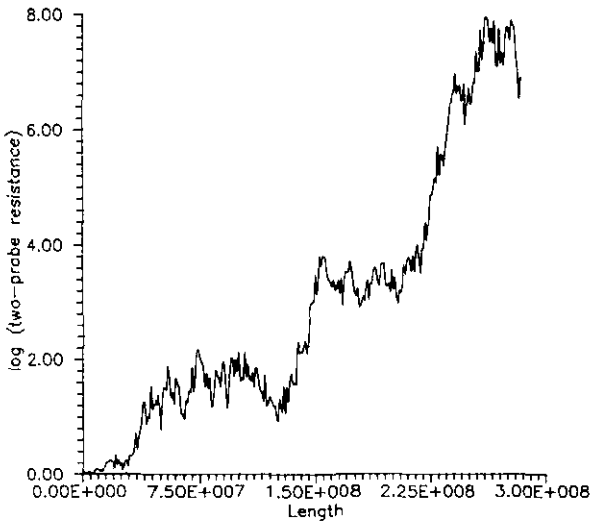
Chain Length $N$	Energy domain of resonance cluster core around $E = \epsilon_B = 0.4$	Number of resonances inside core	Width of each resonance inside core
$5 \times 10^2$	0.3672–0.4240	6	$6.4 \times 10^{-3}$
$1 \times 10^3$	0.3766–0.4091	7	$3.1 \times 10^{-3}$
$5 \times 10^3$	0.397 40–0.404 24	7	$6.3 \times 10^{-4}$
$1 \times 10^4$	0.397 28–0.403 50	12	$3.4 \times 10^{-4}$
$5 \times 10^4$	0.399 105–0.402 065	27	$6.6 \times 10^{-5}$
$1 \times 10^5$	0.399 68–0.400 54	16	$3.3 \times 10^{-5}$
$5 \times 10^5$	0.399 717–0.400 229	46	$6.6 \times 10^{-6}$

system size). The number of such states is found to increase as  $\sqrt{N}$ . Thus what we find is that *not all* of the  $c\sqrt{N}$  states are ballistic as claimed by DWP ( $c < 1$ , in contrast with DWP and Wu *et al* (1992) who claim that  $c = 1$ ), but rather that these are the states whose localization length is system spanning and thus include the states both inside the cluster core and in the fragmentation region as defined by us. This result is also in agreement with the recent observation by Bovier (1992) who, using perturbation theory and an invariant measure formalism, claimed that for a random dimer system the number of states for which the localization length exceeds the size  $N$  of the system is proportional to  $N^{1/2}$ . Furthermore the overpowering role of disorder becomes very clear if one looks at figure 7, where  $|\epsilon_A - \epsilon_B| = 1.6$ , and compares with figure 2 or 3 for  $|\epsilon_A - \epsilon_B| = 0.8$ . It is evident that as the amount of disorder increases, i.e. as  $|\epsilon_A - \epsilon_B|$  approaches  $2V$ , there is much more 'fragmentation' in the

resonance structure both inside and outside the cluster core. Even though our figures are for the higher site energy (i.e.  $E = \epsilon_B$ ) we have checked that all the statements above are also true for Fermi energies near the lower site energy (i.e.  $E = \epsilon_A$ ).

That there could be a very large number of states (around the site energies) which look like extended states, but whose localization lengths are much larger than the typical system sizes (albeit quite large ones) considered, may be demonstrated very easily by studying the evolution of the two-probe resistance  $R_2$  with the chain length for Fermi energies close to  $\epsilon_A$  or  $\epsilon_B$ . In figure 8 we have shown the logarithm of the two-probe resistance (negative of the logarithm of transmittance) as a function of length for  $E = 0.4004$ , where  $\epsilon_B = 0.4$ . The existence of an essentially exponential localization is quite clear here and the localization length (two times the inverse of the slope for the best fitting straight line) for this particular realization turns out to be about  $9.0 \times 10^7$ . We would like to mention two points here. First, in this particular curve representing states close to one of the site energies, the resistance tends to increase with rather sharp jumps and a concomitant noisy plateau-like structure, the plateaux themselves being reminiscent of the behaviour in a generalized Harper model (Thakur *et al* 1992). In the latter model the plateau structure is very systematic, the potential being deterministic with a slowly varying period. It would be interesting to know what gives rise to this plateau-like structure in a random potential. Second, it should be noted that the resistance for this sample remains fixed at an average value of about  $\exp(1.5)$  from a length of about  $4.0 \times 10^7$  to about  $12.0 \times 10^7$ , and thus the average localization length in this rather large domain (or in any other plateau-like region) would *seem* to be zero. Thus it is not surprising that the diffusion characteristic of this state would look, in this length scale, not quite like a Bloch state (whose MSD grows as  $t^2$ ), but like a somewhat resistive, a so-called 'super-diffusive', state with the MSD growing as  $t^{3/2}$ , for relatively short time scales. Yet indeed it is an exponentially localized state, and to know the exponentially localized nature of this state one would have to study its diffusion for times much larger than those considered by DWP (typically of the order of  $10^5$  in units of 'average' hopping time). The possibility of many such states even for quite large system sizes must be at the heart of the misplaced conclusions of DWP. To justify this statement even more convincingly we will first show that a quadratically diverging localization length at a single, isolated energy in this region is indeed consistent with a square-root-wise growth of the number of states ( $\Delta\lambda$ ) with system spanning localization length. For that purpose, let us assume that  $\xi \sim |E_F - \epsilon_B|^{-\mu}$ . Then one may write for the energy domain with  $N \leq \xi \leq \infty$ ,  $\Delta E \sim \xi^{-1/\mu} \Big|_N^\infty = N^{-1/\mu}$ . Now if one uses an *ansatz* that the density of states is rather flat on average and equal to  $N^{-1}$  (this is reasonably true for states away from the ends of the spectrum: see our DOS calculation later on), then we actually find that  $\Delta\lambda \sim N^{1-(1/\mu)}$ . Now using the fact that  $\Delta\lambda$  actually grows as  $N^{1/2}$ , we see that  $\mu = 2$ . This certainly proves our assertion, except for the fact that the approximate nature of the *ansatz* seems to mar the proof to some extent. So, to prove our assertion in a different (numerical) fashion, we have numerically calculated, by using the method mentioned above, the inverse localization lengths for states with reduced energy differences,  $|(E_F - \epsilon_B)/\epsilon_B|$ , covering more than two decades (from both sides of  $\epsilon_B$ ) and have shown them in a double logarithmic plot in figure 9. A straight line is seen to fit the data in an excellent fashion, and the slope of 1.97 of the best fitted line clearly indicates that the localization length diverges as  $\xi - |E_F - \epsilon_B|^{-2}$ . There is an identical behaviour for energies close to  $\epsilon_A$ . These results clearly show that (i) as opposed to DWP, there are *no Bloch states* except possibly at

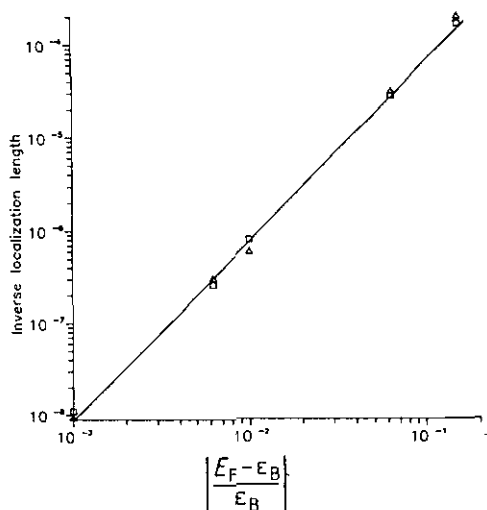
$\epsilon_A$  and  $\epsilon_B$  and (ii) as opposed to Wu *et al* (1992), there is certainly *no mobility edge* in this random dimer model, separating a domain of extended states from a domain of localized states.



**Figure 8.** Logarithm of the two-probe resistance ( $R_2$ ) for a particular sample ( $\epsilon_B = -\epsilon_A = 0.4$ ) as a function of length for a Fermi energy of  $E_F = 0.4004$ . The existence of a generic exponential localization is quite clear here. But the noisy, plateau-like structure continuing for very large domains of length (for  $E_F$  very close to  $\epsilon_A$  or  $\epsilon_B$ ) may easily lead one to totally wrong conclusions regarding the localization behaviour if one is not careful enough.

In a recent study (Basu *et al* 1991b) on the nature of Azbel resonances, we found that their multifractal spectra are critical-like, i.e. they behave like the states at a mobility edge (Thakur *et al* 1992, see also Schreiber and Grussbach 1991). We conjecture that for energies inside the cluster cores of the random dimer model, the multifractal spectra would also be critical-like and that for energies inside the fragmentation region the multifractal spectra will be like that for an exponentially localized state (Thakur *et al* 1992). Work in this direction is under progress. We make a remark in passing that whereas Schreiber and Grussbach (1991) apply multifractal analysis to the wavefunction only at criticality and surmise whether the analysis could distinguish between critical, extended and localized states, we (Thakur *et al* 1992) have actually applied the analysis to transmittance and have shown that it can distinguish between these three types of situations very effectively.

The occurrence of these special resonance structures near the two site energies in the case of a random dimer is also understandable from the following argument. As a basis for comparing the random dimer chain with the purely random (monomer) chain, let us compare the parent ordered chain for these two cases. The parent ordered chain for the random dimer model is AABBAABB... type. When one solves the tight-binding equation for this infinite ordered chain one obtains four subbands (Kar Gupta and Sen 1992). The two outer bands will have equal but smaller band widths and the two inner bands will have equal but larger band widths. Now the parent ordered chain for the purely random system (taken from a binary distribution) is of the form ABAB... Here one can show as before (Kar Gupta and Sen 1992) that there will be two subbands (instead of four) with equal band widths. But the



**Figure 9.** Double logarithmic plot of the inverse localization length against reduced energy difference from  $\epsilon_B$ , namely  $|(E_F - \epsilon_B)/\epsilon_B|$ . The symbols  $\Delta$  stand for  $E_F < \epsilon_B$  and the symbols  $\square$  stand for  $E_F > \epsilon_B$ . A straight line gives an excellent fit to the data covering more than two decades and the slope is about 1.97 indicating a power-law divergence of the localization length around  $E_F = \epsilon_B$ .

interesting thing to note is that for an AABBAABB... perfectly ordered chain the band gap at the centre is much smaller than that of an ABAB... ordered chain. For example, when  $\epsilon_B = -\epsilon_A = 0.4$ , the band gap for an ABAB... ordered chain is 0.8 but for an AABBAABB... ordered chain it reduces to 0.154. So the short range order even in the atomic scale for the dimer can reduce the band gap appreciably. If we increase  $\epsilon_A$  and  $\epsilon_B$  within the allowed region, i.e.  $|\epsilon_A - \epsilon_B| < 2V$ , the widths of the four bands decrease and the band gaps increase. The most important point to note is that the two site energies  $\epsilon_A$  and  $\epsilon_B$  always fall within the two inner broad bands as long as  $|\epsilon_A - \epsilon_B| < 2V$ , but as  $|\epsilon_A - \epsilon_B|$  approaches  $2V$ , the two site energies move gradually outwards and finally for  $|\epsilon_A - \epsilon_B| > 2V$ , they fall outside the two inner bands, within the band gap where only the localized states exist. For example, when  $\epsilon_B = -\epsilon_A = 0.4$ , the band edges for the central left band are at energies  $-1.166$  and  $0.077$ ; and those for the central right band are at  $0.077$  and  $1.166$ . Corresponding energies for  $\epsilon_B = -\epsilon_A = 0.95$  are  $(-1.001, -0.379)$ , and  $(0.379, 1.001)$ , i.e. the two central bands still include the site energies  $\epsilon_A$  and  $\epsilon_B$ . But when  $\epsilon_B = -\epsilon_A = 1.1$ , the respective bands are from  $\pm 1.005$  to  $\pm 0.489$  respectively. So it is evident that in this case the site energies are excluded from the central bands and fall inside the band gap since the outer two bands extend from  $\pm 2.326$  to  $\pm 2.486$ .

Now as randomness is introduced in the binary distribution, both the bands of the ABAB... chain disappear and almost all states become exponentially localized. For the random dimer chain on the other hand, as localization enters strongly from the outer edges of the spectrum, the two outer smaller bands become completely fragmented and so we see exponentially decaying states outside the central core as in the case of a perfectly random system. But since for the random dimer chain one or more than one pair of A (or B) atoms do occur on consecutive lattice sites

(there is some short range correlation at energies equal to the site energies), it may be expected that the parent ordered band structure is not fully forgotten but is manifested in *finite length dimer chains* by the occurrence of a close bunching of near resonance states around the two site energies only if they are included inside the two inner, comparatively broad bands of the parent ordered AABBB... chain, i.e. if and only if  $|\epsilon_A - \epsilon_B| \leq 2V$ . In figure 10, we have shown the density of states (DOS) of a random dimer chain of size  $N = 5000$  by direct diagonalization of the ensuing tridiagonal Hamiltonian. We can see clearly that the DOS in a small region around  $E = \pm 0.4$  is reasonably flat (yet not completely flat which would have indicated extended band states), but at all other energies (including those around  $E = 0$ ) the DOS is high fragmented, hinting at the possible occurrence of localized states. (Note that on average the DOS is still flat except near the ends of the spectrum: a fact we used earlier for calculating the divergence exponent of localization length). Furthermore the almost flat region of the DOS occurs at almost the same region where the cluster core in transmittance occurs (see table 1). Comparison with the results for other sizes tends to suggest that this flat region shrinks to zero with chain size in a similar fashion as the cluster core does. To get some idea about the nature of the states in the core and the fragmentation region, we plotted the probability of finding the electron  $|c_n|^2$  against  $n$  for two different eigenstates (for  $N = 500$ ), one well within the cluster core (figure 11(a)) and the other in the fragmentation region (figure 11(b)). We chose a small system size in these cases for the sake of clarity, the results being qualitatively the same for higher system sizes. While it is clear that in the fragmentation region the wavefunction decays fast enough, it is also evident that *in the core region the wavefunction is certainly not Bloch type* (in contrast to DWP's claim). Further, these *apparently* perfectly transmitting resonance states are not like Pendry's necklace states either. Thus these resonances are quite new by all counts.

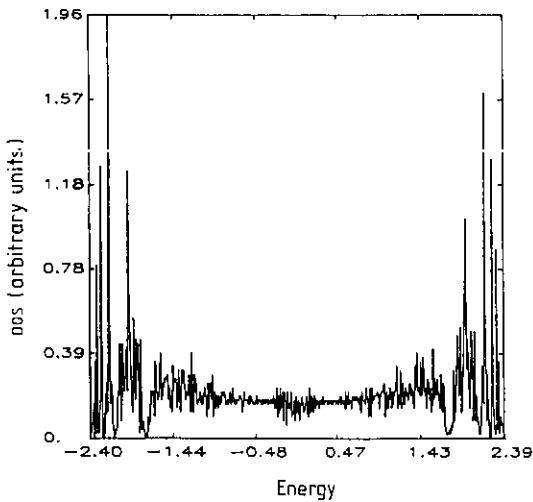
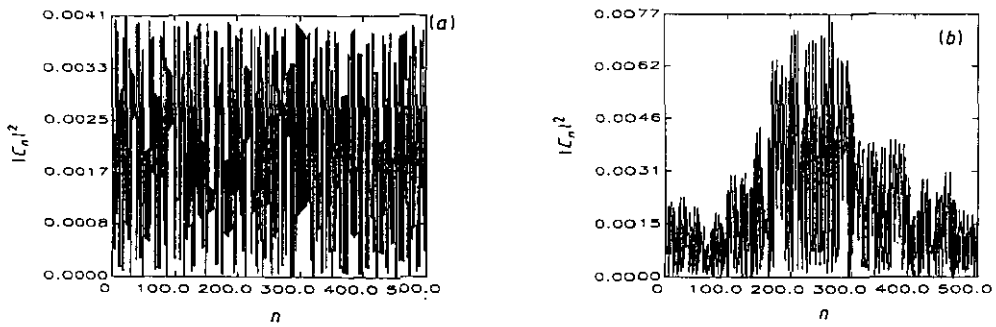


Figure 10. Density of electronic states for a particular random dimer chain of length  $N = 5000$  obtained by direct diagonalization.

Now we want to consider the possibility of quantum diffusion in this random dimer model. Let us consider a fixed Fermi energy of the electrons depending on their number density. If this Fermi energy does not fall inside one of the clusters, the conductance decays with length very fast (actually exponentially, very much like that



**Figure 11.** (a) Probability of finding the electron at different sites for a Fermi energy equal to one of the exact eigenstates ( $E = 0.406\,058\,546\,391\,26$ ) which lies at the centre of one cluster core for a random dimer with  $N = 500$ . This state does not look at all like a Bloch state even though it seems to be of non-decaying type. (b) The same as (a) but for an eigenstate ( $E = 0.257\,191\,728\,259\,09$ ) which is deep inside the fragmentation region. Clearly the wavefunction for this state is spatially decaying.

for a purely random chain) as indicated by our figure 1. But for small length samples the total probability that this Fermi energy falls within the cluster core around one of the site energies is not insignificant. For such Fermi energies, the conductance does not seem to have an overall decay with increasing chain lengths as long as the Fermi energy remains within the cluster core for all such lengths. But as one increases the system size, there will always be a length (depending upon how far the Fermi energy is from the nearest site energy) above which the cluster narrows enough in energy domain to exclude the given Fermi energy from its core. From this length onwards, on further increment of length, the conductance starts decaying slowly at first and eventually exponentially. These are the results that are expected according to our analyses above for very large but finite-length dimer chains. Finally, as the length approaches infinity, the total cluster width approaches zero and the number of resonance states inside it approaches infinity as well. Thus, an infinite degeneracy of states occurs at each of the two site energies which behave as isolated (zero-width) resonances in the infinite length limit. The total measure of these resonance states is thus zero. This fact is also supported by Bovier (1992) who finds that in the random dimer model the localization length diverges in an infinite length sample strictly at two exceptional energies *only*, namely the site energies. Now it is also well known that transmission through isolated resonances of zero width at zero temperature and in the absence of an external field *does not naturally occur* (in linear response theory, the applied *static* electric field is assumed to be vanishingly small). Hence our transfer matrix study indicates that almost all the states, except for *isolated resonances of total measure zero*, are localized in the given random dimer model and thus there is an absence of quantum diffusion in an infinite random dimer chain.

Finally we would like to comment on the issue of the diffusion of a particle initially localized at a certain site. Since the initial wavefunction is a Kronecker delta, its diffusion has contributions from all the energy eigenstates. Though in experimental situations, the transport in a Fermi system does *not* take place in this fashion (that is not by taking contributions from all the available energy eigenstates, as we stressed at the beginning of this section), we will still consider this problem for purely conceptual reasons. According to DWP for  $|\epsilon_A - \epsilon_B| \leq 2V$ , there is an absence of localization

in this system and, in fact, the transport becomes super-diffusive (diffusive) when the inequality (equality) holds. But the results of the transfer matrix study as discussed above tend to indicate otherwise. To find some clue on how the effects of disorder show up in the diffusion behaviour we solved the time dependent Hamiltonian (1) numerically and calculated the MSD as discussed in the introduction for a purely random (monomer) chain. For this random 'monomer' case, we find a short time scale up to which the MSD diverges as  $t^{3/2}$ , but beyond which one can see a crossover to the expected bounded nature due to localization. For the random 'monomer' with  $\epsilon_B = -\epsilon_A = 0.4$ , this time scale is of the order of only 100 in units of average hopping time. This short time scale in the monomer problem may be related to the exponential decay of almost all the eigenstates and the exponential decay of the width of the perfect resonance states. For the random dimer case, since the widths of the individual resonance states inside the decaying cluster core decay themselves as  $1/N$  but their number inside this core increases algebraically, there is no particular length (or time) scale for the decay of the diffusion 'constant' in this way of looking at the diffusion of a fermion in a somewhat 'classical' fashion. Thus one may not be able to assign a single time beyond which there is a crossover in the behaviour of the MSD from a diverging to a bounded nature. Hence in numerical computations one may see super-diffusive or diffusive behaviour for quite a while. Absence of a single length or time scale in this problem may probably be related to the existence of a group of critical-like (resonance) states inside the cluster core (which exists only for a finite size sample). But the critical states are known to decay in a power-law fashion. Thus it seems that at best a 'sub-diffusive' behaviour should show up for a very large but finite sample. In any case, even in this way of looking at the transport of an initially localized fermion, eventually in the infinite length limit the diffusion constant seems to approach zero since the support from each of the individual zero-width resonances must approach zero.

The effect of disorder in the random dimer chain becomes very vivid if one studies the situation where the hopping energies are perfectly correlated with neighbouring site energies. For example instead of keeping the hopping term constant ( $= 1$ ) one may choose the hopping to be 0.94 when an A and a B site are neighbours and 1 otherwise. This is one example of a correlated random dimer model which seems to be relevant in the transport of the polymer polyaniline (Wu and Phillips 1991). This very slight change in the hopping seems to remove the cluster core completely and the effect of fragmentation (i.e. localization) appears very emphatically everywhere, as we have shown elsewhere (Sen and Gangopadhyay 1992).

#### 4. Conclusions

There is a close clustering of resonance states in the random dimer chain for Fermi energies close to each of the two site energies as long as the site energies satisfy the relation  $|\epsilon_A - \epsilon_B| < 2V$ . The energy domains within which the core of the clusters occur are found to decay algebraically as  $N^{-2/3}$  as the chain size increases. The number of resonances within the cluster core increases as  $N^{1/3}$  and the width of each of the resonance states inside this core is also found to decay algebraically as  $1/N$  where  $N$  is the chain length. This characteristic of the dimer chain in contrast to the random 'monomer' chain is significantly different. In the immediate neighbourhood of the region where the cluster core occurs, there is a fragmentation region where

the width of each of the resonance states falls off very rapidly (exponentially) just as in the case of a purely random chain. Thus for large chain sizes, they cannot contribute to the conductance any more. If the Fermi energy falls within the cluster region, then the conductance will be significantly large and would not seem to fall off with increasing chain size up to some maximum size. But since with increasing chain size the energy domain of the cluster gets narrower and narrower, ultimately this particular Fermi energy becomes excluded from the cluster core region and the conductance starts decaying exponentially. We have clearly demonstrated that *all* states around each site energy have *finite localization lengths* and that the divergence of the localization length as the Fermi energy approaches one of these energies is given by  $\xi \sim (E_F - \epsilon_S)^{-2}$ , where  $S = A, B$ . Because of this reason and because the cluster width decays algebraically (in contrast to a perfectly random chain), a very much larger system size would be required to see the crossover to exponential decay in the conductance if the Fermi energy is even slightly closer to one of the site energies. As far as the diffusion of the initially localized particle at the centre of the chain (site 0) is concerned, it is true that transport almost without scattering will be supported by clusters of an algebraically increasing number of resonance states near the two site energies. Furthermore, this support will continue for a very much longer time for the dimer than the monomer because the resonances decay algebraically and not exponentially. Thus one may see an apparent super-diffusive behaviour for a very long time (length). But finally in the infinite length limit all the resonances decay to zero width and it is well known that resonances of zero width cannot support transport. Thus the initially localized particle cannot obtain any more support of its transport from all these perfectly transmitting states since they are isolated resonances of zero width. Thus our studies indicate that the above-mentioned random dimer model with its short range correlation will *not* give rise to delocalization of an initially localized particle in the *truly infinite length limit* and that there is *no metal-insulator transition* in this random dimer model.

In spite of all these, it must be noted that the model has two remarkable properties. First, two very broad resonance structures occur at two predictable Fermi energies (namely the site energies), and those at the site energies survive, with infinite degeneracy, even in the infinite length sample. This predictability is not observed for the Azbel resonances for a random monomer chain. Second, each of the resonance cluster cores along with the individual resonances inside them decay *algebraically* with length. Thus the states inside the resonance cluster cores survive unusually long times and have *very long localization lengths*. It is highly remarkable that short range order on the atomic scale in the random dimer model has been able to affect physical properties on a macroscopic or at least mesoscopic scale. These two facts together make the two resonance states very attractive for possible use in mesoscopic quantum-mechanical switching devices, because these states are robust enough and not too 'delicate' to use technologically (in contrast with the Azbel resonances).

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