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Abstract. We have calculated the critical exponent of the metal–insulator transition for a three-dimensional network of random wires. The Hamiltonian of this model is not explicitly defined, and so we do not bias our results towards the models with diagonal or off-diagonal disorder, which produce conflicting exponents. The result is $s = \nu = 1.10 \pm 0.05$, which is in agreement with other models using tight-binding Hamiltonians with off-diagonal disorder. We suggest that pure wave interference is not the dominant mechanism for Hamiltonians with diagonal disorder and therefore some other physical process must be responsible for generating exponents of $s = \nu \simeq 1.5$.

1. Introduction

Since the formulation of the scaling theory [1,2], great advances have been made in the study of Anderson localization. Of particular importance to this paper was the numerical confirmation of the scaling theory and the existence of the metal–insulator transition in three dimensions using a finite-size scaling technique [3,4]. Calculation of the critical exponents for the metal–insulator transition was also made possible by this method. Previously, an exponent for the metal–insulator transition of $s = \nu = 1$ had been obtained from the non-linear σ-model using a truncated series expansion. However, the validity of this truncation has been called into question [5,6]. Numerical techniques, on the other hand, are limited only by the availability of computer memory and CPU time and should therefore have provided us with definitive answers concerning the critical behaviour. Unfortunately, it is the results of these very techniques that have presented us with another problem.

Consider the usual tight-binding Hamiltonian

$$\mathbf{H} = \sum_i |i\rangle \varepsilon_i \langle i| + \sum_{\langle ij \rangle} |i\rangle V_{ij} \langle j| \tag{1}$$

where ε_i labels the site energies and V_{ij} is the interaction between nearest-neighbour sites. We could consider introducing disorder into the Hamiltonian in one of two ways:

(i) Choose ε_i randomly from a uniform distribution of width W, while keeping V_{ij} fixed. This is the model studied by Anderson in his original paper on the 'Absence of diffusion in certain random lattices' [7].

(ii) Keep ε_i constant and vary the off-diagonal coupling.

Both these models belong to the orthogonal universality class and are thus predicted to exhibit identical critical behaviour [8]. However, results from extensive numerical experiments clearly show that they do not [9]. Model (i) gives an exponent of $s = \nu \simeq 1.5$,

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while model (ii) gives $s = \nu \simeq 1.0$. When these numerical experiments are performed, the two models are driven through the transition in different ways: for model (i), the disorder characterized by the width of the site energy distribution is varied, while for model (ii) it is the energy that is changed. Whether the difference in the critical exponents is due to fundamentally different physical processes, or due to the numerical method of forcing the transition, is not clear.

In this paper, we have studied the metal–insulator transition using a network of random one-dimensional wires. The underlying Hamiltonian of this model is not explicitly defined and thus we are not biased towards one or other of the two models outlined above. Such network models have been used before for studying, amongst other things, the integer quantum Hall effect [10] and the quantum percolation problem [11].

2. The model

Our system consists of a d-dimensional network of random one-dimensional wires. For simplicity, an example of a two-dimensional system is shown in figure 1. For those requiring physical justification of this model, it can be thought of as the underlying lattice formed by a system constructed from disordered hypercubes. In direct analogy with the long-strip method of MacKinnon and Kramer [3, 4], we consider continually adding $M^{(d-1)}$ hypercubes, in the form of a slice, to the system. Then, the system has a finite cross section of $M^{(d-1)}$, but an effectively unbounded length since we can add an arbitrary number of slices (see figure 2).

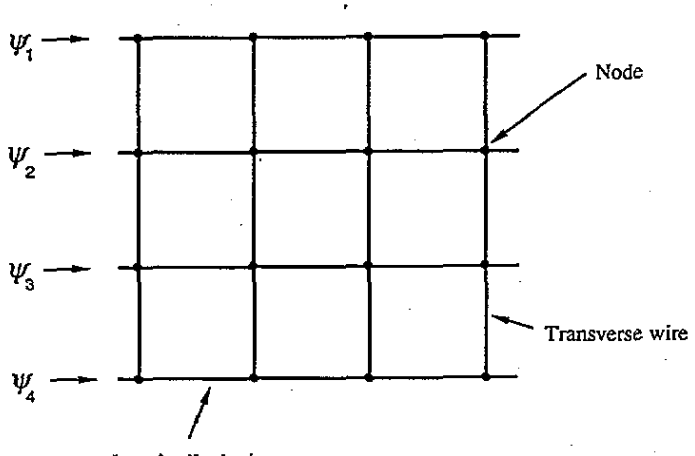

Figure 1. A two-dimensional network of random wires. The waves are fed in along the longitudinal wires and propagate through the system, satisfying certain conditions at the nodes. The system is finite in the transverse direction, but effectively unbounded in the longitudinal direction.

Now, close to the metal–insulator transition electronic transport is dominated by a single channel [12, 13]. Since this is the region of interest, each hypercube can be considered simply as d one-dimensional wires (the conducting channels) connecting opposite faces and the wire network picture of figure 1 begins to emerge.

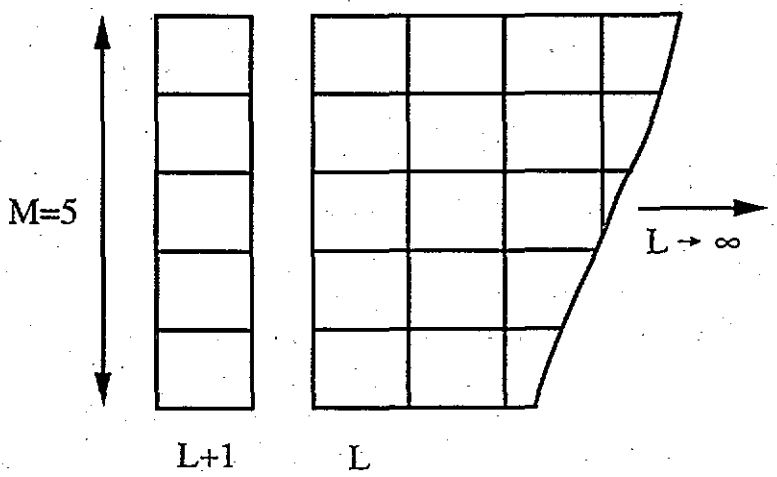

Figure 2. Building the system from two-dimensional hypercubes. A slice of width $M = 5$ is added to the system, increasing the length from L to $L + 1$. This process is continued until L is sufficiently large.

Waves propagating on this network must satisfy certain conditions at each node, where the wires intersect with each other. For a d-dimensional network, these conditions are (from elementary quantum mechanics):

(i) The wavefunction must be single valued at any point in space. Thus, if the waves on the $2d$ wires connected by a given node are $\psi_1, \psi_2, \ldots, \psi_{2d}$, then the condition at the node is

$$\psi_1 = \psi_2 = \ldots = \psi_{2d}. \tag{2}$$

(ii) The first derivative of the wavefunctions must be continuous at any point in space, which is just equivalent to current conservation. Thus, at the node

$$\sum_{n=1}^{2d} \frac{\mathrm{d}\psi_n}{\mathrm{dx}} = 0 \tag{3}$$

where all the derivatives are defined as positive towards the node.

3. Algorithm

Consider the situation illustrated in figure 3, which is a two-dimensional network. (In fact this discussion is sufficiently general that it is valid for any dimension, but the graphical representation is far simpler and more obvious in only two dimensions. Furthermore, in this paper we present results for a three-dimensional network only.)

If we can derive a transfer matrix $\mathbf{T}_{\mathrm{real}}$ relating the amplitude and derivative of a wave at one end of a one-dimensional wire to the amplitude and derivative at the other end, then we can calculate the amplitude and derivative of all the waves into the nodes labelled set 1 by applying $\mathbf{T}_{\mathrm{real}}$ in turn to the set of input wave amplitudes $(\psi_1, \ldots, \psi_M)$ and derivatives $(\psi'_1, \ldots, \psi'_M)$.

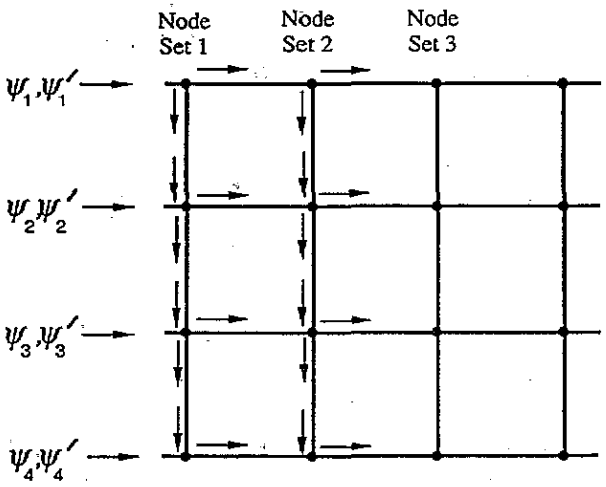

Figure 3. A two-dimensional system of cross section $M = 4$. The transfer matrix $\mathbf{T}_{\text{real}}$ is applied to the input waves and their derivatives, ψ_1, ψ_1' etc to determine the amplitudes of the waves at each node on node set 1. The derivative of the waves into the nodes on node set 1 is also determined by this calculation. The downward pointing arrows indicate the derivatives of the waves along the transverse wires on node set 1, calculated using matrix $\mathbf{T}_{\text{der}}$. With this information, the derivatives of the waves leaving node set 1 towards node set 2 can be calculated using condition (3) and the process can be repeated for node set 2. Periodic boundary conditions are used in the transverse direction.

Now given a matrix $\mathbf{T}_{\text{der}}$, which determines the derivatives at either end of a one-dimensional wire given the amplitudes, we can calculate the derivatives into and out of each node along the transverse wires on set 1, since we know the amplitudes at these nodes.

Finally, by applying condition (3) the derivatives of the waves leaving the nodes on set 1 can be determined. The entire process can then be repeated for the nodes on set 2 and so on. In effect we have a recursion relation, which we simply continue to iterate.

All that is left to do is to determine the matrices $\mathbf{T}_{\text{real}}$ and $\mathbf{T}_{\text{der}}$.

4. Deriving the matrices

Because of the time-reversal symmetry, we can follow the behaviour of wavefunctions of the form

$$\psi_1 = A_1 \cos kx + B_1 \sin kx \tag{4}$$

where A_1, B_1 are real amplitudes. Now, let ψ_1 be the wavefunction on one side of a one-dimensional random wire and let ψ_2 be the wavefunction on the other side. If we reset the origin to be on the same side of the wire as ψ_1, then the amplitude and derivative of ψ_1 on that side will be

$$\psi_1(0) = A_1 \qquad \psi_1'(0) = kB_1. \tag{5}$$

Now, we assume that at each node the wires are connected by a small piece of uniform material. Then, even in the limit that this piece of material becomes vanishingly small, the

value of k for the waves on the $2d$ wires, connected by a given node, will be the same at that node. Then, k becomes irrelevant in the current conservation condition (3) and can therefore be ignored in our calculations. So we can write

$$\psi_1'(0) = B_1. \tag{6}$$

Thus, it is possible to write

$$\begin{bmatrix} \psi_2(x) \\ \psi_2'(x) \end{bmatrix} = \mathbf{T}_{\text{real}} \begin{bmatrix} \psi_1(0) \\ \psi_1'(0) \end{bmatrix} \tag{7}$$

where $\mathbf{T}_{\text{real}}$ is a real 2×2 transfer matrix for the one-dimensional wire. This transfer matrix is easily derived from the conventional transfer matrix for travelling waves

$$\mathbf{T} = \begin{bmatrix} 1/t & r/t \\ (r/t)^* & (1/t)^* \end{bmatrix} \tag{8}$$

where r and t are the complex reflection and transmission coefficients for the wire. If the travelling waves on either side of the wire have amplitudes, for the forward and reverse travelling parts, which are complex conjugates of each other, $\mathbf{T}_{\text{real}}$ can be obtained by superposing these parts and calculating the real amplitudes to give

$$\mathbf{T}_{\text{real}} = \begin{bmatrix} (1/|t|)\cos\phi_t + (|r|/|t|)\cos(\phi_r - \phi_t) & (-1/|t|)\sin\phi_t - (|r|/|t|)\sin(\phi_r - \phi_t) \\ (1/|t|)\sin\phi_t - (|r|/|t|)\sin(\phi_r - \phi_t) & (1/|t|)\cos\phi_t - (|r|/|t|)\cos(\phi_r - \phi_t) \end{bmatrix} \tag{9}$$

where ϕ_r and ϕ_t are the reflection and transmission phase respectively.

Now, our model also requires us to determine the matrix $\mathbf{T}_{\text{der}}$, which relates the derivatives at both end points of a wire to the amplitudes at those end points. Rearranging the top row of equation (7) gives

$$\psi_1'(0) = \left\{ \left[(1/|t|)\cos(\phi_t) + (|r|/|t|)\cos(\phi_r - \phi_t) \right] / \left[(1/|t|)\sin(\phi_t) + (|r|/|t|)\sin(\phi_r - \phi_t) \right] \right\} \times \psi_1(0) - \left\{ 1/\left[(1/|t|)\sin(\phi_t) + (|r|/|t|)\sin(\phi_r - \phi_t) \right] \right\} \psi_2(x). \tag{10}$$

Equation (7) can then be rearranged to give

$$\begin{bmatrix} \psi_1(0) \\ \psi_1'(0) \end{bmatrix} = \mathbf{T}_{\text{real}}^{-1} \begin{bmatrix} \psi_2(x) \\ \psi_2'(x) \end{bmatrix} \tag{11}$$

and the top row of this matrix equation gives

$$\psi_2'(x) = \left\{ 1/\left[(1/|t|)\sin(\phi_t) + (|r|/|t|)\sin(\phi_r - \phi_t) \right] \right\} \psi_1(0) - \left\{ \frac{\left[(1/|t|)\cos(\phi_t) - (|r|/|t|)\cos(\phi_r - \phi_t) \right]}{\left[(1/|t|)\sin(\phi_t) + (|r|/|t|)\sin(\phi_r - \phi_t) \right]} \right\} \psi_2(x). \tag{12}$$

Because we have chosen to define the derivative out of a node to be negative in condition (3)

$$\begin{bmatrix} \psi_1'(0) \\ \psi_2'(x) \end{bmatrix} = \mathbf{T}_{\text{der}} \begin{bmatrix} \psi_1(0) \\ \psi_2(x) \end{bmatrix} \tag{13}$$

where

$$\mathbf{T}_{\mathrm{der}} = \begin{bmatrix} \dfrac{(-1/|t|)\cos(\phi_t)-(|r|/|t|)\cos(\phi_r-\phi_t)}{(1/|t|)\sin(\phi_t)+(|r|/|t|)\sin(\phi_r-\phi_t)} & \dfrac{1}{(1/|t|)\sin(\phi_t)+(|r|/|t|)\sin(\phi_r-\phi_t)} \\ \dfrac{1}{(1/|t|)\sin(\phi_t)+(|r|/|t|)\sin(\phi_r-\phi_t)} & \dfrac{(-1/|t|)\cos(\phi_t)+(|r|/|t|)\cos(\phi_r-\phi_t)}{(1/|t|)\sin(\phi_t)+(|r|/|t|)\sin(\phi_r-\phi_t)} \end{bmatrix}. \tag{14}$$

It is important to note that there is a possibility for the elements of $\mathbf{T}_{\mathrm{der}}$ to become infinite. These events can plague numerical experiments and so we define our model so that this eventuality cannot occur. By studying the eigenvalues of the transmission matrix for a simple system consisting of only one transverse wire, we determined that the elements of $\mathbf{T}_{\mathrm{der}}$ becoming infinite corresponded to a situation where either the symmetric or the antisymmetric part of the wavefunction was transmitted and the other part was reflected back along the longitudinal links. For this situation to occur, it is necessary for the values of t, ϕ_r and ϕ_t to be chosen appropriately from their own particular distributions. These events were found to happen so rarely (perhaps once every 1 000 000 times) that we concluded that they could be ignored. This was done by choosing the value of the transmission phase from a restricted distribution, the portion being forbidden lying in the range that would cause a numerical instability. This is an inherent problem with the transfer matrix method: in effect the problem we are solving is, 'What went in, in order to give these outputs?'. We have obviously then found situations where no combinations of the inputs can possibly give these outputs, hence there is no solution to the problem in this formulation. In any case, universality arguments allows us to ignore these events since we do not expect that the exponents will be changed by doing so, even though the critical disorder might be.

Disorder is introduced into our model by the choice of the phase and amplitude of the reflection and transmission coefficients appearing in matrices (9) and (14). Azbel [14] and Pendry [15] argue that the transmission through disordered one-dimensional systems is dominated by tunnelling via eigenstates in the system. Azbel has studied the tunnelling via a single eigenstate, while Pendry suggests that, for very long systems, the transmission occurs via a series of eigenstates, which he terms a necklace. Azbel determined a very simple expression for the distribution of the transmission amplitude

$$P(|t|) = \left(\frac{L_0}{L}\right)\frac{1}{|t|} \qquad \exp\left(-L/L_0\right) \leqslant |t| \leqslant 1 \tag{15}$$

where the ratio L/L_0 defines the disorder in the system. For our purposes, the expression obtained by Azbel is perfectly adequate. Furthermore, it is particularly easy to implement numerically. Azbel's formula is the simplest, physically justifiable distribution that we can choose. Again, universality arguments suggest that the actual form of the distribution should not change the values of the exponents.

If we assume only elastic scattering, then current conservation gives

$$|t|^2 + |r|^2 = 1 \tag{16}$$

so determining $|t|$ also fixes the value of $|r|$. As is usual in these calculations, we assume phase randomization across the wires and no correlation between the reflection and transmission phase. Thus, our matrices (9) and (14) are parameterized by three numbers: the transmission amplitude $|t|$, which is selected from the distribution (15) for a given disorder, and the reflection and transmission phases, which are selected randomly and independently from a uniform $[0, 2\pi)$ distribution, subject to the constraint that the elements of matrix $\mathbf{T}_{\mathrm{der}}$ remain finite.

Our model of propagating real wavefunctions in a random network is now completely described.

5. Scaling

MacKinnon and Kramer [3, 4] showed that the renormalized localization length

$$\Lambda = \lambda_M / M \tag{17}$$

where λ_M is the localization length for a system of cross-section M^{d-1}, obeys a scaling relationship of the form

$$\mathrm{d} \ln \Lambda / \mathrm{d} \ln \mathrm{M} = \chi(\ln \Lambda) \tag{18}$$

where

$$\Lambda = f(\xi / M) \tag{19}$$

and ξ can be identified as the localization length of the infinitely wide system. Close to the metal–insulator transition $\chi(\Lambda) \simeq 0$ and therefore

$$\ln \Lambda = \ln \Lambda_c + (\tau - \tau_c) A M^{\alpha} \tag{20}$$

where τ is the disorder parameter, which is changed to drive the system through the transition and

$$\alpha = \partial \chi / \partial \ln \Lambda \big|_{\chi=0}$$

is the logarithmic derivative of χ at $\chi = 0$.

Comparing equations (19) and (20) we see that

$$\xi \simeq |\tau - \tau_c|^{-1/\alpha}. \tag{21}$$

A similar fixed-point analysis on the β function of Abrahams *et al* [2] gives the following relations

$$\sigma \simeq |\tau - \tau_c|^{s} \tag{22}$$

for the conductivity σ on the extended side and

$$\xi \simeq |\tau - \tau_c|^{-\nu} \tag{23}$$

on the localized side of the transition. Since $\sigma \simeq \xi^{-1}$ in the localized regime, we have

$$s = \nu = 1/\alpha \tag{24}$$

and thus calculating α gives us the required exponents s and ν.

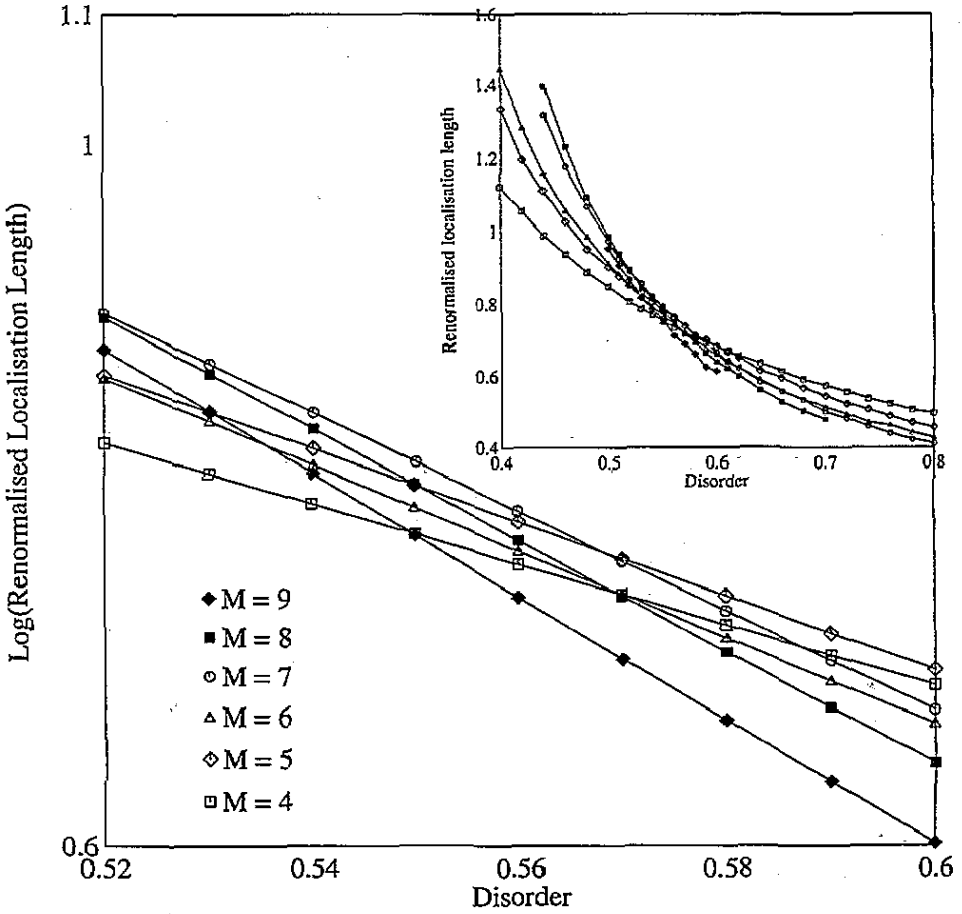

Figure 4. Results obtained for the three-dimensional network. The localization lengths have been determined to a statistical accuracy of 0.5%. The inset graph shows the results obtained for systems with widths $M = 4$ to $M = 9$. The main graph shows a plot of $\log \Lambda$ versus disorder L/L_0 in the region of the transition. It is clear that there is no common crossing point, hence the need for the width-dependent constant $B(M)$ in equation (25).

6. Analysis

Simulations in two-dimensions were performed with perfect transmission on the one-dimensional wires in the network, the only disorder occurring being due to a random phase change across each wire. In this case, we found that all states were localized as we expected. No further analysis was performed in this case since the model was defined in order to study the transition in three dimensions.

To calculate a value for the critical exponent, we use equation (20) and study the behaviour of Λ as the system cross section M^{d-1} and disorder are varied. The localization lengths are extracted using the method outlined in references [4] and [16]. If we plot $\ln \Lambda$ as a function of disorder, for various values of M, then the critical disorder is determined by the intersection of the curves for differing M. It is normally found that not all the curves cross in exactly the same place (see figure 4). For this reason, we modify equation (20) by the addition of some width-dependent constant B, which corrects for the fact that the

curves do not all cross at the same point:

$$\ln \Lambda = \tau A M^{\alpha} + B(M). \tag{25}$$

We then select points in the transition region and perform a non-linear least squares fit to determine the value of α. The transition region can be determined by varying the disorder 'window', over which points are selected in order to carry out the fit. If the disorder 'window' is too large, that is we have selected points too far from the transition point, then the quality of the fit becomes very poor, indicating that we need to select fewer points.

7. Results and discussion

We obtain for the exponent α a value of

$$\alpha = 0.91 \pm 0.04 \tag{26}$$

corresponding to the exponents for the metal–insulator transition of

$$s = \nu = 1.10 \pm 0.05 \tag{27}$$

which is in close agreement with the exponents obtained for models with off-diagonal disorder. The quality of the fit can be quantified by comparing the value of the χ^2 function with the number of degrees of freedom: χ^2 should have a value approximately equal to the number of degrees of freedom. For this value of α we have a χ^2 of 47.73 and the number of degrees of freedom is 45.

Most of the literature on numerical investigations of the exponents has been done on the diagonal models and the exponents obtained of $s = \nu \simeq 1.5$ are not in question. Little published work exists on the off-diagonal models [17], save for the results of one of the authors of this paper [9]. Our result confirms that exponents of $s = \nu \simeq 1.0$ can be obtained from numerical experiment and therefore results from off-diagonal models are not due to some numerical error. We have also established some insight into the physical processes responsible for these exponents. Clearly, the only physical process occurring in our model is the interference of the waves propagating through the network. Thus we suggest that this is not the dominant mechanism in the models with diagonal disorder and some other physical process must be responsible for producing exponents of $s = \nu \simeq 1.5$.

Acknowledgments

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