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Anderson localisation from a generalised master equation

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Abstract. We consider here a tight-binding model for the motion of a single electron and an energetically disordered lattice. We show that the Anderson transition in this model can be studied using a generalised master equation with a nearest-neighbour memory function. It is first demonstrated that because the generalised master equation with a nearest-neighbour memory function is isomorphic to a classical bond-percolation problem, an exact expansion can be constructed for the diffusion constant using the bond flux method of Kundu, Parris and Phillips. We show that at the effective medium level, the diffusion constant vanishes for any non-zero value of the disorder. We then calculate the probability distribution of the self-energy for the bond flux Green function on a Cayley tree of connectivity K . Our approach predicts an Anderson transition at $W/V = 13$ for $K = 2$ and $W/V = 20$ for $K = 3$. W is the width of the distribution for the site energies and V , the nearest-neighbour matrix element. These results are in good agreement with the exact values of $W/V = 17$ ($K = 2$) and $W/V = 29$ ($K = 3$). Further applications of the generalised master equation to disordered systems and the prospect of constructing the exact memory function for Anderson localisation are discussed.

1. Introduction

We consider here the transport of a single electron on an energetically-disordered lattice. We treat this system in the tight binding approximation in which one orbital and a single random site energy are assigned to each lattice site. A constant nearest-neighbour matrix element, V , mediates transport among the lattice sites. It was originally shown by Anderson [1] that for a uniform distribution of site energies of width W , delocalised (current carrying) electronic states fail to occur when W/V exceeds a critical value [1]. In this work, we study the localisation–delocalisation transition in the Anderson model using a generalised master equation (GME) [2–7] with an approximate memory function. While the GME has been used extensively [3–5] as a tool for bridging the gap between coherent and incoherent motion in ordered systems, few applications of the GME to quantum transport in disordered systems exist [7]. In fact, the present study represents the first application of the GME to the Anderson transition.

Because of the relevance of the Anderson transition to insulator–metal transitions and the residual resistivity in metals, much effort has been expended in an attempt to form a clear understanding of this model [8–19]. For example, the early work of Thouless

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[9, 10], Wegner [11], the subsequent work of Abrahams and co-workers and MacKinnon and Kramer [12] led to the scaling theory of Anderson localisation. This work established that the metal–insulator transition is a continuous function of the energy in three dimensions and that all states are localised for finite disorder in one and two dimensions. Subsequent analyses by Vollhardt and Wölfle (vw) showed that the results of scaling theory can be reproduced by a self-consistent diagrammatic expansion of the density response function for a system of independent particles moving in a random potential [13]. The basic principle underlying the work of vw [13] is that the coherent back-scattering which leads to Anderson localisation can be described by some type of average density relaxation kernel or memory function. Recently, Loring and Mukamel [19] have attempted to implement the basic idea of the VW work. They start with a stochastic equation of motion for the density matrix. The stochastic term in their equations corresponds to a constant site off-diagonal dephasing process. For equation of motion methods see [18]. However, Parris and Phillips [20] have recently proved that a constant site off-diagonal dephasing process will always thwart quantum localisation at long durations.

In this work we study the Anderson transition using a memory function approach. The starting point for our analysis is a generalised master equation for the site occupation probabilities. The central quantity in any GME [2–7] is the memory function which in this case describes the interaction of the electron with the disordered environment. In our analysis we employ a nearest-neighbour approximation [2] to the exact memory function for a tight-binding Hamiltonian. The question on which we focus is as follows: can a GME with a nearest-neighbour memory function for a tight-binding Hamiltonian describe Anderson localisation? As we shall see, on a Cayley tree the answer to this question is an unequivocal *yes*. Hence, this method appears to be a promising tool for studying localisation in other disordered systems. Two methods are employed to study the role of disorder. In the first, we capitalise on the isomorphism between the GME in the Laplace domain for a nearest-neighbour memory kernel and classical bond percolation. The bond flux transformations developed by Kundu, Parris, and Phillips [21] are then used to calculate the diffusion coefficient. The resultant diffusion coefficient is then studied at the level of the effective medium approximation. Within this approximation, it is shown that the diffusion constant vanishes in all spatial dimensions for any non-zero value of the disorder.

In the second approach, we investigate the properties of the Green function for the probability fluxes. By examining the self energy of the flux Green function, we are able to determine whether the energy spectrum corresponds to a collection of stationary (localised) states or delocalised states. We show that the vanishing of the imaginary part of the self-energy that appears in the probability flux Green function is the signature of Anderson localisation. To facilitate an exact calculation of the self energy we specialise to a Cayley tree of connectivity K and compute the probability distribution of the self-energy. We show that for $K = 1$ all states are localised for a flat distribution of site energies of width W . For $K = 2$ and 3 we show that the nearest-neighbour memory kernel predicts a localisation transition at $W/V = 13$ and 20, respectively. These results are in excellent agreement with the exact results of $W/V = 17$ ($K = 2$) and $W/V = 29$ ($K = 3$) predicted by the method of Abou-Chacra, Anderson and Thouless (AAT) [8].

In the next section we discuss the validity of the GME for Anderson localisation. A derivation of the equations of motion is also given for a nearest-neighbour memory function. The diffusion constant is calculated in § 3 and in § 4 the self-energy calculations for the site-return Green function are presented and the existence of a localisation

transition on the Cayley tree is demonstrated. We close with a general discussion of the prospects for constructing a self-consistent equation for the memory function.

2. Equations of motion

The Hamiltonian describing our system is

$$H = \sum_n \varepsilon_n a_n^\dagger a_n + \sum_{n,m} V_{nm} a_n^\dagger a_m \quad (2.1)$$

where ε_n are the random site energies and V_{nm} the matrix element connecting sites n and m . V_{nm} is zero unless sites n and m are nearest neighbours. The operator a_n^\dagger (a_n) creates (destroys) an electron at site n . A standard [1, 8, 17] way of studying the dynamics determined by (2.1) is the Heisenberg equation of motion

$$i\dot{a}_n = \varepsilon_n a_n + \sum_m V_{nm} a_m \quad (2.2)$$

for the operators a_n . An obvious alternative to (2.2) is of course the Liouville equation of motion

$$i\dot{\rho}_{nm} = \sum_l (V_{nl}\rho_{lm} - \rho_{nl}V_{lm}) + (\varepsilon_n - \varepsilon_m)\rho_{nm} \quad (2.3)$$

for the density matrix ρ . Equation (2.3) provides a direct route to the dynamics because any transport property can be computed once the site probabilities or equivalently the site diagonal elements (ρ_{nn}) of the density matrix are known. However, calculation of the ρ_{nn} values directly from (2.3) is problematic because (2.3) involves both diagonal and off-diagonal elements of the density matrix. Zwanzig [2] and others [3, 4] have shown how to construct a closed equation of motion involving only the site probabilities and an appropriate memory function. For a localised initial condition [2, 3], the appropriate equation for the time evolution of the site probabilities ($P_n(t)$) is the generalised master equation (GME)

$$\dot{P}_n = \int_0^t \sum_m [W_{mn}(t-t')P_m(t') - W_{nm}(t-t')P_n(t')] dt'. \quad (2.4)$$

In equation (2.4) $W_{nm}(t-t')$ is the memory function responsible for transport between sites n and m . The Markovian approximation to the memory function in (2.4) corresponds to a memory that is a delta function in time, $W_{nm}\delta(t-t')$. In this limit equation (2.4) reduces to the standard master equation

$$\dot{\bar{P}}_n = \sum_m (W_{mn}P_m(t) - W_{nm}(t)) \quad (2.5)$$

which describes incoherent transport and W_{nm} is the rate of transport between sites n and m .

We emphasise that equation (2.4) is a fully quantum mechanical exact equation. In this respect, then, it is different in kind from the GME derived by Klafter and Silbey [6] in the context of incoherent or master equation dynamics. The memory function that appears in the Klafter–Silbey work arises when projection operators are introduced to average over the disorder [6].

In an ordered infinite one-dimensional system with nearest-neighbour matrix elements $V_{nm} = V$, and $\varepsilon_n = \varepsilon_m$ for all $n \neq m$, the exact memory function [3]

$$W_{mn}(t) = \frac{1}{t} \frac{d}{dt} J_{m-n}^2(2Vt) \quad (2.6)$$

connects every pair of sites. To lowest order in V^2 , the exact memory function, equation

(2.6), reduces to $W_{nm} \rightarrow 2V^2 \delta_{n,m+1}$ which connects nearest neighbours only. It is well known that this approximate memory function is sufficient to generate the exact mean-square displacement $2V^2 t^2$ for an ordered system even though the nearest-neighbour approximation may result in negative site probabilities [3, 4]. The result for the mean-square displacement is easily established because in an ordered system with a nearest-neighbour memory function, the diffusion coefficient is simply the time integral of the memory function [3]. As a result simple rules can be formulated that relate the long time dependence behaviour of the memory function to the asymptotic properties of the diffusion constant [3]. For example, in an ordered system with a nearest-neighbour memory function, a purely oscillatory (in time) memory will result in localisation. On the other hand, diffusion or incoherent transport obtains if the memory function decays to zero at long times.

For disordered systems the memory function is considerably more complicated. We propose here to study the Anderson transition with the nearest-neighbour approximation to the memory for (2.1). Using the procedure outlined by Zwanzig [2], it is straightforward to show that

$$F_{n,n\pm 1}(t) = 2V^2 \cos(\varepsilon_n - \varepsilon_{n\pm 1})t \quad (2.9)$$

is the nearest-neighbour approximation to the memory function for equation (2.1). For a one-dimensional system then, the corresponding equation of motion for the site probabilities is

$$\begin{aligned} \dot{P}_n(t) = 2V^2 \left(\int_0^t \cos[(\varepsilon_n - \varepsilon_{n+1})(t-t')] (P_{n+1}(t') - P_n(t')) \right. \\ \left. + \int_0^t \cos[(\varepsilon_n - \varepsilon_{n-1})(t-t')] (P_{n-1}(t') - P_n(t')) \right) dt'. \end{aligned} \quad (2.10)$$

It should be clear from (2.10) that because the memory function changes from site to site, the diffusion constant is no longer simply related to the time integral of the memory function. Consequently, the simple rule that an oscillatory memory will give rise to localisation might not be valid. The memory function (2.9) is well known to predict [3] localisation rather than coherent transport when the site energies alternate ($\pm \Delta$) along a chain or whenever any long-range periodicity is associated with the site energies. Clearly, the nearest-neighbour approximation to the memory function cannot account for any long-range periodicity and is consequently doomed to fail in such cases. Hence, whether the memory function (2.9) is adequate to describe a localisation–delocalisation transition in a disordered system is an open question. We now turn to the answer to this question. In the next section we show how to construct an exact expansion for the diffusion constant for equation (2.10) and its d -dimensional analogue. The expansion is then analysed in the effective medium approximation.

3. Diffusion coefficient

3.1. One dimension

To formulate the diffusion coefficient for the model defined in (2.9), it is expedient to consider the Laplace transformed equations of motion. Let us define the quantities

$$\Delta_m = (\varepsilon_{m+1} - \varepsilon_m)/\sqrt{2V} \quad (3.1)$$

and

$$F_m(s) = s/(s^2 + \Delta_m^2) \quad (3.2)$$

where $s = \varepsilon/\sqrt{2V}$, ε the Laplace transform variable conjugate to time. Noting that $F_m(s)$

is the Laplace transform of the memory function (2.9), we rewrite the equations of motion as

$$sP_n(s) - P_n(t=0) = F_n(s)(P_{n+1}(s) - P_n(s)) + F_{n-1}(s)(P_{n-1}(s) - P_n(s)). \quad (3.3)$$

We point out that in the Laplace domain, the master equation for nearest-neighbour transport

$$sP_n(s) - P_n(t=0) = W_n(P_{n+1}(s) - P_n(s)) - W_{n-1}(P_{n-1}(s) - P_n(s)) \quad (3.4)$$

closely resembles the Laplace transformed nearest-neighbour GME. The only difference between (3.4) and (3.3) is that the hopping rates $F_n(s)$ in (3.3) are frequency dependent, whereas in (3.4) the W_n values are static. We now show that the similarity between (3.3) and (3.4) can be exploited to construct an expansion for the diffusion constant for (3.3).

We proceed by introducing the flux or probability current

$$J_n(s) = F_{n-1}(s)(P_n(s) - P_{n-1}(s)) \quad (3.5)$$

between sites n and $n - 1$. For classical bond-disordered systems, Kundu, Parris and Phillips [21] (KPP) have shown that (3.5) provides a direct route to the diffusion constant. Because (3.3) is of the bond-disordered form, the same techniques apply here as well. Only one change is necessary, namely $W_n \rightarrow F_n(s)$. Hence, we will be brief but self-contained in our presentation. We first rewrite equation (3.3) in a more transparent form

$$sP_n(s) - P_n(t=0) = J_{n+1}(s) - J_n(s). \quad (3.6)$$

For the localised initial condition $P_n(0) = \delta_{n,0}$

$$s \sum_n n^2 P_n(s) = \sum_n J_n(s) - 2 \sum_n n J_n(s) \quad (3.7)$$

or equivalently

$$D(s) = \frac{sl^2}{2} \left(\left\langle \sum_n J_n(s) \right\rangle - 2 \left\langle \sum_n n J_n(s) \right\rangle \right). \quad (3.8)$$

The angle brackets in (3.8) signify an average over the distribution of site energies and l the lattice spacing. Equation (3.8) suggests that once the probability current generating function

$$F(q, s) = \sum_n e^{iqn} J_n(s) \quad (3.9)$$

is known, the diffusion constant can be constructed because [21]

$$D(s) = \frac{sl^2}{2} \left(\langle F(q=0, s) \rangle + 2i \frac{\partial}{\partial q} \langle F(q, s) \rangle \Big|_{q=0} \right). \quad (3.10)$$

As in the classical problem [21], an integral equation can be constructed for $F(q, s)$ by subtracting the equations of motion for $P_n(s)$ and P_{n-1} , multiplying through by e^{iqn} and summing over n . The result is

$$s \sum_n e^{iqn} \frac{J_n}{F_n} = -2(1 - \cos q)F(q, s) + (1 - e^{iq}). \quad (3.11)$$

The final expression for the integral equation

$$F(q, s) = (1 - e^{iq})/[s^2 + c(s) + 2(1 - \cos q)] - \frac{1}{2\pi} \int_{-\pi}^{\pi} dq' \left[\left(\sum_m \delta(\Delta_m^2) e^{i(q-q')m} F(q', s) \right) [s^2 + c(s) + 2(1 - \cos q)]^{-1} \right] \quad (3.12)$$

is obtained by expanding about a uniform system with a frequency-dependent nearest-neighbour energy difference $c(s)$ and recalling that J_n is the inverse Fourier transform of $F(q, s)$. In (3.12) the fluctuation $\delta(\Delta_m^2) = \Delta_m^2 - c(s)$.

Equation (3.12) can be solved by successive iteration. For example, the n th term in the iteration will contain n factors of the site energy fluctuation $\delta(\Delta_m^2)$. In the classical one-dimensional problem [21], however, the hopping rate fluctuation $\delta(W_m^{-1})$ was paired with a factor of the frequency, s . As a consequence, the n th term in the iteration of the integral equation was of the form $s^n \times (n \text{ factors of } \delta(1/W_m))$. In the limit of small frequencies ($s \rightarrow 0$, the long-time limit) the resultant expansion for the diffusion constant was convergent and yielded the exact long-time behaviour. As is clear from (3.12), such is not the case here. The fluctuation $\delta(\Delta_m^2)$ is not paired with a factor of s . This has two consequences. First, the magnitude of successively higher order fluctuation terms is not necessarily decreasing. Consequently, the expansion determined by (3.12) might not be convergent. Second, there are an infinite number of terms that contribute to the DC conductivity and each successive frequency correction to the diffusion constant.

While neither of these problems can be circumvented entirely, it is possible to construct a slightly more convergent form of (3.12). We proceed by rewriting (3.12) so that certain classes of higher-order terms are summed exactly. For example, all terms involving repeated scattering from the same site can be resummed by introducing the single site t -matrix [22, 23]

$$t_m = \frac{\delta(\Delta_m^2)}{1 - g_0(s)\delta(\Delta_m^2)} \quad (3.13)$$

where

$$g_0(s) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dq [s^2 + c(s) + 2(1 - \cos q)]^{-1} = \frac{1}{2\pi} \int_{-\pi}^{\pi} g(q, s) dq. \quad (3.14)$$

To obtain the diffusion coefficient, we note that $\langle F(q, s) \rangle$ is diagonal in q space. Hence $\langle F(q, s) \rangle|_{q=0} = 0$ as a result of the $(1 - e^{iq})$ factor that multiplies each term in the expansion. The only non-zero contribution to $D(s)$, then, must arise from the second term in (3.10) when the q derivative acts on $(1 - e^{iq})$. Let us define

$$\pi_{qq'} = [g(q', s) - g_0(s)]\delta(q - q'). \quad (3.15)$$

The matrix π will act as the propagator in the t -matrix expansion of the diffusion constant. From (3.10)–(3.14) it follows that [21, 22]

$$D(s)\delta(q') = sl^2 \lim_{q \rightarrow 0} [g(q, s) + g\langle t \rangle g + g\langle t\pi t \rangle g + \dots]_{q, q'} \quad (3.16)$$

is the t -matrix expansion for the diffusion coefficient. We point out that (3.16) might still not be a convergent expansion. However, (3.16) sums up many more terms order by order than does (3.12).

Consider the first two terms

$$D(s) \approx \frac{sl^2}{s^2 + c(s)} \left(1 + \frac{1}{s^2 + c(s)} \langle t \rangle \right) \quad (3.17)$$

in (3.16). If we choose as the uniform system $c(s) = \langle \Delta_m^2 \rangle = \langle \Delta^2 \rangle$ we see that the first term is $\langle 1/F_n \rangle^{-1} l^2 = l^2 s / (s^2 + \langle \Delta^2 \rangle)$. In the incoherent bond problem in one dimension,

$l^2\langle 1/W_n \rangle^{-1}$ is the exact zero-frequency diffusion coefficient [21]. We see in the quantum mechanical case that $\langle 1/F_n \rangle^{-1}$ is just the leading term in an infinite series. It is clear however that $\langle 1/F_n \rangle^{-1}$ vanishes as $s \rightarrow 0$ for any non-zero value ($\langle \Delta^2 \rangle \neq 0$) of the disorder and diverges (for $s \rightarrow 0$) when $\langle \Delta^2 \rangle = 0$. This result is consistent with an absence of diffusion in one-dimensional systems for any non-zero value of the disorder.

Equation (3.17) can also be used to construct an effective medium approximation (EMA) for the diffusion constant. In the EMA, the uniform system $c(s)$ is chosen so that $\langle t \rangle = 0$. When $\langle t \rangle = 0$, $D_0 = sl^2/(s^2 + c(s))$ will be the exact diffusion constant through second order in the t -matrix expansion. If for all values of the disorder $c(s) \simeq c_0$ (a constant) as $s \rightarrow 0$, D_0 will vanish; that is, the electron will be localised. We solve the effective medium equation

$$\langle t \rangle = \langle (\Delta_n^2 - c(s)) / [1 + g_0(\Delta_n^2 - c(s))] \rangle = 0 \quad (3.18)$$

or equivalently

$$\langle 1/[1 + g_0(\Delta_n^2 - c(s))] \rangle = 1 \quad (3.19)$$

in the case that the disorder is determined by the uniform distribution

$$P(\Delta_n) = \begin{cases} 1/W & -1/2W \leq \Delta_n < 1/2W \\ 0 & \text{otherwise.} \end{cases} \quad (3.20)$$

We find that

$$\frac{2}{W[g_0(1 - g_0c)]^{1/2}} \tan^{-1} \left[\frac{W}{2} \left(\frac{g_0}{1 - g_0c} \right)^{1/2} \right] = 1. \quad (3.21)$$

Substitution of the integral $g_0 = [(s^2 + c(s))(s^2 + 4 + c(s))]^{-1/2}$ into (3.21) leads to

$$\frac{W}{2} \left(\frac{c_0^2 + 4c_0}{1 - c_0(4c_0 + c_0^2)^{1/2}} \right)^{1/2} = \tan \left(\frac{W}{2} \{ (c_0^2 + 4c_0)^{1/2} [1 - c_0(c_0^2 + 4c_0)^{1/2}] \}^{1/2} \right) \quad (3.22)$$

as the final self-consistent equation for c_0 in the limit that $s \rightarrow 0$. Recall $c(s) \rightarrow c_0$ as $s \rightarrow 0$. Equation (3.22) was solved numerically. We found that (3.22) always admits a non-zero solution for arbitrarily small values of the disorder, W . In particular the solutions to (3.22) have the following property. For small W , $c_0 \propto W^2$ and for large W , $c_0 \propto W$. Hence, localisation obtains as it should in one-dimension and for any non-zero value of the disorder. We show in the Appendix that the argument presented here for a uniform distribution can be generalised to any distribution of site energies.

3.2. Higher dimensions

We now generalise the calculation of the diffusion coefficient presented in the previous section to d dimensions. Here again the d -dimensional t -matrix expansion for the diffusion coefficient developed in [22, 23] in the context of incoherent transport in bond-disordered systems is the basis for our calculation. To proceed we write the GME

$$\begin{aligned} \dot{P}_n = 2V^2 \int_0^t \sum_{\alpha=1}^d & [\cos(\varepsilon_n - \varepsilon_{n+\alpha})(t - t')(P_{n+\alpha}(t') - P_n(t')) \\ & + \cos(\varepsilon_n - \varepsilon_{n-\alpha})(t - t')(P_{n-\alpha}(t') - P_n(t'))] dt' \end{aligned} \quad (3.23)$$

in d dimensions for a nearest-neighbour memory kernel. In (3.23) $\mathbf{n} = (n_1, n_2, \dots, n_d)$ is

a direct lattice vector and α is a unit vector pointing along the α direction from site n to its nearest-neighbour along that direction. Throughout this paper, we will use Greek superscripts to denote spatial components of a matrix. As before, it is instructive to rewrite the equations of motion in the Laplace domain

$$sP_n - P_n(t=0) = \sum_{\alpha=1}^d F_n(P_{n+\alpha} - P_n) + F_{n-\alpha}^\alpha(P_{n-\alpha} - P_n) \quad (3.24)$$

where $F_n^\alpha = s/(s^2 + \Delta_{n,\alpha}^2)$ is the frequency-dependent hopping rate and $\Delta_{n,\alpha} = (\varepsilon_{n+\alpha} - \varepsilon_n)/\sqrt{2V}$ the dimensionless energy difference between sites n and $n + \alpha$. Let us define the probability current or bond flux

$$J_n^\alpha(s) = F_{n-\alpha}^\alpha(s)(P_n(s) - P_{n-\alpha}(s)) \quad (3.25)$$

between sites n and $n - \alpha$ along the α direction and the corresponding generating function

$$Q^\alpha(q, s) = \sum_n \exp(iq \cdot n) J_n^\alpha(s). \quad (3.26)$$

Each of the flux generating functions is related to the frequency-dependent diffusion constant [21]

$$D^{\alpha\alpha}(s) = \frac{sI^2}{2} \left(\langle Q^\alpha(q=0, s) \rangle + 2i \frac{\partial}{\partial q_\alpha} \langle Q^\alpha(q, s) \rangle \Big|_{q=0} \right) \quad (3.27)$$

along the α direction in the crystal. We will consider here an isotropic distribution of site energies. In an isotropic system, $D^{\alpha\alpha}$ is independent of direction. Hence we will drop the subscript on the diffusion constant and set $D(s) = D^{\alpha\alpha}(s)$.

We now construct a coupled set of integral equations for the Q^α terms. This can be done by Fourier transformation of the equations of motion

$$\frac{sJ_n^\alpha}{F_n^\alpha} - \frac{J_n^\alpha(0)}{F_n^\alpha} = \sum_{\alpha=1}^d J_{n+\alpha}^\alpha + J_{n-\alpha}^\alpha - 2J_n^\alpha \quad (3.28)$$

for the fluxes and expanding about a uniform system with frequency-dependent hopping rate $(c^\alpha(s))^{-1}$. The result

$$[sc^\alpha(s) + \mathbf{Z} - \mathbf{Y}]Q = j(0) \quad (3.29)$$

is most easily written in matrix form. In (3.29), we have introduced the column vectors Q and $j(0)$ with components $Q^\alpha(q, s)$ and $[1 - \exp(iq_\alpha)]$, respectively. The matrices \mathbf{Z} and \mathbf{Y} are defined as follows

$$\mathbf{Z}_{qq'}^{\alpha\mu} = [1 - \exp(iq_\alpha)][1 - \exp(-iq_\mu)]\delta(q - q') \quad (3.30a)$$

and

$$\mathbf{Y}_{mn}^{\alpha\mu} = s(c^\alpha(s) - 1/F_n^\alpha(s))\delta_{mn}\delta_{\alpha\mu} = \mathbf{Y}_m^\alpha. \quad (3.30b)$$

The remainder of our analysis will focus on the matrix $\mathbf{G} = [sc^\alpha(s) + \mathbf{Z} - \mathbf{Y}]^{-1}$. The form of this matrix in one dimension is given implicitly through equations (3.11) and (3.12). In one dimension, we showed that $\langle \mathbf{G} \rangle$ is diagonal in q space. The same is true for the d dimensional case as noted by Parris [22]. Consequently, because the elements of $j(0)$ vanish as $q \rightarrow 0$, $\langle Q^\alpha(q=0, s) \rangle = 0$ and only the q derivative of the diagonal part of $\langle \mathbf{G} \rangle j(0)$

$$D = D_{\alpha\alpha}(s) = sI^2 \langle \mathbf{G} \rangle_{q,q}^{\alpha\alpha} \Big|_{q=0} \quad (3.31)$$

is needed to define the diffusion coefficient.

Following [22] for incoherent transport, we divide the Green operator into perturbed and unperturbed parts. We choose as the unperturbed system one in which the diffusion constant is $c^\alpha(s)$. For an isotropic system $c^\alpha(s) = \bar{c}(s)$ and the unperturbed propagator is $g = (s\bar{c}(s) + \mathbf{Z})^{-1}$ whose matrix elements are

$$g_{qq'}^{\alpha\mu} = \left(\delta_{\alpha\mu} - \frac{[1 - \exp(q_\alpha)[1 - \exp(-iq_\mu)]]}{s\bar{c}(s)[s\bar{c}(s) + \sum_\lambda 2(1 - \cos q_\lambda)]} \right) \delta(q - q'). \quad (3.32)$$

A Dyson expansion

$$\langle \mathbf{G} \rangle = g + \langle g\mathbf{Y}\mathbf{G} \rangle = g + g\langle \mathbf{Y} \rangle g + g\langle \mathbf{Y}g\mathbf{Y}g \rangle + \dots \quad (3.33)$$

for the average Green function follows immediately. This expansion can be resummed by introducing the single site t matrix [22, 23]

$$t_{mn}^{\alpha\mu} = \mathbf{Y}_m^\alpha (1 - g_0^{\alpha\mu} \mathbf{Y}_m^\alpha)^{-1} \quad (3.34)$$

and an effective propagator $\pi_{qq'}^{\alpha\mu} = g_{qq'}^{\alpha\mu} - g_0^\alpha \delta_{\alpha\mu} \delta(q - q')$. The d -dimensional form of the self-propagator is

$$g_0^\alpha(s) = \frac{1}{(2\pi)^d} \int d\mathbf{q} d\mathbf{q}' g_{qq'}^{\alpha\alpha} = \frac{d-1}{d(s\bar{c})} + \frac{1}{d(2\pi)^d} \int \left(s\bar{c} + \sum_{\alpha=1}^d 2(1 - \cos q_\alpha) \right)^{-1}. \quad (3.35)$$

Substitution of (3.34) into (3.33) leads to the desired expansion

$$D(s) = D^{\alpha\alpha}(s) = sl^2 \lim_{q \rightarrow 0} [g + g\langle t \rangle g + g\langle t\pi t \rangle g + \dots]_{q,q}^{\alpha\alpha} \quad (3.36)$$

for the diffusion constant.

Equation (3.36) can be used to formulate an expression for $D(s)$ valid through arbitrary order in the t matrix. For the present analysis, we focus on the first two terms in (3.36). As $q \rightarrow 0$, $g \rightarrow (s\bar{c}(s))^{-1}$ and

$$D(s) \sim \frac{sl^2}{s\bar{c}(s)} \left[1 + \frac{\langle t \rangle}{s\bar{c}(s)} \right]. \quad (3.37)$$

For the nearest-neighbour memory kernel in which $F_n^\alpha = s/(s^2 + \Delta_{n,\alpha}^2)$, the frequency-dependent hopping rate $\bar{c}(s)^{-1}$ is of the form $\bar{c}(s) = (s^2 + b(s))/s$. Here $b(s)$ is the site energy difference in the uniform system. If we choose $b(s)$ to be $\langle \Delta^2 \rangle$, then the first term in (3.37) is exactly $\langle 1/F_n^\alpha \rangle^{-1}$. As remarked previously, this term vanishes for all non-zero values of the disorder ($\langle \Delta^2 \rangle \neq 0$). Hence, the first term in (3.37) always predicts localisation whenever the disorder is non-zero irrespective of the spatial dimension.

To improve on this calculation, we derive a self-consistent equation for $\bar{c}(s)$ at the effective medium level. We must solve, then, the d -dimensional analogue of equation (3.18). As $s \rightarrow 0$, the integral (Kundu and Phillips [21]) in $g_0^\alpha(s)$ is negligible relative to the first term. If we let $\lim_{s \rightarrow 0} \bar{c}(s)/d \rightarrow R^{-1}$, the self-consistency condition becomes

$$R = \left\langle 1 / \left(\bar{F} + \frac{d-1}{d} R \right) \right\rangle^{-1} \quad (3.38)$$

with \bar{F} the $s = 0$ limit of the Laplace transform of the memory function. The vanishing of R is the signature of localisation. The properties of (3.38) are best illuminated by rewriting (3.38)

$$R = \left(\int_{-\infty}^{\infty} \frac{\rho(\Delta) d\Delta}{\bar{F}(\Delta) + [(d-1)/d]R} \right)^{-1} \quad (3.39)$$

in terms of the site energy distribution function $\rho(\Delta)$. For the nearest-neighbour memory

function (2.9), $\tilde{F}(\Delta)$ is $\lim_{s \rightarrow 0} s/(s^2 + \Delta^2) = \pi^{-1}\delta(\Delta)$. Because $\tilde{F}(\Delta)$ only contributes at $\Delta=0$ and $\rho(\Delta)$ is normalised, the self-consistency condition implies that $R = (d-1)R/d$ or $R = 0$. Hence, the EMA also predicts a vanishing of the diffusion constant regardless of the spatial dimension and the magnitude of the disorder. We remind the reader that because we have truncated the memory function to order V^2 , the effective medium developed here is based on an expansion for the average probability from the localised side. This is in stark contrast to the standard coherent potential approximation, which introduces an effective medium for the average amplitude [24, 25]. Consequently, the exact behaviour of the diffusion constant in our model is still an open question, because of the approximate nature of the analysis presented thus far. Our subsequent exact analysis of the flux self-energy on a Cayley tree in § 4 strongly suggests, however, that the nearest-neighbour memory approximation is sufficient to describe Anderson localisation. As a consequence, the higher order terms in (3.36) should certainly be investigated to see if they lead to a localisation–delocalisation transition in $d = 3$.

Although the EMA fails to describe the Anderson transition in $d = 3$, it is worth exploring just what type of transition, if any, the EMA in this model predicts. The integral in (3.39) is finite at $R = 0$ only if $\rho(\Delta)/\tilde{F}(\Delta)$ is a bounded function as $\Delta \rightarrow \infty$. The quantity $\rho(\Delta)/\tilde{F}(\Delta)$ can be thought of as the ratio of distributions. $\rho(\Delta)/\tilde{F}(\Delta)$ will diverge as $\Delta \rightarrow \infty$ if the width of the distribution $\rho(\Delta)$ is wider than that for $\tilde{F}(\Delta)$. Should this state of affairs obtain, equation (3.39) will predict a localisation–delocalisation transition. Consider the case in which $\tilde{F}(\Delta)$ is non-zero only over a finite interval $[-\Delta_{\max}, \Delta_{\max}]$. Under such circumstances, (3.39) can be rewritten as

$$R = \left[\frac{(1-P)d}{(d-1)R} + \int_{-\Delta_{\max}}^{\Delta_{\max}} \left(d\Delta\rho(\Delta)/\tilde{F}(\Delta) + \frac{d-1}{d}R \right) \right]^{-1} \quad (3.40)$$

where $(1-P)$ is the probability that $\rho(\Delta)$ is defined outside the interval $[-\Delta_{\max}, \Delta_{\max}]$. As a consequence, the self-consistent condition is

$$1 = \frac{d-1}{d(1-P)} \quad (3.41)$$

which implies that $P_c = 1/d$. We see then that the EMA (3.39) is capable of predicting the EMA for classical percolation [24] transitions ($P_c = 1/d$) only. Such transitions come about from purely incoherent or decaying (in time) memory function. At the EMA level, transport thresholds are determined by the incoherent rather than the coherent part of the memory function. This certainly clarified why the EMA in this model fails for the Anderson transition.

4. Anderson transition

We now show that the GME with a nearest-neighbour memory kernel can lead to an Anderson transition on a Cayley tree of connectivity K . The quantity on which we focus is the energy spectrum of the Green function for the bond fluxes. In the frequency domain, the singularities of the Green function determine the energy spectrum. If all the singularities are real simple poles, then the Green function describes a stationary system in which no transport obtains. Singularities with non-zero imaginary parts indicate the presence of branch points. This signifies the existence of delocalised states. Though the calculation of the energy spectrum [8, 17, 25] is typically performed with the

Green function for the amplitudes, the Green function for the fluxes and site probabilities, as we will see, suffice just as well to establish the existence of branch points.

To proceed, consider the equations of motion for the bond fluxes

$$\frac{sJ_n^\alpha}{F_n^\alpha} - \frac{J_n^\alpha(t=0)}{F_n^\alpha} = -2J_n^\alpha + \sum_{\alpha=1}^d J_{n+\alpha}^\alpha + J_{n-\alpha}^\alpha. \quad (4.1)$$

The long-time properties of our system are determined along the axis $\text{Re}(s) = 0$ or the $\text{Im}(s)$ axis. If all the states are localised, then the probability of remaining at the initial site (the origin) is either unity for all times or recurs to unity with a non-infinite recurrence time. For this state of affairs to obtain, all the singularities of the probability Green function must correspond to simple poles which lie along the $\text{Im}(s)$ axis. From equations (3.24) and (4.1) it follows that the probability Green function G_p and the Green function for the flux at the origin G_j are related through

$$G_p(\mathbf{0}, \mathbf{0}; s) = \frac{1}{s} - \frac{1}{s} \sum_{\alpha=1}^d [G_j^\alpha(\mathbf{0} + \boldsymbol{\alpha}, \mathbf{0} + \boldsymbol{\alpha}; s) + G_j^\alpha(\mathbf{0}, \mathbf{0}; s) - G_j^\alpha(\mathbf{0}, \mathbf{0} + \boldsymbol{\alpha}; s) - G_j^\alpha(\mathbf{0} + \boldsymbol{\alpha}, \mathbf{0}; s)] \quad (4.2)$$

where

$$G_j^\alpha(n + \boldsymbol{\alpha}, n + \boldsymbol{\alpha}; s) = [s^2 + \Delta_{n,\alpha}^2 + 2 - \Gamma^\alpha(n + \boldsymbol{\alpha}; s)]^{-1} \quad (4.3)$$

is the single-point Green function for the flux site $n + \boldsymbol{\alpha}$. In (4.3) $\Gamma^\alpha(n + \boldsymbol{\alpha}; s)$ is the self-energy along the α direction for the flux between sites n and $n + \boldsymbol{\alpha}$. It is evident from (4.3) and (4.2) that except at $s = 0$, the singularities of the probability Green function $G_p^\alpha(\mathbf{0}, \mathbf{0}; s)$ cannot be simple poles along the $\text{Im}(s)$ axis unless $\text{Im} \Gamma^\alpha(\mathbf{0} + \boldsymbol{\alpha}; s)$ and $\text{Im} \Gamma^\alpha(\mathbf{0}; s)$ are both identically zero with probability unity. If we require that the probability distributions of $\text{Im} \Gamma^\alpha(\mathbf{0} + \boldsymbol{\alpha}; s)$ and $\text{Im} \Gamma^\alpha(\mathbf{0}; s)$ be identical, then $\text{Im} \Gamma^\alpha(\mathbf{0} + \boldsymbol{\alpha}; s) = 0$ necessarily implies that $\text{Im} \Gamma^\alpha(\mathbf{0} - \boldsymbol{\alpha}; s) = 0$ as well. Hence, we need only focus on the probability distribution of either $\text{Im} \Gamma^\alpha(\mathbf{0}; s)$ to analyse the Anderson transition.

4.1. Self-energy for $K = 1$

At this point we specialise to a Cayley tree facility an exact calculation of the Green function

$$G_j(0; s) = (s^2 + \Delta_0^2 + 2 - \Gamma(0; s))^{-1}$$

for the flux in the bond at the origin. We have dropped the superscript on $G_j(0; s)$ and $\Gamma(0; s)$ because directionality is not defined on a Cayley tree. By way of illustration, consider first the $K = 1$ lattice. We number the sites according to figure 1(a). The self-energy $\Gamma(0; s)$ is computed by summing over all closed skeleton paths that return to the origin [25]. Clearly there are only two such paths: $0 \rightarrow 1 \rightarrow 0$ and $0 \rightarrow -1 \rightarrow 0$. The resultant self-energy at the origin

$$\Gamma(0; s) = \Gamma(0, 0(1)) + \Gamma(0, 0(-1)) \quad (4.5a)$$

$$= [s^2 + 2 + \Delta_{-1}^2 - \Gamma(-1, -1(0))]^{-1} + [s^2 + 2 + \Delta_1^2 - \Gamma(1, 1(0))]^{-1} \quad (4.5b)$$

can be written as the sum of two self-energies $\Gamma(0, 0(1))$ and $\Gamma(0, 0(-1))$. These quanti-

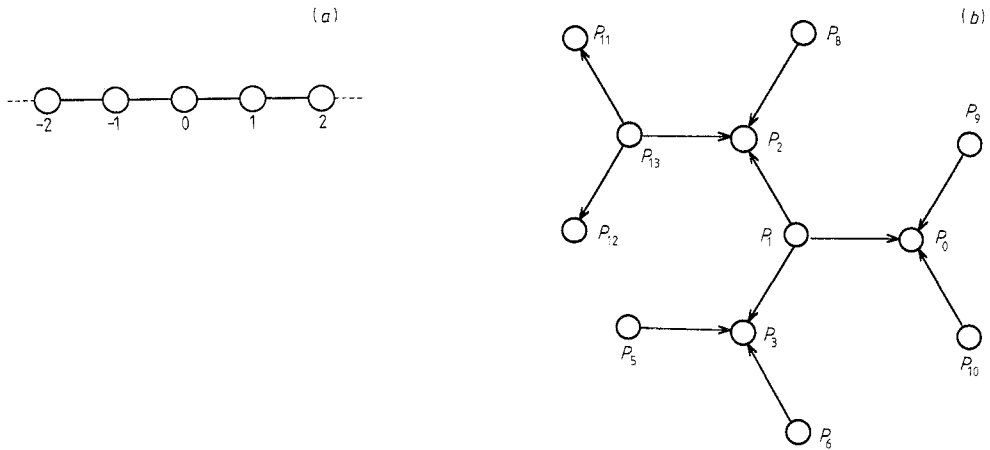


Figure 1. (a) The tight binding model in one dimension. The sites are labelled with integers, and the interactions between the sites are nearest-neighbour only, as indicated by the connecting bonds. (b) The Cayley tree of connectivity $K = 2$. Each site probability P_n is connected to three nearest-neighbours. The directional arrows are superimposed on the bonds to assist in the construction of the equations for the flux. With the flux between any two sites defined, as in (4.7), as $J_{m,n}(S) = F_{m,n}(s)(P_n(s) - P_m(s))$, where m and n are taken in the order specified by the direction of the arrows, the equations for the evolution of the fluxes take on the simple form shown in (4.9), in which the terms on the right-hand side of the equation are all negative.

ties exclude all paths that visit sites 1 and -1 , respectively. In general $\Gamma(n, n(m, l, \dots))$ is the self-energy at site n which excludes all paths that visit sites (m, l, \dots) . Self-consistency is introduced by requiring that the probability distribution for $\Gamma(0, 0(1))$, $\Gamma(0, 0(-1))$, $\Gamma(-1, -1(0))$ and $\Gamma(1, 1(0))$ be equal [8]. This self-consistency condition is justified because the probability distribution for a self energy of the form $\Gamma(n, n(m))$ should be independent of n and m . Now the signature of Anderson localisation is the vanishing of $\text{Im } \Gamma(0; s)$. Equation (4.5a) implies that for $\text{Im } \Gamma(0; s) = 0$, $\text{Im } \Gamma(0, 0(1))$ and $\text{Im } \Gamma(0, 0(-1))$ must both vanish. However, because $\Gamma(0, 0(1))$ and $\Gamma(0, 0(-1))$ obey the same probability distribution, $\text{Im } \Gamma(0, 0(1)) = 0$ necessarily implies that $\text{Im } \Gamma(0, 0(-1)) = 0$ as well. Hence, the question of localisation can be answered in one dimension by investigating the properties of either $\Gamma(0, 0(1))$ or $\Gamma(0, 0(-1))$.

Consider then the defining equation

$$\Gamma(0, 0(-1)) = [s^2 + 2 + \Delta_1^2 - \Gamma(1, 1(0))]^{-1} \quad (4.6)$$

for $\Gamma(0, 0(-1))$. We employed the Monte Carlo procedure of AAT [8] to solve equation (4.6) for the probability distribution of $\text{Im } \Gamma(0, 0(-1))$. A flat distribution of 1000 members was used to generate random values for the site energies and $\Gamma(1, 1(0))$. The $\text{Im } \Gamma(0, 0(-1))$ was computed with $s = iu$ and u chosen so that the mean of $\text{Im } \Gamma(0, 0(-1))$ was maximised. The choice of u ($s = iu$) such that $\text{Im } \Gamma(0, 0(-1))$ is maximised guarantees that when $\text{Im } \Gamma(0, 0(-1))$ vanishes, all the fluxes are localised. We found that $\text{Im } \Gamma(0, 0(-1))$ vanished for all values of W/V and for all values of u (even for infinitesimally small values of W/V). Hence, the nearest-neighbour memory function corroborates the well known result [12–15] in $d = 1$ that all states are localised in the presence of disorder.

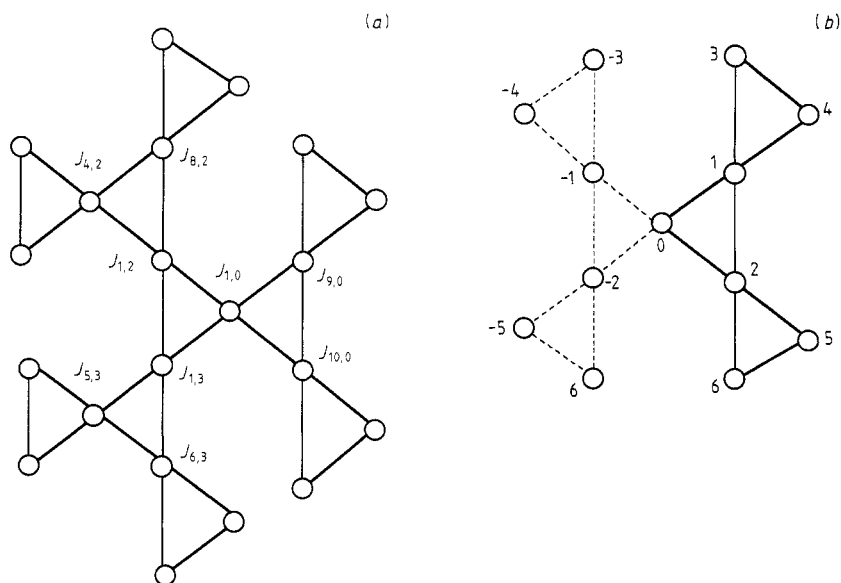


Figure 2. (a) The structure of equation (4.9) for the fluxes in the Cayley tree of connectivity $K = 2$ is that of an expanded cactus of triangles in which each flux $J_{m,n}$ is represented by a 'flux-site' in the cactus, and is connected to four neighbouring fluxes. The expanded cactus can be generated via a bond-to-site transformation of the Cayley tree; the bonds in the Cayley tree become the sites in the expanded cactus. (b) It is convenient to replace the double label $J_{m,n}$ for each flux 'site' on the expanded cactus of (a) with a single integer. In order to calculate the self-energy $\Gamma(0, 0(-1, -2))$ on the expanded cactus, one must sum over all of the self-avoiding paths which exclude the 'flux-sites' -1 and -2 . There are three such paths, $0 \rightarrow 1 \rightarrow 0$, $0 \rightarrow 2 \rightarrow 0$ and $0 \rightarrow 1 \rightarrow 2 \rightarrow 0$. These paths are decorated with paths over sites 3, 4, 5, and 6, etc. The entire left side of the figure is avoided for this calculation, as represented by the broken lines. Similarly, when calculating $\Gamma(0, 0(1, 2))$, the entire right side of the figure is avoided, i.e. none of the sites labelled by the positive integers are visited.

4.2. Self-energy for $K = 2, 3$

The calculation for Cayley trees of higher connectivity is considerably more complicated. Consider the $K = 2$ lattice shown in figure 1(b). The arrows indicate the direction in which the fluxes should be computed. Let us define the flux between sites n and m as

$$J_{n,m}(s) = F_{m,n}(s)(P_m(s) - P_n(s)) \quad (4.7)$$

where $F_{m,n}(s) = s/(s^2 + \Delta_{n,m}^2)$ and $\Delta_{n,m} = (\epsilon_n - \epsilon_m)/\sqrt{2V}$. In figure 1(b) an arrow pointing from site $n \rightarrow m$ defines the flux $J_{n,m}$. Using the numbering of the sites shown in figure 1(b), we see that the equation of motion in the Laplace domain for the probability to remain at the origin.

$$sP_0(s) - P_0(t=0) = -J_{9,0} - J_{10,0} - J_{1,0} \quad (4.8)$$

involves only the fluxes for the three nearest neighbours. In contrast, the equation of motion for the flux at the origin

$$\frac{sJ_{1,0}}{F_{1,0}} - \frac{J_{1,0}(t=0)}{F_{1,0}} = -2J_{1,0} - J_{1,3} - J_{1,2} - J_{9,0} - J_{10,0} \quad (4.9)$$

is determined by the next-nearest neighbour fluxes as well. Equation (4.9) is the $K = 2$ Cayley tree analogue of equation (4.1). It is clear from (4.9) that the flux equations do not map onto a simple Cayley tree of connectivity K . It is possible however, to construct a decorated Cayley tree on which the flux equations can be generated by summing over the nearest-neighbour sites only. The fluxes correspond to free bonds in the Cayley tree, each connected to $2K$ nearest-neighbour bonds. If one transforms the Cayley tree so that the bonds are represented as points, the resulting structure is the expanded cactus shown in figure 2(a).

On this lattice, the flux equations for a given site can be generated by summing over the vertices of the two triangles emanating from the flux site of interest. The form of the flux equations will always be that of equation (4.9), with the nearest-neighbour fluxes appearing with a minus sign.

We must compute the self-energy by summing over all non-intersecting skeleton paths on the expanded cactus shown in figure 2(a). To simplify the notation, we drop the double subscript on the fluxes and number the sites according to figure 2(b). Here again the quantity of interest is the self-energy

$$\Gamma(0, 0; s) = \Gamma(0, 0(1, 2)) + \Gamma(0, 0(-1, -2)) \tag{4.10}$$

at the origin. As in the one-dimensional case, we need only focus on one of the terms in (4.10). Consider $\Gamma(0, 0(-1, -2))$. Three paths, $0 \rightarrow 1 \rightarrow 0$, $0 \rightarrow 2 \rightarrow 0$, and $0 \rightarrow 2 \rightarrow 1 \rightarrow 0$, contribute to the self-energy

$$\begin{aligned} \Gamma(0, 0(-1, -2)) &= [s^2 + 2 + \Delta_1^2 - \Gamma(1, 1(0))]^{-1} + [s^2 + 2 + \Delta_2^2 - \Gamma(2, 2(0))]^{-1} \\ &\quad - [s^2 + 2 + \Delta_2^2 - \Gamma(2, 2(0))]^{-1} [s^2 + 2 + \Delta_1^2 - \Gamma(1, 1(2, 0))]^{-1}. \end{aligned} \tag{4.11}$$

The self-energies that exclude one site can be expressed as

$$\Gamma(1, 1(0)) = \Gamma(1, 1(2, 0)) + [s^2 + 2 + \Delta_2^2 - \Gamma(2, 2(1, 0))]^{-1} \tag{4.12}$$

and

$$\Gamma(2, 2(0)) = \Gamma(2, 2(1, 0)) + [s^2 + 2 + \Delta_1^2 - \Gamma(1, 1(2, 0))]^{-1}. \tag{4.13}$$

We can now express $\Gamma(0, 0(-1, -2))$ entirely in terms of self-energies that exclude the two sites

$$\begin{aligned} \Gamma(0, 0(-1, -2)) &= \frac{[s^2 + 2 + \Delta_2^2 - \Gamma(2, 2(1, 0))] + [s^2 + 2 + \Delta_1^2 - \Gamma(1, 1(2, 0))] - 1}{[s^2 + 2 + \Delta_2^2 - \Gamma(2, 2(1, 0))] \times [s^2 + 2 + \Delta_1^2 - \Gamma(1, 1(2, 0))] - 1}. \end{aligned} \tag{4.14}$$

Let us define $\Gamma(n, n(m, l)) = \Gamma_{nR} + i\Gamma_{nI}$ and $X_n = s^2 + 2 + \Delta_n^2 - \Gamma_{nR}$ for any site n and pair of sites (m, l) . The real and imaginary parts of $\Gamma(0, 0(-1, -2))$ can be expressed in terms of these quantities. For $\text{Im } \Gamma(0, 0(-1, -2))$ we obtain

$$\begin{aligned} \text{Im}\Gamma(0, 0(-1, -2)) &= \Gamma_{0I} \\ &= \frac{\Gamma_{2I}(\Gamma_{1I}\Gamma_{2I} + X_1^2 - X_1 + 1) + \Gamma_{1I}(\Gamma_{1I}\Gamma_{2I} + X_2^2 - X_2 + 1)}{(X_1X_2 - \Gamma_{2I}\Gamma_{1I} - 1)^2 + (\Gamma_{2I}X_1 + \Gamma_{1I}X_2)^2}. \end{aligned} \tag{4.15}$$

The imaginary $s(s = iu)$ axis was scanned, and it was found, as is evident from figure 3, that the maximum value of W/V needed to cause a transition was $W/V = 13$ at a value of $u = 1.8$. This result is in good agreement with the exact value of AAT of $W/V = 1.7$.

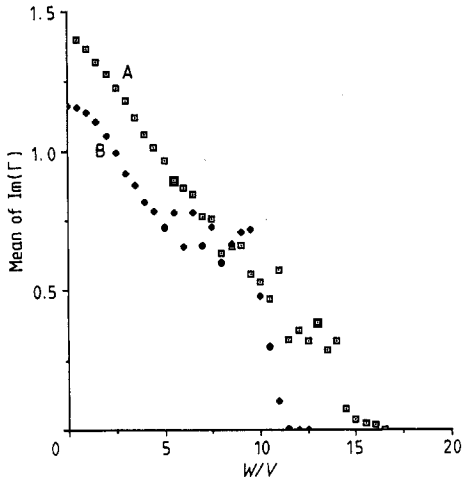


Figure 3. The geometric mean of the imaginary part of the self-energy $\Gamma(0, 0)$, as a function of the ratio of the full width of the disorder W and the nearest-neighbour overlap integral V , for the Cayley tree of connectivity $K = 2$. The points shown represent the average of the last 20 of 100 iterations of the self-consistent equation, with an ensemble of 500 members. The curves are A: the self-energy for the amplitudes, which is generated from the exact expressions of AAT [8] with $u = 0$; B, the self-energy for the fluxes, which is generated from (4.14), with $u = 1.8V$. Curve A approaches zero at $W/V = 17$, while curve B approaches zero at $W/V = 13$.

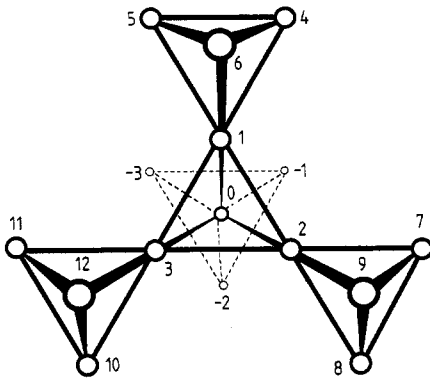


Figure 4. For the Cayley tree of connectivity $K = 3$, the corresponding expanding cactus for the fluxes is a network of tetrahedrons, such that each 'flux-site' is connected to six nearest-neighbours. In order to calculate $\Gamma(0, 0(-1, -2, -3))$, it is necessary to sum over nine self-avoiding paths which completely exclude the sites labelled by the negative integers. The excluded sites are shown connected by broken lines. Three of the self-avoiding paths are the single-edge routes $0 \rightarrow 1 \rightarrow 0$, $0 \rightarrow 2 \rightarrow 0$, and $0 \rightarrow 3 \rightarrow 0$. Three others define the faces of the tetrahedron: $0 \rightarrow 1 \rightarrow 2 \rightarrow 0$, $0 \rightarrow 1 \rightarrow 3 \rightarrow 0$, and $0 \rightarrow 3 \rightarrow 2 \rightarrow 0$. The three remaining paths are $0 \rightarrow 1 \rightarrow 2 \rightarrow 3 \rightarrow 0$, $0 \rightarrow 2 \rightarrow 3 \rightarrow 1 \rightarrow 0$ and $0 \rightarrow 3 \rightarrow 1 \rightarrow 2 \rightarrow 0$.

The discrepancy between the value of AAT and the GME results stems of course from the $0(V^2)$ or nearest-neighbour approximation we have made to the memory function. This approximation effectively decreases the magnitude of the nearest-neighbour matrix element, V . Consequently, the electronic states become localized at a smaller value of the disorder W . As we will see the $K = 3$ results also follow this pattern. It is likely then that inclusion of higher order terms in the memory function should improve the estimate of the critical value of W/V .

We now turn to the $K = 3$ calculation. For $K = 3$, the equations of motion for the flux at site n can be obtained by summing over all the six nearest-neighbour fluxes of site n on the expanded cactus in figure 4. The lattice in figure 4 can be obtained by decorating each lattice site of a standard $K = 3$ Cayley tree with a tetrahedron. In analogy with the $K = 2$ calculation, the localisation-delocalisation transition can be studied from the self-energy $\Gamma(0, 0(-1, -2, -3))$. The expression for $\Gamma(0, 0(-1, -2, -3))$ is easily obtained by summing over the skeleton paths enumerated in the caption for figure 4. We solved the self-consistent equation for $\text{Im}[\Gamma(0, 0(-1, -2, -3))]$ using the Monte Carlo method of AAT [8]. Our results are shown in figure 5. They indicate that the maximum value of $\text{Im} \Gamma(0, 0(-1, -2, -3))$ which occurs at $u = 2.0$ vanishes for $W/V \approx 20$ as opposed to the exact [8] value $W/V \approx 29$. Here again we obtain satisfactory agreement between the

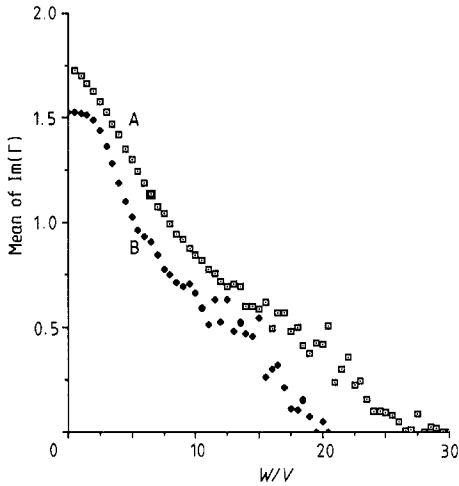


Figure 5. The geometric mean of the imaginary part of the self-energy $\Gamma(0,0)$, as a function of the ratio of the full width of the disorder W and the nearest-neighbour overlap integral V , for the Cayley tree of connectivity $K = 3$. The points shown represent the average of the last 20 of 100 iterations of the self-consistent equation, with an ensemble of 500 members. The curves are A: the self-energy for the amplitudes, which is generated from the exact expressions of AAT [8] with $u = 0$; B, the self-energy for the fluxes, which is generated from (4.16), with $u = 2.0V$. Curve A approaches zero quickly at $W/V = 29$, while curve B approaches zero at $W/V = 20$.

localisation of the GME with a nearest-neighbour memory kernel and that predicted by the exact amplitude equation.

5. Final remarks

We have demonstrated how a generalised master equation can be used to study Anderson localisation. At the effective medium level, the GME approach with a nearest-neighbour memory function fails to predict an Anderson transition on a cubic lattice for $d = 3$. Only localised solutions exist to the effective medium equations regardless of the magnitude of the disorder. That only localised solutions exist for the effective medium equations is not unexpected because the perturbative t -matrix expansion for the diffusion constant is explicitly based on the localised side of the transition. Our subsequent calculations of the exact self-energy on a Cayley tree for the GME with a nearest-neighbour memory function do, however, predict an Anderson transition in good agreement with the exact Cayley tree results. This suggests that a more exact treatment of the analytical expansion for the diffusion constant beyond the effective medium approximation might predict a localisation–delocalisation transition for $d = 3$. Such an analysis is currently under way as well as numerical simulations in the spirit of those of MacKinnon and Kramer [12] of the localisation length and localisation function for the GME with a nearest-neighbour memory function.

Inasmuch as all information regarding the interaction of the electron with the disordered environment lies in the memory function, the GME is a particularly simple yet powerful tool for studying quantum localisation. Of course, the GME is only as powerful as the memory function is exact. For example, with the exact memory function it is likely that an effective medium theory for the diffusion coefficient would suffice to describe the Anderson transition. In addition, the exact memory function for the Anderson problem defines precisely how coherent backscattering gives rise to loss of phase memory and the onset of quantum localisation. Hence it is worth considering how this quantity can be determined exactly. Zwanzig [2] has outlined a projection operator route to the memory function, $W_{nm}(t - t')$. The method is systematic and leads to an exact expansion

for $W_{nm}(t - t')$ in even powers of the matrix element V . The first term is of course the nearest-neighbour kernel treated here. The next term is $O(V^2)$ and contains sums and products of cosines whose arguments are nearest and next-nearest neighbour energy differences. Each successive term in the series contains more distant connections between the sites. It is certainly worth exploring the possibility of developing a self-consistent analysis of this expansion.

Finally, we comment that aside from offering a direct route to the mean-square displacement, the GME is particularly amenable to the inclusion of phonon interactions. For an energetically disordered system interacting with phonons the exact memory function is simply a product of the memory functions for the energy disorder and the phonon degrees of freedom. Memory functions for quasiparticle transport in the presence of strong linear coupling to phonons are well known [3]. In the nearest-neighbour approximation, the analysis developed here can be used as well. Two problems that can be investigated with such a memory function are (i) the stabilisation of Anderson-localised states [26, 27] at zero temperature by the lattice distortion and (ii) the temperature dependence of polaron hopping in a disordered environment. Solution to these problems will establish the GME as a versatile tool for treating both coherent and incoherent transport in disordered systems.

Acknowledgement

We thank P Parris for no fewer than five insightful remarks and the NSF for funding this work. We thank Connie Barnes for assistance with the artwork.

Appendix

To prove that a non-zero constant c_0 is a solution to equation (3.19) in 1D for any distribution of the disorder, we proceed as follows. In the limit that $s \rightarrow 0$, equation (3.19) becomes

$$\frac{1}{\sqrt{c_0(c_0 + 4)}} = \int_{-\infty}^{+\infty} \frac{\rho(\Delta) d\Delta}{\Delta^2 + \sqrt{c_0(c_0 + 4)} - c_0}. \quad (\text{A1})$$

As $c_0 \rightarrow 0$, the RHS of (A1) may be expanded as

$$\int_{-\infty}^{+\infty} \frac{\rho(\Delta) d\Delta}{\Delta^2 + \sqrt{c_0(c_0 + 4)}} \left(1 + \frac{c_0}{\Delta^2 + \sqrt{c_0(c_0 + 4)}} + \dots \right). \quad (\text{A2})$$

Because $\rho(\Delta)$ is always positive and $\Delta^2 + \sqrt{c_0(c_0 + 4)} > \sqrt{c_0(c_0 + 4)}$, the following inequality holds if $\rho(\Delta) \neq \delta(\Delta)$:

$$\begin{aligned} & \int_{-\infty}^{+\infty} \frac{\rho(\Delta) d\Delta}{\Delta^2 + \sqrt{c_0(c_0 + 4)}} \left(1 + \frac{c_0}{\sqrt{c_0(c_0 + 4)} + \Delta^2} + \dots \right) \\ & < \int_{-\infty}^{+\infty} \frac{\rho(\Delta) d\Delta}{\sqrt{c_0(c_0 + 4)}} \left(1 + \frac{\sqrt{c_0}}{\sqrt{c_0 + 4}} + \dots \right). \end{aligned} \quad (\text{A3})$$

Dropping the higher order terms on the RHS of (A3), we see that for $c_0 \rightarrow 0$

$$\int_{-\infty}^{+\infty} \frac{\rho(\Delta) d\Delta}{\Delta^2 + \sqrt{c_0(c_0 + 4)} - c_0} < \frac{1}{\sqrt{c_0(c_0 + 4)}}. \quad (\text{A4})$$

On the other hand, as c_0 becomes large, the LHS of (A1) goes to zero as $1/c_0$, and the RHS of (A1) becomes

$$\int_{-\infty}^{+\infty} \frac{\rho(\Delta) d\Delta}{\Delta^2 + 2 - 1/c_0 + \dots} \quad (\text{A5})$$

and approaches a constant as $c_0 \rightarrow \infty$.

In summary, as $c_0 \rightarrow 0$, the LHS of (A1) is greater than the RHS of (A1), and as $c_0 \rightarrow \infty$, the LHS of (A1) is less than the RHS of (A1). Therefore, there exists a value of c_0 between zero and ∞ for which (A1) will be satisfied.

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