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1989 J. Phys.: Condens. Matter 1 8471

(http://iopscience.iop.org/0953-8984/1/44/017)

J. Phys.: Condens. Matter 1 (1989) 8471–8479. Printed in the UK

Transport in models with correlated diagonal and off-diagonal disorder

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Received 12 May 1989, in final form 19 July 1989

Abstract. The electrical transport properties of one-dimensional tight-binding models, with correlation between diagonal and off-diagonal disorder, are obtained using Felderhof's method. A new local transformation eliminating the off-diagonal disorder is utilised. The characterisation of the type of correlation for the existence of a critical energy E_c, at which transmission exists, is found. It is a generalisation, in some sense, of the well known transmission at the band centre for the case with only off-diagonal disorder. For the high-wavenumber approximation we find explicitly the inverse localisation length which, close to E_c, behaves as $|E - E_c|^\nu$, with $\nu = 1$ at the edges of the band and $\nu = 2$ otherwise. The transmission for a wavepacket around E_c is analysed for samples of finite size.

1. Introduction

We consider the one-dimensional (1D) tight-binding (TB) Hamiltonian given by

$$H = \sum_l \{\Omega_l |l\rangle\langle l| + \mathscr{D}_{l+1}^* |l\rangle\langle l+1| + \mathscr{D}_l |l\rangle\langle l-1|\} \tag{1.1}$$

where each state $|l\rangle$ is an atomic-like orbital centred at the site l. The sites l form a lattice and the set $\{|l\rangle, l \in Z\}$ is an orthogonal base in the space $l^2(Z)$. The quantity Ω_l is the energy of an electron at the l-position in the absence of the nearest-neighbour transfer rate $\mathscr{D}_l$. We denote by $|\chi\rangle$ the eigenfunction of the operator H with eigenvalue E. Expanding $|\chi\rangle$ in terms of the basis $\{|l\rangle\}$ we have

$$|\chi\rangle = \sum_l \phi_l |l\rangle \qquad \phi_l = \langle l|\chi\rangle \tag{1.2}$$

so the time-independent Schrödinger equation can be written as

$$\mathscr{D}_{l+1}^* \phi_{l+1} + \mathscr{D}_l \phi_{l-1} + (\Omega_l - E)\phi_l = 0. \tag{1.3}$$

In the case where only the Ω_l are random independent variables and $\mathscr{D}_l = 1$ (diagonal disorder) we recover the Anderson model [1]. A remarkable fact is that the wavefunctions are always exponentially localised [2, 3], whereas in the absence of disorder the wavefunctions are extended Bloch states. The static conductivity is given by the Kubo formula and the diffusion constant is zero [4] because of localisation.

0953-8984/89/448471+09$02.50

In the case where only the $\mathscr{D}_l$ are random independent variables and $\Omega_l = 0$ (off-diagonal disorder), it is known that the band centre ($E = 0$) is an extended state [5, 6]. We remark that, physically, off-diagonal disorder may be more directly related to structural characteristics of the disordered medium [7] (liquid-like stucture).

We will discuss the situation in which both diagonal and off-diagonal disorder are present. For this we proceed by finding a transformation that maps the general equation (1.3) to an equation that is of a form similar to the diagonal disorder case. The usual methods for that case (see, for example, [8]) will be adapted to this new equation. We apply this transformation to our models with correlation between diagonal and off-diagonal disorder. We investigate the conditions for the existence of a critical energy E_c at which transmission (delocalisation) exists. This is a generalisation, in some sense, of the case with off-diagonal disorder only where the critical energy is at the band centre [6]. We find that the existence of E_c is linked to the type of correlation between diagonal and off-diagonal disorder, and therefore the microscopic details are important in the transmission properties of the system. Moreover only for a special correlation type does the critical energy exist. The asymptotic behaviour of the inverse of the localisation length l^{-1} can be calculated in the high-wavenumber limit. Close to E_c, when the conditions for the existence (of E_c) are satisfied, this behaviour is given by the form $l^{-1} \sim |E - E_c|^{\nu}$ with $\nu = 2$ if $|E_c| \neq 2$, or $\nu = 1$ if $|E_c| = 2$. $|E| = 2$ corresponds to the band edges.

We note that a large number of physical problems can be described by an equation of general type (1.3)—for example, lattice vibrations of a harmonic chain, electrical lines or classical diffusion in random media [9, 10].

In § 2 we describe the TB model where the diagonal and off-diagonal disorder are correlated at each impurity. In § 3, a new local transformation eliminating the off-diagonal component of disorder is proposed for the general case, and applied to our model. In § 4 Felderhof's method is adapted to study the transport properties in these models. The existence of E_c is discussed in §§ 5 and 6 for the cases where the wavelength is short and the wavelength is not short, respectively. Finally, in § 7 a simple example with two kinds of impurities is given and the critical energy is found explicitly.

2. The model

In the TB equation (1.3), we consider the case with N random impurities where each impurity is placed at a random position x_n ($n = 1, 2, \ldots, N$) on the background. For the binding energy Ω_l, and the transfer rate $\mathscr{D}_l$ we take

$$\Omega_l = \begin{cases} 0 & \text{for } l \neq x_n \\ v_n & \text{for } l = x_n \end{cases} \tag{2.1}$$

$$\mathscr{D}_l = \begin{cases} 1 & \text{for } l \neq x_n, x_n + 1 \\ \mu_n & \text{for } l = x_n, x_n + 1 \end{cases} \tag{2.2}$$

where v_n and $\mu_n > 0$ are real random quantities. Now we introduce the more advantageous variables

$$u_n \doteq \frac{v_n}{\mu_n^2} \tag{2.3}$$

$$w_n \doteq \frac{1 - \mu_n^2}{\mu_n^2}. \tag{2.4}$$

We remark that w_n is directly related to the off-diagonal disorder variable and u_n includes the diagonal disorder variable. For these real random quantities we consider the probability density ρ given by

$$\rho(u_1, w_1, x_1, \ldots, u_N, w_N, x_N) = \delta(x_1) \prod_{n=2}^{n=N} F(\xi_n) \prod_{n=1}^{n=N} G(u_n, w_n) \tag{2.5}$$

where both F and G are normalised to unity and $\xi_n = (x_n - x_{n-1})$. The average over either F or G will be denoted by the brackets $\langle .. \rangle$, whereas the average over the complete probability distribution (2.5) will be denoted by $\langle .. \rangle_{F,G}$. The first impurity is fixed at $x_1 = 0$, and the relative distances ξ_n are independent random variables with the same probability density F. The support of F is such that no overlap between impurities occurs. Further, we assume

$$x_{n+1} - x_n > 2 \tag{2.6}$$

which can be interpreted as a condition of weak density of impurities. The random variables u_n and w_n are correlated, but each impurity (u_n, w_n) is independent and governed by the same distribution G.

Finally, we remark that the TB Hamiltonian H can be represented by the tridiagonal matrix

$$H = \begin{pmatrix} \ddots & 1 & 0 & 0 & 0 \\ 1 & 0 & \mu_n & 0 & 0 \\ 0 & \mu_n & v_n & \mu_n & 0 \\ 0 & 0 & \mu_n & 0 & 1 \\ 0 & 0 & 0 & 1 & \ddots \end{pmatrix}. \tag{2.7}$$

3. Transformation from off-diagonal to diagonal TB

The transmission and spectral properties for systems with only diagonal disorder, in one dimension, are well known. The localisation of the states and the absence of transmission has been rigorously proved [2, 3]. The existence of a transformation from off-diagonal to diagonal TB has therefore practical importance.

We express the wavefunction ϕ_l of the Schrödinger equation (1.3), in terms of a new variable ψ_l defined by the local transformation

$$\psi_l = \phi_l / \varphi_l \tag{3.1}$$

where the quantity φ_l is given by the simple recursion formula

$$\varphi_l^* \varphi_{l-1} = 1/\mathscr{D}_l. \tag{3.2}$$

Then the equation for ψ_l is given by

$$\psi_{l+1} + \psi_{l-1} + |\varphi_l|^2 (\Omega_l - E)\psi_l = 0 \tag{3.3}$$

which involves only diagonal disorder. We remark that this is a generalised eigenvalue equation for ψ_l ($E\psi_l$ is multiplied by $|\varphi_l|^2$). However, the methods for the usual eigenvalue problem are easily adapted to this case.

In the interesting case when the Ω_l are independent identical random variables and $\mathscr{D}_l$ is a deterministic function of l, the equation (3.3) becomes similar to the Anderson model with modulation ($|\varphi_l|^2$). Because, recently, artificial structures with practically arbitrary properties as a function of linear distance have become available in microstructures, the investigation of a random array with modulation has practical interest. For example in [10] the case where $|\varphi_l|^2 \sim l^\kappa$ ($\kappa \leq 0$) was studied and a crossover ($\kappa = -\frac{1}{2}$) between the metallic and insulator regimes was found.

Now we consider the statistical behaviour of the random quantity $|\varphi_l|^2$, when $\mathscr{D}_l$ are random independent variables for any l (this is not the case in the model of § 2). For simplicity we suppose that the $\mathscr{D}_l$ are real quantities governed by the probability distribution g, given by

$$g(\mathscr{D}_l) = \begin{cases} 1/2\eta & \text{for } 1-\eta \leq \mathscr{D}_l \leq 1+\eta \\ 0 & \text{otherwise} \end{cases} \tag{3.4}$$

where η (< 1) is a real positive parameter. Due to (3.2) we have that

$$\varphi_l = \frac{\mathscr{D}_{l-1}}{\mathscr{D}_l} \cdots \frac{\mathscr{D}_1}{\mathscr{D}_2} \varphi_0. \tag{3.5}$$

For convenience we suppose that l is an even number and we take the initial condition $\varphi_0 = 1$.

Then by (3.4) and (3.5) we have that

$$\langle |\varphi_l|^2 \rangle \sim \left(\frac{1 + \frac{1}{3}\eta^2}{1 - \eta^2} \right)^{l/2} \tag{3.6}$$

$$\langle |\varphi_l|^4 \rangle \sim \left(\frac{(1 + 2\eta^2 + \frac{1}{5}\eta^4)(1 + \frac{1}{3}\eta^2)}{(1-\eta^2)^3} \right)^{l/2} \tag{3.7}$$

and due to (3.6) and (3.7) we see that the random quantity $|\varphi_l|^2$ has an anomalous statistical behaviour when $l \to \infty$, because the relative fluctuations

$$\frac{\langle |\varphi_l|^4 \rangle - \langle |\varphi_l|^2 \rangle^2}{\langle |\varphi_l|^2 \rangle^2} \tag{3.8}$$

are exponentially divergent with l.

Finally we remark that the function $\phi_l = \mathrm{i}^l \varphi_l$ is a solution of the TB equation (1.3) (with $\mathscr{D}_l$ real) in the band centre $E = 0$ when only off-diagonal disorder is present ($\Omega_l = 0$).

4. Transfer matrix technique: Felderhof's method

Now we apply the transformation defined in § 3 to the model. In this case the solution of the recursion formula for φ_l is simple and given by

$$\varphi_l = \begin{cases} 1 & \text{for } l \neq x_n \\ 1/\mu_n & \text{for } l = x_n. \end{cases} \tag{4.1}$$

Thus when $l \neq x_n$ we have $\phi_l = \psi_l$ and the transmission and reflection coefficients are the same in both representations. The diagonal equation for the amplitude ψ_l in this case is written as

$$\psi_{l+1} + \psi_{l-1} + (V_l - E)\psi_l = 0 \tag{4.2}$$

with the new random diagonal potential V_l given by

$$V_l = \begin{cases} 0 & \text{for } l \neq x_n \\ u_n - Ew_n & \text{for } l = x_n. \end{cases} \tag{4.3}$$

The random quantities u_n and w_n are given by (2.3) and (2.4) with probability distribution ρ (2.5). Equation (4.2) is similar to the Anderson model with a weak density of impurities ($(x_n - x_{n-1}) > 2$). We can conveniently evaluate the transmission properties using the transfer-matrix technique and in particular Felderhof's method [11]. So we consider that on the left of the system ($l < x_1$), the solution of (4.2) is given by $\psi_l = e^{ikl} + re^{-ikl}$. On the right of the system ($l > x_N$) $\psi_l = te^{ikl}$, and with the usual definition of the transmission and reflection coefficient, $T = |t|^2$, $R = |r|^2$, we have that $R + T = 1$. The wavenumber k is given by the dispersion relation

$$E = 2\cos k \tag{4.4}$$

the condition $|E| < 2$ gives us the appropriate interpretation for the transmission coefficients T and R. We remark that the band edges are given by the relation $|E| = 2$.

The transfer matrix relating the wavefunction across the system, is obtained as the product of individual transfer matrices. Let us consider the interval $x_{n-1} < l < x_n$ where the solution for ψ_l (and ϕ_l) can be written as

$$\psi_l = A_n e^{ikl} + B_n e^{-ikl} \qquad x_{n-1} < l < x_n. \tag{4.5}$$

Now using the condition of weak density of impurities ($\xi_n > 2$) we match the wavefunctions on the right and left of an impurity (located at the x_n position) with the help of (4.2). This yields the transfer matrix $\mathbf{M}(n)$ relating the amplitudes (A_{n+1},B_{n+1}) and (A_n,B_n) by

$$\begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = \mathbf{M}(n) \begin{pmatrix} A_n \\ B_n \end{pmatrix} \tag{4.6}$$

with

$$\mathbf{M}(n) = \begin{pmatrix} e^{-ikx_n} & 0 \\ 0 & e^{ikx_n} \end{pmatrix} \begin{pmatrix} \alpha_n & -i\beta_n \\ i\beta_n & \alpha_n^* \end{pmatrix} \begin{pmatrix} e^{ikx_n} & 0 \\ 0 & e^{-ikx_n} \end{pmatrix} \tag{4.7}$$

and

$$\beta_n = \frac{V_{x_n}}{2\sin k} \qquad \alpha_n = 1 - i\beta_n. \tag{4.8}$$

The ratio between the reflection and transmission coefficients across the sample with N impurities is written as [11]

$$R/T = \tfrac{1}{2}(\Gamma - 1) \tag{4.9}$$

where the quantity Γ is given by a product of the random independent matrices

$$\Gamma = \{\mathbf{K}(N)\mathbf{U}(\xi_N)\dots\mathbf{U}(\xi_2)\mathbf{K}(1)\}_{(2,2)}. \tag{4.10}$$

The symbol $\{..\}_{(2,2)}$ designates the element (2, 2) in the product matrix. The three-dimensional collision matrix $\mathbf{K}$ and the propagation matrix $\mathbf{U}$ are given by

$$\mathbf{K} = \begin{pmatrix} \alpha^2 & -i\alpha\beta & -\beta^2 \\ 2i\alpha\beta & |\alpha|^2+\beta^2 & -2i\alpha^*\beta \\ -\beta^2 & i\alpha^*\beta & \alpha^{*2} \end{pmatrix} \tag{4.11}$$

$$\mathbf{U}(\xi) = \begin{pmatrix} e^{i2k\xi} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{-i2k\xi} \end{pmatrix}. \tag{4.12}$$

We note that every matrix $(\mathbf{K}(n) - \mathbf{I})$ is statistically independent and depends linearly on V_{x_n} and $V_{x_n}^2$.

Due to the form of the probability distribution ρ (2.5) we have that

$$\langle\Gamma\rangle_{F,G} = \{\langle\mathbf{K}(N)\rangle\langle\mathbf{U}(\xi_N)\rangle\dots\langle\mathbf{U}(\xi_2)\rangle\langle\mathbf{K}(1)\rangle\}_{(2,2)}. \tag{4.13}$$

The complete calculation of $\langle\Gamma\rangle_{F,G}$ (or $\langle R/T\rangle_{F,G}$) requires evaluation of a power of the three-dimensional matrix $\langle\mathbf{U}\rangle\langle\mathbf{K}\rangle$, this can be achieved by standard methods (see, for example, [12]). The growth rate of $\langle\Gamma\rangle_{F,G}$ is given by the inverse localisation length $l^{-1} = \ln(\lambda_0)$, where λ_0 is the largest positive real root of the characteristic equation

$$|\lambda\mathbf{I} - \langle\mathbf{U}\rangle\langle\mathbf{K}\rangle| = 0. \tag{4.14}$$

Finally it is interesting to note that the electrical resistivity in a disordered (1D) system is proportional to the ratio R/T as was first argued by Landauer [13, 14].

5. Large-wavenumber limit

We consider now the approximation

$$k(x_{n+1} - x_n) \gg 1. \tag{5.1}$$

Then $\langle e^{ik\xi_n}\rangle \simeq 0$ and the average propagator $\langle\mathbf{U}\rangle$ is given by

$$\langle\mathbf{U}\rangle \simeq \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{5.2}$$

Thus by (4.13) we have that, in this approximation,

$$\langle\Gamma\rangle_{F,G} = \left(1 + \frac{2\sigma^2}{4-E^2}\right)^N \tag{5.3}$$

with

$$\sigma^2 = \langle V_{x_n}^2\rangle = \langle w_n^2\rangle E^2 - 2\langle u_n w_n\rangle E + \langle u_n^2\rangle. \tag{5.4}$$

In this expression the averages (with respect to the distribution G) are n-independent.

Due to the inequality

$$\langle u_n w_n \rangle^2 \leq \langle u_n^2 \rangle \langle w_n^2 \rangle \tag{5.5}$$

satisfied by any distribution G, we always have $\sigma^2 \geq 0$ for every real energy E. So two different types of behaviour ($\sigma^2 > 0$ or $\sigma^2 = 0$) in the transmission properties can be found in the system.

(i) When $\sigma^2 > 0$ there is exponential localisation since by (5.3) we have

$$\langle R/T \rangle_{F,G} \sim \exp(l^{-1}N) \tag{5.6}$$

in the limit $N \to \infty$. The inverse localisation length l^{-1} (we take the distance factor as one) is given by

$$l^{-1} = \ln\left(1 + \frac{2\sigma^2}{4 - E^2}\right). \tag{5.7}$$

We remark that in the band centre, $E = 0$, the localisation length depends only on the second moment of u_n.

It is interesting to note that when the energy is close to the edges of the band ($|E| \sim 2$), the localisation length is close to zero, i.e. the localisation is maximal.

(ii) When $\sigma^2 = 0$ we have total transmission since from (5.3) and (4.9) we have that

$$\langle R/T \rangle_{F,G} = 0. \tag{5.8}$$

The condition $\sigma^2 = 0$ can be satisfied only when the two random quantities u_n and w_n are proportional to each other, or

$$u_n = E_c w_n. \tag{5.9}$$

Here the constant E_c becomes the critical energy when there is transmission. So E_c exists only for a particular form of the distribution G.

In the original variables, the binding energy v_n and the transfer rate μ_n, the relation (5.9) is equivalent to the equation

$$v_n = E_c(1 + \mu_n^2). \tag{5.10}$$

When $E \neq E_c$ and the relation (5.9) is verified, we always have exponential localisation and by (5.7) it is easy to see that, close to E_c, the inverse localisation length behaves as

$$l^{-1} \sim |E - E_c|^{\nu} \tag{5.11}$$

where $\nu = 2$ if $|E_c| \neq 2$ and $\nu = 1$ if $|E_c| = 2$ (the band edges).

Now we discuss briefly the transmission properties for a wavepacket with energy centred around E_c. If we consider a system where (5.9) is verified and with fixed size $N = N_0$, then by (5.11) we have an energy range of width ΔE given by

$$\Delta E \approx 1/\sqrt{N_0} \tag{5.12}$$

around $E_c \neq 2$ where the localisation length l is greater than N_0 (quasi-metallic regime). We therefore conjecture that for a system of finite size N_0, one will find transmission for wavepackets with energy support $[E_c + \frac{1}{2}\Delta E,\ E_c - \frac{1}{2}\Delta E]$. This transmission should therefore be experimentally observable.

6. E_c for arbitrary wavenumber

Here we discuss briefly the conditions for the existence of a critical energy beyond the approximation (5.1). From the expression (4.13) for $\langle \Gamma \rangle_{F,G}$ we see that there is transmission when $\langle \mathbf{K} \rangle = \mathbf{I}$. Since $\langle \mathbf{K} - \mathbf{I} \rangle$ is linear in $\langle V_{x_n} \rangle$ and $\langle V_{x_n}^2 \rangle$, the conditions for transmission are

$$\langle V_{x_n} \rangle = 0 \tag{6.1}$$

$$\langle V_{x_n}^2 \rangle = 0. \tag{6.2}$$

The condition (6.2) has been discussed in the preceding section. Thus the relation (5.9) on G is always necessary for the existence of E_c.

On the other hand the condition (6.1) is also true at $E = E_c$ when (5.9) is verified. So the linear relation between the random variables u and w is a necessary and sufficient condition for the existence of the critical energy $E = E_c$ where transmission ($\langle R/T \rangle = 0$) takes place.

In the next section a simple example with total transmission at E_c is studied.

7. An example: two types of atomic impurities

Here we consider the particular distribution given by

$$G(u, w) = \tfrac{1}{2}\{\delta(u-a)\delta(w-b) + \delta(u+a)\delta(w+b)\} \tag{7.1}$$

where δ is the Dirac function, a and b are real quantities and $|b| < 1$. This can be interpreted as a lattice (background) with two species of atomic impurities, A and B. Thus the binding energy Ω_l and the transfer rate $\mathscr{D}_l$, are given by

$$\left.\begin{aligned} \Omega(\mathrm{A}) &= a/(1+b) \\ \mathscr{D}(\mathrm{A}) &= 1/\sqrt{1+b} \end{aligned}\right\} \quad \text{for impurity A}$$

$$\left.\begin{aligned} \Omega(\mathrm{B}) &= -a/(1-b) \\ \mathscr{D}(\mathrm{B}) &= 1/\sqrt{1-b} \end{aligned}\right\} \quad \text{for impurity B.}$$

The distribution (7.1) is equivalent to a linear relation between the quantities u and w where the constant of proportionality is given by a/b, so the critical energy is given by the simple expression

$$E_c = a/b. \tag{7.2}$$

We remark that when $a = 0$ (i.e. only off-diagonal disorder) one has $E_c = 0$ (band centre) as in [6].

When $b \to 0$, one has that $E_c \to \infty$ and there is no finite critical energy. This is similar to the Anderson model with only diagonal disorder.

Finally, in the large-wavenumber limit we have, due to (5.7), that the inverse localisation length is given explicitly by

$$l^{-1} = \ln\left(1 + 2\frac{(Eb-a)^2}{(4-E^2)}\right) \tag{7.3}$$

and the behaviour close to E_c is given by (5.11).

8. Conclusions

In the TB model with correlation between diagonal and off-diagonal disorder of § 2, the general local transformation of § 3 has been used to eliminate the off-diagonal component of disorder. Then using Felderhof's method we find the characterisation on the correlations for the existence of the critical energy E_c where total transmission takes place. We find that only for a particular relation (or type of correlation) between diagonal and off-diagonal disorder ((5.9) or (5.10)) is transmission possible. This is a generalisation of the well known transmission in the band centre when only off-diagonal disorder [6] is present.

In the large-wavenumber case, the inverse of the localisation length l^{-1} was obtained explicitly (equation (5.7)). Close to E_c, when the special condition on the correlation (5.9) is satisfied, the behaviour is given by $l^{-1} \approx |E - E_c|^{\nu}$ where $\nu = 2$ or $\nu = 1$ depending on whether $|E_c|$ is or is not at the band edges, respectively.

The transmission of a wavepacket in the system with finite size N_0 is briefly analysed (§ 5); we find that for the energy width $\Delta E \approx 1/\sqrt{N_0}$ around $E_c \neq 2$, transmission exists. This implies that this transmission should be measurable.

Finally we remark that very different transport properties can be found depending of the microscopic details (correlation between diagonal or off-diagonal disorder) of the system.

Acknowledgments

It is a pleasure to thank Professor C P Enz and Dr H R Jauslin for stimulating discussions. This work has been partially supported by the Fonds National Suisse de la Recherche Scientifique.

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