Exact solution of the problem of transmission of an electron through a one-dimensional chain of randomly positioned centers

V. I. Perel' and D. G. Polyakov
A. F. Ioffe Physicotechnical Institute, Academy of Sciences of the USSR

(Submitted 20 April 1983)
Pis'ma Zh. Eksp. Teor. Fiz. **37**, No. 11, 539–542 (5 June 1983)

The probability distribution for the wave function of an electron moving through a disordered, one-dimensional chain of scattering centers is found in the short-wavelength limit.

PACS numbers: 72.10.Bg

We are interested in the following problem. We have the equation

$$\frac{d^2\Psi(z)}{dz^2} + [k^2 - 2V(z)]\Psi(z) = 0,$$

where $V(z)$ is the potential created by randomly distributed centers. In the intervals between centers, the wave function has the form

$$\Psi(z) = a_+ e^{ikz} + a_- e^{-ikz} = \Psi_+(z) + \Psi_-(z).$$

Scattering by a center is characterized by the linear transformation

$$a_+ = \alpha_1 \tilde{a}_+ + \beta_1 \tilde{a}_- e^{-2ikz_1}, \quad a_- = \beta_1^* \tilde{a}_+ e^{2ikz_1} + \alpha_1^* \tilde{a}_-, \quad |\alpha_1|^2 - |\beta_1|^2 = 1, \tag{1}$$

where $a_\pm$ and $\tilde{a}_\pm$ are the amplitudes of the wave functions to the right and left of the center, respectively. The coefficients α_1 and β_1 do not depend on the coordinate of the center z_1. The values of the wave functions at the entrance ($z = 0$) and exit of a chain of length z satisfy the relations

$$\Psi_+(z)=\alpha\bar{\Psi}_+(0)+\beta\Psi_-(0),\quad \Psi_-(z)=\beta^*\Psi_+(0)+\alpha^*\Psi_-(0),\quad |\alpha|^2-|\beta|^2=1 \tag{2}$$

The coefficients α, β depend on the specific realization of the distribution of centers along the chain and in this sense are random quantities. The problem is to find their probability distribution.

This problem is the subject of many papers concerning Anderson localization and, in addition, the short-wavelength limit (large k) is of greatest interest. Some results are known for the average values (see, for example, Refs. 1–6 and the review in Ref. 7, concerning similar problems). Mel'nikov found the complete solution of the problem in the case of weak scattering by a separate center ($|\beta_1| \ll 1$) (see also Refs. 1 and 3, where the solution is presented for a potential in the form of Gaussian white noise). The general solution in the short-wavelength limit is obtained below.

We shall introduce the probability density $W(\mathbf{a},z)$ for the probability that the vector $\mathbf{a} = (\mathrm{Re}\, a_+, \mathrm{Im}\, a_+, \mathrm{Re}\, a_-, \mathrm{Im}\, a_-)$ assumes at the point z a given value if at the point $z = 0$ it has the value $\mathbf{a}_0$. It satisfies the following obvious equation:

$$\frac{\partial W(\mathbf{a},z)}{\partial z} = n[\,\widetilde{W}(\mathbf{a},z) - W(\mathbf{a},z)], \tag{3}$$

where n is the density of centers and $\widetilde{W}(\mathbf{a},z) = W(\tilde{\mathbf{a}},z)$, while $\tilde{\mathbf{a}}$ is related to $\mathbf{a}$ by relation (1). This equation is exact, since the probability of finding a center at point z is independent of the probability that the amplitude has a definite value to the left of the center. The boundary conditions for this equation can be prescribed only on the left end of the chain ($z = 0$). We transform to new variables $\rho_+, \rho_-, \phi, \chi$ according to the equation $\Psi_\pm = \rho_\pm \exp[i(\chi \pm \phi)]$. Then Eq. (3) assumes the form

$$\frac{\partial W}{\partial z} + k\frac{\partial W}{\partial \phi} = n(\widetilde{W} - W). \tag{4}$$

We note that the relation between $\widetilde{\Psi}_\pm$ and $\Psi_\pm$ does not contain the coordinate of the center. It is easy to show that $\widetilde{\chi} - \chi$ does not depend on χ, so that (4) retains its form after averaging over χ. In what follows, W is the probability averaged over χ. In the limit of large k, we can seek W in the form of the expansion $W = W^{(0)} + W^{(1)}/k + \cdots$. In the zeroth-order approximation, $\partial W^{(0)}/\partial\phi = 0$, while the condition for solvability of the first approximation leads to the equation

$$\frac{\partial W^{(0)}}{\partial z} = n\int_0^{2\pi}\frac{d\phi}{2\pi}(\widetilde{W}^{(0)} - W^{(0)}). \tag{5}$$

The probability $W^{(0)}$ depends only on ρ_+ and ρ_-. However, $\rho_-^2 - \rho_+^2 = J$ is, according to (2), a conserved quantity (flux). For this reason, we can write $W^{(0)} = \delta(J - J_0)F(I,z)$, where $I = \rho_-^2 + \rho_+^2$. We shall seek F for boundary conditions of the specific form $J_0 = 0$, $I_0 = 1$. As will be evident, this is sufficient for solving completely the problem stated at the beginning of the paper (we note that under such conditions the function F describes the distribution of the electronic density of a localized state). From Eqs. (1) and (5) we find

$$\frac{\partial F(I,z)}{\partial z} = n \int_0^{2\pi} \frac{d\psi}{2\pi} [F(qI,z) - F(I,z)]. \tag{6}$$

Here $q = \gamma_1 + \sqrt{\gamma_1^2 - 1}\cos\psi$, $\gamma_1 = |\alpha_1|^2 + |\beta_1|^2 = 1 + 2R_1/T_1$; R_1, T_1 are coefficients of reflection and transmission for scattering of an electron by the center. From Eq. (6) it is easy to obtain

$$\int_0^{\infty} dI I^s F(I,z) = \exp\{[P_s(\gamma_1) - 1] nz\}, \tag{7}$$

where P_s is a Legendre function [$F(I,z)$ can be obtained from this equation by an inverse Mellin transformation, but this is not our purpose]. We shall show that the result (7) permits obtaining the complete solution for the probability distribution of the transition matrix (2). This matrix contains three independent parameters, which we shall choose as $\gamma = |\alpha|^2 + |\beta|^2 = 1 + 2R/T$ (R and T are the coefficients of reflection and transmission for the entire chain) and the phases of the coefficients α and β. The probability density $w(\gamma,z)$, which gives a statistical description of the transition matrix for the chain, must be determined. Evidently, $F(I,z)$ is expressed in terms of $w(\gamma,z)$:

$$F(I,z) = \int_0^{2\pi} \frac{d\psi}{2\pi} \int_1^{\infty} d\gamma\, w(\gamma,z)\, \delta(I - I(\gamma, \psi, J_0, I_0)), \tag{8}$$

where $I(\gamma,\psi,J_0,I_0) = \gamma I_0 + \sqrt{\gamma^2 - 1}\sqrt{I_0^2 - J_0^2}\cos\psi$ is the sum $|\Psi_+|^2 + |\Psi_-|^2$, written in terms of initial values J_0, I_0 with the help of the transformation (2). Setting here $J_0 = 0, I_0 = 1$, multiplying (8) by I^s, integrating over I, and using (7), we obtain for $w(\gamma,z)$ the integral equation

$$\int_1^{\infty} d\gamma\, w(\gamma,z) P_s(\gamma) = \exp\{[P_s(\gamma_1) - 1] nz\}. \tag{9}$$

This equation is solved using a Möhler-Fock transformation[8]:

$$w(\gamma,z) = \int_0^{\infty} dt\, P_{-\frac{1}{2}+it}(\gamma)\, t\,\mathrm{th}(\pi t) \exp\{[P_{-\frac{1}{2}+it}(\gamma_1) - 1] nz\}. \tag{10}$$

Equation (10) is the solution of this problem.

From (9) it is easy to find the averages for the integral powers γ (setting $s = 1,2,...$) and for $\ln[(\gamma+1)/2] = \ln(1/T)$ (differentiating it with respect to s and letting s approach 0):

$$\langle\gamma\rangle = 2\langle 1/T\rangle - 1 = \exp[(2R_1/T_1) nz], \quad \langle\ln(1/T)\rangle = nz\ln(1/T_1).$$

Multiplying (10) by $T = 2/(\gamma+1)$ and integrating, we obtain a general expression for the average transmission coefficient of the chain

$$\langle T\rangle = 2\pi \int_0^{\infty} dt\, t \frac{\mathrm{th}(\pi t)}{\mathrm{ch}(\pi t)} \exp\{[P_{-\frac{1}{2}+it}(\gamma_1) - 1] nz\}.$$

For weak scattering and a white noise potential, the well-known results[1-5] follow from the equations presented above (here the distribution (10) goes over into the distribu-

tions in Refs. 1, 3, and 5). Other limiting cases are also easily obtained from (10): $R_1 \to 1$, large x, etc. Substituting R_1 and T_1 which correspond to delta-function centers, the equations for $\langle 1/T \rangle$ and $\langle \ln(1/T) \rangle$ coincide with those obtained in Ref. 6, where scattering was not assumed to be weak.

We note some exact results following from (3) for arbitrary k. Multiplying (3) by $|a_+|^2, |a_-|^2, (a_+ a_-^*)$, we can obtain a closed system of first-order differential equations with constant coefficients for the corresponding average values. Assuming all averages to be $\propto \exp(\nu n z)$, we find the characteristic equation $\nu^3 + \delta\nu^2 + [\delta + 4k^2 n^{-2} + 8(\mathrm{Re}\,\alpha_1)(\mathrm{Im}\,\alpha_1)kn^{-1}]\nu - 8|\beta_1|^2 k^2 n^{-2} = 0$, $\delta = 4 - 4(\mathrm{Re}\,\alpha_1)^2$. For the boundary conditions $|a_{+0}| = 0, |a_{-0}| = 1$, the quantity $|a_-|^2$ is equal to $1/T$. Thus $\langle 1/T \rangle$ can be found exactly for arbitrary values of z and k. We note that the z dependence of $\langle 1/T \rangle$ contains oscillating terms. The root of the characteristic equation for which $\mathrm{Re}\,\nu$ is maximum determines the behavior of $\langle 1/T \rangle$ for large z: $\langle 1/T \rangle \propto \exp(z/l)$. In the simple case of delta-function centers, $1/l = 2(k_b^2 n)^{1/3}$ for $|k_b + k^2/n| \ll |k_b (k_b/n)^{1/3}|$ and $1/l = 2k_b^2/(2k_b + k^2/n)$ when the inverse inequality is satisfied and $2k_b + k^2/n > 0$ ($-\hbar^2 k_b^2/2m$ is the energy of the bound or virtual state in the field of an isolated center). In the short-wavelength limit, ($kl \gg 1, |k_b|l \gg 1$) $1/l = 2nk_b^2/k^2 = 2nR_1/T_1$.

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Translated by M. E. Alferieff
Edited by S. J. Amoretty