Probability distribution for the transmission of an electron through a chain of randomly placed centers

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The probability distribution for the transmission coefficient T is derived in the short-wave limit for an arbitrary matrix for scattering by an individual center. The behavior of this probability at values of T near unity is determined by those configurations of centers for which the transmission is resonant. The effect of an external electric field is analyzed. Exact results are derived for $\langle 1/T \rangle$ without using the short-wave approximation.

The passage of an electron through a disordered one-dimensional 1D) chain has been the subject of many studies (see Refs. 1–8, for example) in connection with the problem of Anderson localization. A significant point here is that the classical Boltzmann equation cannot be used to describe the 1D motion of an electron which is scattered elastically by random inhomogeneities.[1,9–13] The reason is that the Boltzmann equation completely ignores the interference effects which are strong in this case.

In the present paper we solve the steady-state problem with purely elastic scattering. Our basic result is an exact expression for the probability distribution for the transmission coefficient T in the short-wave limit (T is directly related to the conductivity of the chain[3,14–19]). This distribution has been derived previously under the assumption that the scattering by an individual center is weak[1,2,5,6]; we do not use this assumption here. Exact expressions have also been derived for expectation values.[5,7] The distribution of the transmission coefficient is of particular interest, however, because of the well-known circumstance that T is not a self-averaging quantity.

In Section 1 we derive the basic equation for the probability for the value of the wave function after an electron has traversed a part of the chain of a given length z with identical centers arranged in a random manner. Exact results for certain expectation values ($\langle 1/T \rangle$, for example) follow directly from this equation; these results are derived in §6. In §2, the basic equation is used to derive an equation which holds in the short-wave limit (at large values of the wave vector). This equation is solved exactly, and it yields an expression for the probability distribution $w(\gamma,z)$ ($\gamma = 2/T - 1$). This expression is analyzed in §3. In particular, it yields expressions for $\langle T \rangle$ and $\langle \ln T \rangle$ for an arbitrary probability for scattering by an individual center. In §4, a generalization is made to the case in which the centers are not identical, and only the probability matrix for the scattering by the center is given. The case of a fixed number (N) of centers on the chain is examined in the same section. In this case we can clearly see the role played by those configurations which result in a resonant transmission. For example, it turns out that the functions $w_N(\gamma,z)$ in the cases $N = 2$ and 4 have a singularity at $T = 1$ (they become infinite; at $N > 4$, the functions w_N remain finite). This singularity is of course retained in the problem with a fluctuating number of centers on the chain. The effect of a static external electric field on the transmission is studied in §5. It is shown that if the effect of the field on the scattering event itself is ignored than the field dependence of $w(\gamma,z)$ is governed entirely by the dependence of the scattering matrix of the center on the kinetic energy of the electron. If the chain is long enough, the electron acquires such a high kinetic energy in this field that the scattering becomes unimportant, and the transmission coefficient of the chain becomes independent of its length. In the final section we derive exact results for $\langle 1/T \rangle$ and certain other expectation values without resorting to the short-wave approximation.

There is a point worth noting here: In scaling theory[3] it is usually assumed that at small values of z the results should be the same as those found by solving the classical Boltzmann equation. This assumption generates a relationship among the parameters in the expressions for the various expectation values ($\langle 1/T \rangle$, $\langle \ln T \rangle$, etc.). The results derived below show that this procedure is not correct (even in the short-wave limit) if the scattering by an individual center is not assumed weak. This circumstance was also pointed out in Ref. 7, where $\langle 1/T \rangle$ and $\langle \ln T \rangle$ were calculated for scattering by δ-shaped centers.

§1. BASIC EQUATION

We consider a $1D$ chain of randomly placed centers which create a potential $V(z)$. The wave function of an electron in this chain satisfies the equation

$$\frac{d^2\Psi}{dz^2} + [k^2 - 2V(z)]\Psi = 0. \tag{1}$$

The concentration of centers is assumed to be small enough that the scattering by each center is independent of the other centers. In the intervals between centers the wave function is

$$\Psi(z) = a_+ e^{ikz} + a_- e^{-ikz} = \Psi_+(z) + \Psi_-(z). \tag{2}$$

The scattering by a center is characterized by the linear transformation

$$\begin{aligned} a_+ &= \alpha_1 \tilde{a}_+ + \beta_1 \tilde{a}_- e^{-2ikz_1}, \\ a_- &= \beta_1^* \tilde{a}_+ e^{2ikz_1} + \alpha_1^* \tilde{a}_-, \quad |\alpha_1|^2 - |\beta_1|^2 = 1, \end{aligned} \tag{3}$$

where $a_\pm$ and $\tilde{a}_\pm$ are the amplitudes of the wave function respectively to the right and to the left of the center. The coefficients α_1 and β_1 do not depend on the coordinate z_1 of the center; they are related to the reflection amplitude r_1 and

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the transmission amplitude t_1 for scattering by a center at the origin:

$$\alpha_1=1/t_1^*, \quad \beta_1=-r_1^*/t_1^*. \tag{4}$$

We introduce a probability density $W(\mathbf{a}, z)$ such that at the point z the vector $\mathbf{a}=(\mathrm{Re}\,a_+, \mathrm{Im}\,a_+, \mathrm{Re}\,a_-, \mathrm{Im}\,a_-)$ takes on a given value under the condition that it has the value $\mathbf{a}_0$ at the point $z=0$. For W we can write

$$W(\mathbf{a}, z+dz)=ndzW(\tilde{\mathbf{a}}, z)+(1-ndz)W(\mathbf{a}, z)$$

(n is the concentration of centers). This relation is exact, since the probability for a given value of the wave function to the left of the point z and the probability ndz for the center to be in the interval $(z, z+dz)$ are independent. We thus find the differential equation

$$\frac{dW(\mathbf{a}, z)}{dz}=n[\bar{W}(\mathbf{a}, z)-W(\mathbf{a}, z)], \quad \bar{W}(\mathbf{a}, z)=W(\tilde{\mathbf{a}}, z), \tag{5}$$

where $\tilde{\mathbf{a}}$ is related to $\mathbf{a}$ by the transformation inverse to (3). In the spirit of this derivation, the boundary conditions on this equation should be specified at the left end of the chain.

We transform to the new variables ρ_+, ρ_-, Φ, χ by means of

$$a_\pm=\rho_\pm \exp[i(\chi\pm\varphi\mp kz)], \quad \Psi_\pm=\rho_\pm \exp[i(\chi\pm\varphi)].$$

Equation (5) then becomes

$$\frac{\partial W}{\partial z}+k\frac{\partial W}{\partial \varphi}=n(\bar{W}-W). \tag{6}$$

Now W means the probability density for the quantities ρ_+, ρ_-, Φ, and χ ($d\mathbf{a}=\rho_+ d\rho_+ \rho - d\rho - d\varphi d\chi$). Equation (6) is the basic equation for the calculations below. Using (3), one can show easily that in the course of the scattering the phase χ acquires a shift independent of itself ($\tilde{\chi}-\chi$ is independent of χ). For this reason, Eq. (6) remains the same in form after an integration over χ. Below, W will denote the probability integrated over χ. A further simplification results from the circumstance that the flux $J=\rho_-^2-\rho_+^2$ is conserved under transformation (3). As the two other variables it is convenient to choose the intensity $I=\rho_-^2+\rho_+^2$ and the phase φ. Setting $W(J, I, \varphi)=\delta(J-J_0)W(I, \varphi)$, we find for $W(I,\varphi)$ an equation which is the same as (6), in which J is a parameter determined by the boundary condition.

Finally, we write a transformation law for I and φ for scattering by a center:

$$I=\gamma_1\tilde{I}+(\gamma_1^2-1)^{1/2}(\tilde{I}^2-J^2)^{1/2}\cos\psi, \quad \psi=2\tilde{\varphi}+\varphi_{\alpha_1}-\varphi_{\beta_1},$$
$$(I^2-J^2)^{1/2}e^{2i\varphi}=2\alpha_1\beta_1\tilde{I}+(\tilde{I}^2-J^2)^{1/2}(\beta_1^2e^{-2i\tilde{\varphi}}+\alpha_1^2e^{2i\tilde{\varphi}}), \tag{7}$$

where $\gamma_1=|\alpha_1|^2+|\beta_1|^2=1+2R_1/T_1$, R_1 and T_1 are the reflection and transmission coefficients, and φ_{α_1} and φ_{β_1} are the phases of α_1 and β_1.

§2. SHORT-WAVE LIMIT

In the limit of large k we seek W as the expansion $W=W^{(0)}+W^{(1)}/k+\ldots$ (Appendix 1). In a zeroth approximation we find $\partial W^{(0)}/\partial\varphi=0$ from (6). We thus see that $W^{(0)}$ depends on the one variable I. Going on to the first approximation, we find the equation

$$\frac{\partial W^{(0)}}{\partial z}+\frac{\partial W^{(1)}}{\partial \varphi}=n(\bar{W}^{(0)}-W^{(0)}).$$

From the condition for the solvability of this equation (the condition that $W^{(1)}$ is periodic in φ) we find an equation for $W^{(0)}$:

$$\frac{\partial W^{(0)}}{\partial z}=n\left(\int_0^{2\pi}\frac{d\varphi}{2\pi}\bar{W}^{(0)}-W^{(0)}\right). \tag{8}$$

It turns out that this equation can be solved exactly. To solve it we first consider the case of a zero flux, $J=0$, in which case Eq. (7) simplifies considerably:

$$I=\tilde{I}(\gamma_1+(\gamma_1^2-1)^{1/2}\cos\psi). \tag{9}$$

We specify the boundary condition

$$W^{(0)}(I, z=0)=\delta(I-1)$$

(the intensity has unity value at the beginning of the chain). We multiply Eq. (8) by I^s and integrate the result over I. Using (9) and $dId\varphi=d\tilde{I}d\tilde{\varphi}$, we find a differential equation for the expectation value of I^s. Solving it under the boundary condition $I^s=1$ at $z=0$, we find

$$\int_0^\infty dI\, I^sW^{(0)}(I, z)=\exp\{[P_s(\gamma_1)-1]nz\}, \tag{10}$$

where P_s is the Legendre function

$$P_s(\gamma_1)=\int_0^{2\pi}\frac{d\psi}{2\pi}(\gamma_1+(\gamma_1^2-1)^{1/2}\cos\psi)^s. \tag{11}$$

Taking the inverse Mellin transform, we find $W^{(0)}(I, z)$ at $J=0$ from (10), but at present we are not interested in this function itself. We will now show that the result (10) is sufficient basis for calculating the probability distribution of the transmission coefficient of the chain.

The values of the wave function at the beginning of the chain ($z=0$) and at an arbitrary point $z>0$ are related by the matrix

$$\begin{pmatrix}\alpha & \beta\\ \beta^* & \alpha^*\end{pmatrix}, \quad |\alpha|^2-|\beta|^2=1. \tag{12}$$

This relation is

$$\Psi_+(z)=\alpha\Psi_+(0)+\beta\Psi_-(0), \quad \Psi_-(z)=\beta^*\Psi_+(0)+\alpha^*\Psi_-(0). \tag{13}$$

The matrix elements in (12) are expressed in terms of the reflection and transmission amplitudes of a chain of length z by means of equations analogous to (4). In particular, we have $|\beta|^2=R/T$, where R and T are the intensity reflection and transmission coefficients. Matrix (12) can contain three independent parameters; we choose them to be

$$\gamma=1+2R/T=2/T-1$$

and the phases of α and β. The function $W^{(0)}(I,z)$ is expressed in terms of the probability density $w(\gamma, z)$ alone (Appendix 2):

$$W^{(0)}(I, z)=\int_0^{2\pi}\frac{d\psi}{2\pi}\int_1^\infty d\gamma w(\gamma, z)\delta(I-I(\gamma, \psi, J, I_0)), \tag{14}$$

where $I(\gamma, \psi, J, I_0)$ is determined by (7) with $\alpha_1, \beta_1\to\alpha, \beta$ and $\tilde{I}\to I_0$ (I_0 is the intensity at the beginning of the chain). Setting

$J = 0$ and $I_0 = 1$, multiplying (14) by I^s, integrating over I, and using (10), we find an integral equation for $w(\gamma, z)$:

$$\int_1^\infty d\gamma w(\gamma_1, z) P_s(\gamma) = \exp\{[P_s(\gamma_1) - 1]nz\}. \tag{15}$$

This equation can be solved by a Mehler-Fock transformation[20]:

$$w(\gamma, z) = \int_0^\infty dt P_{-1/2+it}(\gamma)\, t\, \mathrm{th}(\pi t) \exp\{[P_{-1/2+it}(\gamma_1) - 1]nz\}. \tag{16}$$

Expression (16) gives the complete solution for the probability distribution for the transmission coefficient of a chain of length z for an electron.

Under the boundary conditions $J = I_0 = 1$ (which mean that there is no flux incident on the chain from the left, while the outgoing flux is unity) the wave intensity at the point z is related to the transmission coefficient of a chain of length z by $I = \gamma$. Such boundary conditions correspond to the transmission of an electron through a chain after incidence from the right. In this case we have $W^{(0)}(I, z) = w(\gamma, z)$, so that $w(\gamma, z)$ must satisfy Eq. (8), with I related to $\tilde{I}$ by (7) at $J = 1$. Using the addition theorem for Legendre functions, we find quite easily by direct substitution that expression (16) is in fact a solution of Eq. (8) corresponding to the boundary condition $w(\gamma, 0) = \delta(\gamma - 1)$. We also note that by solving this equation with other boundary conditions we can easily find the transition probability.[2] Using it, we can find (for example) the intensity distribution in the chain for a given flux incident from the right.

The contents of this section have been published in summary form elsewhere.[21]

To conclude this section we note that the appearance of the functions $P_{-1/2+it}$, called the "cone" functions,[20] in the problem of 1D wave transmission is "not fortuitous": The group of transformations specified by (2×2) matrices of unit modulus is isomorphic to the proper Lorentz group.[22] Transformation (3) is specified by precisely this type of matrix, and it can be associated with a special type of Lorentz transformation which conserves the coordinate Z. We understand the coordinates X and Y and the time τ here as meaning $2\rho_+\rho_- \cos(2\varphi)$, $2\rho_+\rho_- \sin(2\varphi)$, and $\rho_+^2 + \rho_-^2$, respectively; the velocity (v) of the moving coordinate system is related to γ_1 by $\gamma_1 = 1/(1 - v^2)^{1/2} (c = 1)$. Transformation (3) thus describes, in the space X, Y, τ, the motion of a world point along the surface of the hyperboloid $X^2 + Y^2 - \tau^2 = \text{const}$ (in the particular case of a zero flux, with $\rho_+ = \rho_-$, it describes the motion of the world point along the surface of the light cone), and the cone functions play the same role as that played by the spherical harmonics in the rotation group. We wish to call attention to the fact that the problem of the $1D$ transmission in the case of weak scattering was first solved by Gertsenshteĭn and Vasil'ev[23] back in 1959 precisely by making an analogy with the case of a random walk in a Lobachevskiĭ space, whose motion group is isomorphic to the Lorentz group.

§3. ANALYSIS OF $w(\gamma, z)$

To find certain expectation values it is convenient to use Eq. (15), which gives average values of the Legendre polynomials $P_s(\gamma)$ for integer values of s. In particular, for $s = 1$ we have

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

Differentiating (15) with respect to s, and taking the limit as s goes to zero, we find, using (11),

$$\left\langle \ln\frac{\gamma+1}{2}\right\rangle \equiv \left\langle \ln\frac{1}{T}\right\rangle = nz \ln\frac{1}{T_1}. \tag{17}$$

We find the expectation value of the transmission coefficient $T = 2/(\gamma + 1)$ from (16):

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

These equations yield the results found previously[1,2,5,6] for weak scattering and a white-noise potential. When we substitute in the values of R_1 and T_1 corresponding to δ-shaped centers, we find expressions for $\langle 1/T\rangle$ and $\langle \ln(1/T)\rangle$ which are the same as those found in Ref. 7, where the scattering was not assumed weak.

Let us examine the expression for $\langle T\rangle$. At small R_1 we have

$$P_{-1/2+it}(\gamma_1) \approx 1 - (t^2 + 1/4) R_1$$

and

$$\langle T\rangle = 2\pi e^{-R_1 nz/4} \int_0^\infty dt\, t \frac{\mathrm{th}(\pi t)}{\mathrm{ch}(\pi t)} e^{-tR_1 nz}, \quad R_1 \ll 1.$$

At $R_1 nz \gg 1$ this integral can be evaluated easily; the result is the known expression

$$\langle T\rangle = (\pi^{3/2}/2)(R_1 nz)^{-3/2} \exp[-R_1 nz/4]. \tag{18}$$

In the opposite limit of strong scattering ($R_1 \to 1$) we have $P_{-1/2+it}(\gamma_1) \to 0$, so that

$$\langle T\rangle = \exp(-nz), \quad R_1 = 1.$$

This result is obvious, since the right side is the probability for the absence of centers from a chain of length z. The expression for $\langle T\rangle$ at large z but arbitrary R_1 is given below [expression (22)].

Interestingly, the expectation value of the quantity T/R (which is proportional to the conductivity of the chain according to Refs. 3 and 14–19) is always equal to infinity (as has been pointed out by Landauer[14] and Mel'nikov[5]). The reasons are the finite probability for the absence of centers from a chain of any length and the possibility of a resonant passage (§4).

Let us examine the behavior of $w(\gamma, z)$ at large z. When γ is not very large (see below), the integral in (16) is dominated by small values of t. In this case it is convenient to use the integral representation[20]

$$P_{-1/2+it}(\gamma) = \frac{1}{\pi} \int_0^\theta dx \frac{\cos tx}{[2(\mathrm{ch}\,\theta - \mathrm{ch}\,x)]^{1/2}}, \quad \mathrm{ch}\,\theta = \gamma.$$

It follows from this representation that at small t we have

$$P_{-1/2+it}(\gamma)=P_{-1/2}(\gamma)-t^2 f(\gamma),$$

where $f(\gamma)$ is positive. If $\gamma \gg 1$, then

$$P_{-1/2}(\gamma)=\frac{2\ln\gamma}{\pi(2\gamma)^{1/2}}, \quad f(\gamma)=\frac{(\ln\gamma)^3}{3\pi(2\gamma)^{1/2}} \tag{19}$$

Expanding the argument of the exponential in (16) at small values of t, we find

$$w(\gamma,z)=P_{-1/2}(\gamma)\frac{\pi^{1/2}}{4[f(\gamma_1)nz]^{1/2}}\exp\{[P_{-1/2}(\gamma_1)-1]nz\}. \tag{20}$$

The function $P_{-1/2}(\gamma)$ can be expressed in terms of the complete elliptic integral:

$$P_{-1/2}(\operatorname{ch}\theta)=2K(\operatorname{th}(\theta/2))/\pi\operatorname{ch}(\theta/2), \quad P_{-1/2}(1)=1.$$

This function falls off monotonically with increasing γ, but very slowly [see (19)]. It is not difficult to show that Eq. (20) holds if

$$\ln\gamma \ll [f(\gamma_1)nz]^{1/2}. \tag{21}$$

This interval of γ values does not determine the normalization of the probability and does not include typical values of $\ln\gamma$. The average transmission coefficient $T=2/(\gamma+1)$, however, is determined by the values $\gamma\sim 1$, for which Eq. (20) holds. Using this equation for large z and arbitrary γ_1, we find the expression

$$\langle T\rangle=\frac{\pi^{5/2}}{2[f(\gamma_1)nz]^{1/2}}\exp\{[P_{-1/2}(\gamma_1)-1]nz\}. \tag{22}$$

The same z dependence was found by Gogolin[24] in a calculation of the density-density correlation function.

We turn now to the $w(\gamma, z)$ dependence at large z and large γ. We use the asymptotic expansion[20]

$$P_{-1/2+it}(\gamma)=2\operatorname{Re}\frac{1}{(2\pi\gamma)^{1/2}}\frac{\Gamma(it)}{\Gamma(1/2+it)}e^{it\ln(2\gamma)}.$$

Substituting this expression into (16), and evaluating the integral by the method of steepest descent, we find

$$w(\gamma,z)=\frac{\Gamma(it_0)t_0\operatorname{th}(\pi t_0)}{\Gamma(1/2+it_0)}\left(\frac{2}{|\Phi''(t_0)|}\right)^{1/2}e^{\Phi(t_0)},$$
$$\Phi(t)=(it-1/2)\ln(2\gamma)+[P_{-1/2+it}(\gamma_1)-1]nz, \tag{23}$$

where t_0 is the saddle point, determined by the equation $\Phi'(t_0)=0$, i.e.,

$$\ln(2\gamma)+(\partial P_s(\gamma_1)/\partial s)_{s=-1/2+it_0}nz=0$$

(it can be shown that this point lies on the imaginary axis). Under condition (21), t_0 is small, and Eq. (23) converts into (20) with exponential accuracy. The correct coefficient of the exponential function could have been found in this case by taking into account in the integration the rapid change in the factor $t\tanh(\pi\tau)$ at small t.

The distribution of $\ln\gamma$ about its most probable value is Gaussian.[1,3,5-8] This result is easily derived from (23). To show this, we denote by $p(x)$ the probability density for $x=\ln\gamma$,

$$p(x)=w(e^x,z)e^x.$$

We see that the value of t_0 corresponding to the most probable value of x is found from the equation $d(\Phi+x)/dx=0$. In the differentiation here we should treat t_0 as a function of x and make use of $(\partial\Phi/\partial t)_{t=t0}=0$. We find $d(\Phi+x)/dx=it+1/2$; i.e., the unknown is $t_0=i/2$. The condition $(\partial\Phi/\partial t)_{t=i/2}=0$ then determines the most probable value of x, which we denote by x_T. Using (11) and the relation $P_s=P_{-s-1}$, we find

$$x_T=nz\left(\frac{\partial P_s(\gamma_1)}{\partial s}\right)_{s=0}=nz\ln\frac{1}{T_1}. \tag{24}$$

Comparison with (17) shows that $x_T=\langle x\rangle$ at $\langle x\rangle\gg 1$. Expanding $\Phi(t_0)$ in powers of $x-x_T$ and retaining terms of up to second order, we find a Gaussian distribution,

$$p(x,z)=\frac{1}{(2\pi)^{1/2}\sigma}\exp\left\{-\frac{(x-x_T)^2}{2\sigma^2}\right\}, \tag{25}$$

where

$$\frac{1}{\sigma^2}=-\left(\frac{d^2\Phi}{dx^2}\right)_{x=x_T}=-i\left(\frac{dt_0}{dx}\right)_{x=x_T}$$
$$=\left[nz\left(\frac{\partial^2 P_s(\gamma_1)}{\partial s^2}\right)_{s=0}\right]^{-1}.$$

Hence

$$\sigma^2=nz\int_0^{2\pi}\frac{d\psi}{2\pi}[\ln(\gamma_1+(\gamma_1^2-1)^{1/2}\cos\psi)]^2, \tag{26}$$

in agreement with the result derived by Mel'nikov.[5]

At large z, the rms deviation is $\sigma \ll x_T$, so that in most configurations the value of x is very accurately x_T. We must emphasize, however, that the corresponding meaning should not be extended to the quantity $\gamma_T=e^{x_T}$ (the chain resistance corresponding to this value is usually called the "typical" or "scaling" value[3]), since even if the scattering by the center is weak, in which case we would have $\gamma\sim\gamma_T$ in most configurations, the fluctuations of γ about γ_T are not small (they are on the order of γ_T).

There is the interesting question of which values of γ basically determine the expectation value $\langle\gamma\rangle$. It is easy to see that these values lie outside the range of applicability of Gaussian distribution (25). The use of (25) to calculate $\langle 1/T\rangle$ thus leads to an incorrect result, as has been pointed out previously.[5,6] To find $\langle\gamma\rangle$ we need to evaluate the integral

$$\langle\gamma\rangle=\int_0^\infty dx\, e^x p(x,z).$$

By a method similar to that used in the derivation of (24) it can be shown that the integrand has a sharp peak at

$$x=nz\left(\frac{\partial P_s(\gamma_1)}{\partial s}\right)_{s=1}$$
$$=nz\int_0^{2\pi}\frac{d\psi}{2\pi}(\gamma_1+(\gamma_1^2-1)^{1/2}\cos\psi)\ln(\gamma_1+(\gamma_1^2-1)^{1/2}\cos\psi),$$

and it is this which determines the values of $x=\ln\gamma$ that dominate $\langle\gamma\rangle$. These values are $x=3R_1nz$ at $\gamma_1\approx 1(R_1\ll 1)$ and $x=nz\gamma_1\ln\gamma_1$ at $\gamma_1\gg 1(R_1\approx 1)$.

Finally, we note that the function $w(\gamma, z)$ actually has integrable singularities at $\gamma = 1$, $\gamma = \gamma_1$, and $\gamma = 2\gamma_1^2 - 1$ (§4), because of the contribution of large values of t to integral (16). At large values of z, however, these singularities are not influential.

§4. OTHER MODELS

Certain other models can be examined by the same method. Let us assume that the scattering centers are different and that we are given the probability matrix of the scattering by a single center. In Eq. (5) we should then understand $\tilde{W}$ to be the quantity $W(\tilde{\mathbf{a}}, z)$, averaged over various values of γ_1 and β_1. Repeating the calculations of §2, we find, in the short-wave limit, some equations which differ from (15) and (16) in that the Legendre function in the exponential function is averaged over the values of γ_1. The analog of expression (15), for example, is

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

The symbol $\langle \ldots \rangle_{\gamma_1}$ denotes an average over γ_1. For the expectation values we find

$$\langle 1/T\rangle = {}^1/_2\{\exp[2\langle R_1/T_1\rangle_{\gamma_1} nz] + 1\},$$

$$\langle \ln(1/T)\rangle = nz\langle \ln(1/T_1)\rangle_{\gamma_1},$$

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

We wish to emphasize that for $\langle 1/T\rangle$ and $\langle T\rangle$ the averaging over γ_1 must be carried out in the argument of the exponential function, while for $\langle \ln(1/T)\rangle$ the quantity $\ln(1/T_1)$ must be averaged. At large values of z we have the following analog of Eq. (22):

$$\langle T\rangle = \frac{\pi^{5/2}}{2(\langle f(\gamma_1)\rangle_{\gamma_1} nz)^{3/2}} \exp\{[\langle P_{-1/2}(\gamma_1)\rangle_{\gamma_1} - 1] nz\}.$$

Another model which we will consider here and which has been discussed in the literature[1,4,5,7,8,14] assumes that the number of centers in the chain, N, is given and that the centers are again distributed at random. We then find, instead of Eq. (5),

$$\frac{dW_N(\mathbf{a}, z)}{dz} = \frac{N}{z}[W_{N-1}(\mathbf{a}, z) - W_N(\mathbf{a}, z)], \tag{27}$$

where $W_N(\mathbf{a}, z)$ is the probability density of the value of $\mathbf{a}$ for a chain of length z on which there are N centers. There is a distinction from Eq. (5) in that we have made the natural substitution $n \to N/z$ here. We have also taken into account the circumstance that if the center is in an interval dz then there are $N-1$ centers to its left. We could solve a recurrence system of Eqs. (27); we would naturally expect that its solution in the short-wave limit would not depend on the chain length z, but only on the number of centers in the chain. However, we will take a different approach. The solution found above for the problem with a fluctuating number of centers on the chain, $w(\gamma, z)$, is related to the probability of interest here, w_N, by averaging over a Poisson distribution:

$$w = \sum_N w_N (nz)^N e^{-nz}/N!.$$

If we assume that w_N does not depend on z, then we can find it immediately by expanding $\exp(nz)w(\gamma, z)$ in a Taylor series in z. Using (15) and (16), we find

$$w_N(\gamma) = \int_0^\infty dt P_{-1/2+it}(\gamma)\, t \operatorname{th}(\pi t)\, [P_{-1/2+it}(\gamma_1)]^N, \tag{28}$$

$$[P_s(\gamma_1)]^N = \int_1^\infty d\gamma w_N(\gamma) P_s(\gamma).$$

Direct substitution easily shows that expression (28) satisfies the equation

$$w_N(\gamma) = \int_0^{2\pi} \frac{d\psi}{2\pi} w_{N-1}(\gamma\gamma_1 + (\gamma^2-1)^{1/2}(\gamma_1^2-1)^{1/2}\cos\psi),$$

$$\frac{dw_N(\gamma)}{dz} = 0, \tag{29}$$

which is found from (27) in the short-wave limit under the boundary conditions $J = I_0 = 1$.

The expectation values are

$$\langle\gamma\rangle = 2\langle 1/T\rangle - 1 = \gamma_1^N,$$

$$\langle \ln(1/T)\rangle = N \ln(1/T_1),$$

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

Let us compare these expressions with those found previously for the case of a fluctuating number of centers. It is easy to see that expression (17) for $\langle \ln(1/T)\rangle$ is determined primarily by configurations for which the average number of centers is nz. For $\langle 1/T\rangle$ and $\langle T\rangle$, on the other hand, this is true only in the case of weak scattering ($R_1 \ll 1$) and for chains which are not very long ($nzR_1^2 \ll 1$). In the opposite case, $\langle 1/T\rangle$ and $\langle T\rangle$ are determined by configurations for which the number of centers is respectively greater than and less than the average value.

For $N = 0$ and 1 we find trivial results from (28):

$$w_0(\gamma) = \delta(\gamma - 1), \quad w_1(\gamma) = \delta(\gamma - \gamma_1).$$

It is also a straightforward matter to derive an expression for $w_2(\gamma)$. For this purpose it is convenient to use recurrence relation (29); we find

$$w_2(\gamma) = \pi^{-1}(\gamma-1)^{-1/2}(2\gamma_1^2 - 1 - \gamma)^{-1/2}, \quad 1 < \gamma < 2\gamma_1^2 - 1. \tag{30}$$

Outside the indicated range of γ values, the quantity w_2 is zero. Expression (30) could be derived in a different way—by twice applying transformation (3) directly and by taking an average of $\delta(\gamma - \gamma_2)$ over the relative positions of the centers. Here γ_2 is the value of $2/T - 1$ for the passage by two centers separated by a distance Δz:

$$\gamma_2 = \gamma_1^2 + (\gamma_1^2 - 1)\cos(2k\Delta z + 2\varphi_{\alpha_1}). \tag{31}$$

This quantity lies between the value $\gamma_2 = 1$, which corresponds to the resonant transmission of an electron through the pair of centers, and the value $\gamma_2 = 2\gamma_1^2 - 1$, which corre-

sponds to maximum reflection [Eq. (31) actually describes the transmission of a wave through a Fabry-Perot resonator]. We see that the function w_2 has singularities at these extreme points. A remarkable result is that the expectation value of T/R (a quantity associated with the conductivity) is infinite for a system of two centers. This result shows that the divergence of $\langle T/R \rangle$ in the problem with a fluctuating number of centers results not only from the possible absence of centers from the chain but also from the configurations for which the centers fall in a regular order, allowing a resonant transmission. Lifshitz and Kirpichenkov[1,25] have pointed out the role played by resonant transmission in a disordered system.

We can also derive an expression for the probability $w_3(\gamma)$:

$$w_3(\gamma)=\frac{2}{\pi^2(c-a)^{1/2}(b-1)^{1/2}}K\left(\frac{(b-a)^{1/2}(c-1)^{1/2}}{(c-a)^{1/2}(b-1)^{1/2}}\right), \quad \gamma<\gamma_1, \tag{32}$$

where K is the complete elliptic integral,

$$a=\gamma\gamma_1+(\gamma^2-1)^{1/2}(\gamma_1^2-1)^{1/2}, \quad b=\gamma\gamma_1-(\gamma^2-1)^{1/2}(\gamma_1^2-1)^{1/2},$$

$$c=2\gamma_1^2-1.$$

For $\gamma_1(4\gamma_1^2-3)>\gamma>\gamma_1$ we need to make the replacements $b\rightleftarrows c$ in (32). This expression is valid for $\gamma<\gamma_1(4\gamma_1^2-3)$ (i.e., for $a<c$); at larger values of γ, we have $w_3(\gamma)=0$. At values of its argument near unity the function K diverges logarithmically; i.e., $w_3(\gamma)$ has a singularity at $\gamma=\gamma_1(b=c)$. This situation corresponds to a configuration in which there is a resonant transmission through two of three centers. It can be shown that $w_4(\gamma)$ diverges logarithmically in the limit $\gamma\to1$, while $w_N(\gamma)$ has no singularities at all at $N>4$. In other words, the weight of the resonant configurations is relatively small at $N>4$. Nevertheless, it is the resonant transmission which is responsible for the fact that $w_N(\gamma)$ does not vanish in the limit $\gamma\to1$.

§5. TRANSMISSION IN AN ELECTRIC FIELD

When there is an external electric field, the potential $V(z)$ in Eq. (1) contains a regular component $u(z)$ in addition to the random potential of the impurities. Between centers we then have the following instead of (2):

$$\Psi(z)=k^{-1/2}(z)$$
$$\times\left[a_+\exp\left\{i\int_0^z k(z')\,dz'\right\}+a_-\exp\left\{-i\int_0^z k(z')\,dz'\right\}\right],$$
$$k(z)=[k^2(0)-2mu(z)/\hbar^2]^{1/2},$$

where $k(z)$ is the semiclassical wave vector. At the point $z=0$, we take the potential u to be zero. We assume that k is large enough that the semiclassical description can be used to describe the motion between centers. Furthermore, the electric field is assumed weak enough that it does not affect the scattering. Under the assumptions, the amplitudes $a_\pm$ to the right of the center are again related to those $\tilde a_\pm$ to the left by Eqs. (3), except that in the latter equations we need to make the replacement

$$\exp(2ikz_1)\to\exp\int_0^{z_1}2ik(z')\,dz',$$

and Eqs. (5) and (6) hold as before. Repeating the calculations of §2, we find the following replacement for (16) in the short-wave limit:

$$w(\gamma,z)=\int_0^\infty dtP_{-1/2+it}(\gamma)\,t\,\mathrm{th}(\pi t)\exp\left\{n\int_0^z dz'[P_{-1/2+it}(\gamma_1)-1]\right\}, \tag{33}$$

with a corresponding analog of Eq. (15). The effect of the electric field on the probability $w(\gamma,z)$ and thus on the transmission by the chain is due entirely to the dependence of the scattering matrix on the kinetic energy [the dependence $\gamma_1(k)$], which makes γ_1 a function of the position of the center. The expectation values in this case are

$$\langle 1/T\rangle=1/2\left\{\exp\left[2n\int_0^z dz'(R_1/T_1)\right]+1\right\},$$
$$\langle\ln(1/T)\rangle=n\int_0^z dz'\ln(1/T_1). \tag{34}$$

It is also a simple matter to derive the other expectation values.

We recall that in our formulation of the problem an electron is incident on the chain from the right and leaves at the point $z=0$. It is interesting to examine the asymptotic behavior of the expectation values for long chains and at a fixed energy of the incident electron, $\hbar^2k^2(z)/2m=\epsilon_0$. We assume that the field E is uniform and directed in such a manner that the electron is accelerated toward decreasing z. At the exit the electron acquires a large kinetic energy. We can then use the Born approximation for the scattering of the electron by an individual center, and R_1 approaches zero more rapidly than $1/k^2$. The integrals in Eqs. (34) thus converge as $z\to\infty$. Consequently, an arbitrarily weak field, in the absence of energy loss, leads to a breakdown in the sense that the probability for transmission through a long chain does not depend on its length. Hypothetically, there is the exceptional case of δ-shaped centers, for which we would have $R_1\propto1/k^2$. In this case the integrals diverge logarithmically, and $\langle\ln(1/T)\rangle$, for example, increases logarithmically with increasing length of the chain, and from (33) at large z we find an analog of Eq. (18) for $\langle T\rangle$:

$$\langle T\rangle=4\pi^{5/2}a^{3/2}\left(\ln\frac{\varepsilon_0+eEz}{\varepsilon_0}\right)^{-3/2}\left(\frac{\varepsilon_0}{\varepsilon_0+eEz}\right)^{1/16a}, \tag{35}$$

where $a=eE/4n\epsilon_b$. In deriving this expression we assumed $R_1=\epsilon_b/\epsilon$, where ϵ is the kinetic energy of the electron, and ϵ_b is determined by the strength of the center (the Born approximation for δ-shaped centers).

An expression very similar to (35) was derived by Prigodin[26] for the density-density correlation function in a white-noise potential. The exponent in Prigodin's expression, however, is $(1-a)^2/8a$ instead of the $1/16a$ in (35); Prigodin pointed out[26] that his expression was valid only for $a<1$. Furthermore, he suggested that the field corresponding to $a=1$ is a threshold field and that the electron states become delocalized at $a>1$ (Ref. 26). Our result (35) shows that there is no singularity in the average transmission coefficient at $a=1$.

§6. EXACT RESULTS FOR $\langle\alpha\rangle$, $\langle\beta\rangle$, and $\langle 1/T\rangle$

Equation (5) can be used to find exact expressions for certain expectation values at arbitrary values of k. To illustrate the procedure we will calculate the expectation values of α and β. For this purpose it is sufficient to determine $\langle\Psi_+\rangle$ and $\langle\Psi_-\rangle$ under the boundary conditions $\Psi_+(0)=0$ and $\Psi_-(0)=1$. From (13) we see that we have

$$\langle\alpha\rangle=\langle\Psi_-(z)\rangle^*, \quad \langle\beta\rangle=\langle\Psi_+(z)\rangle$$

in this case. In finding $\langle\alpha\rangle$ and $\langle\beta\rangle$, we might note, we are finding the expectation values of $1/t$ and r/t, since $\alpha=1/t^*$ and $\beta=-r^*/t^*$ (r and t are the reflection and transmission amplitudes of the chain). We multiply Eq. (5) by a_+ and a_- and integrate over $\mathbf{a}$. In the first term on the right side we switch to an integration over the variables $\tilde{\mathbf{a}}$, and we use transformation (3). We then find a system of linear equations with constant coefficients for $\langle\alpha\rangle$ and $\langle\beta\rangle$:

$$\frac{1}{n}\frac{d\langle\beta\rangle}{dz}=(\alpha_1-1+ikn^{-1})\langle\beta\rangle+\beta_1\langle\alpha\rangle^*,$$
$$\frac{1}{n}\frac{d\langle\alpha\rangle^*}{dz}=\beta_1^*\langle\beta\rangle+(\alpha_1^*-1-ikn^{-1})\langle\alpha\rangle^*,$$

which are to be solved under the boundary conditions $\langle\alpha\rangle=1$ and $\langle\beta\rangle=0$ at $z=0$. As a result we find

$$\langle\beta\rangle=\frac{\beta_1}{\nu_1-\nu_2}(e^{\nu_1 nz}-e^{\nu_2 nz}),$$
$$\langle\alpha\rangle^*=\frac{1}{\nu_1-\nu_2}[(\nu_1-\alpha_1+1-ikn^{-1})e^{\nu_1 nz} \tag{36}$$
$$-(\nu_2-\alpha_1+1-ikn^{-1})e^{\nu_2 nz}],$$

where ν_1 and ν_2 are the roots of the characteristic equation

$$\nu_{1,2}=\eta\pm(\eta^2+2\eta-k^2n^{-2}-2kn^{-1}\operatorname{Im}\alpha_1)^{1/2}, \quad \eta=\operatorname{Re}\alpha_1-1.$$

We see that $\langle\alpha\rangle$ and $\langle\beta\rangle$ may either increase or decrease with increasing z. This result should be interpreted as evidence of a competition between two factors: Anderson localization, which should cause $\langle|\alpha|\rangle$ and $\langle|\beta|\rangle$ to increase with increasing z, and the transition of the phases of α and β to a stochastic state. Interestingly, in the simplest case of δ-shaped centers we would have $\eta=0$, and under the condition $k^2n^{-2}+2kn^{-1}\operatorname{Im}\alpha_1>0$ (which holds for attracting centers and also for repelling centers if they are not too strong) these factors cancel out exactly, on the average, so that the roots $\nu_{1,2}=\pm i(k^2n^{-2}+2kn^{-1}\operatorname{Im}\alpha_1)^{1/2}$ are purely imaginary.

In the short-wave limit, expression (36) can be derived directly from Eq. (3). Taking an average of (3) over the position of the center, z_1, we find $\langle a_-\rangle=\alpha_1^*\langle a_-\rangle$. It follows that the expectation value of the amplitude a_1 at the end of a chain containing N centers is $(\alpha_1^*)^N a_{-0}$, so that we have [1] $\langle\alpha\rangle=\alpha_1^N\exp(ikz)$. After taking an average over N with a Poisson distribution, we find from this expression $\langle\alpha\rangle=\exp[\alpha_1-1)nz+ikz]$, which agrees with (36) at large k.

In a similar way, we can evaluate the expectation values of quadratic combinations of α and β. For

$$\langle I\rangle=\langle|\Psi_+|^2\rangle+\langle|\Psi_-|^2\rangle, \quad q=\langle\Psi_+\Psi_-^*\rangle,$$

for example, we have

$$\frac{1}{n}\frac{d\langle I\rangle}{dz}=2|\beta_1|^2\langle I\rangle+\alpha_1\beta_1^*q+\alpha_1^*\beta_1q^*,$$
$$\frac{1}{n}\frac{dq}{dz}=\alpha_1\beta_1\langle I\rangle+(\alpha_1^2-1+2ikn^{-1})q+\beta_1^2q^*.$$

Assuming all the expectation values to be proportional to $\exp(\nu nz)$, we find the characteristic equation

$$\nu^3+4[1-(\operatorname{Re}\alpha_1)^2]\nu^2+4[k^2n^{-2}+2(\operatorname{Re}\alpha_1)(\operatorname{Im}\alpha_1)kn^{-1}+1$$
$$-(\operatorname{Re}\alpha_1)^2]\nu-8|\beta_1|^2k^2n^{-2}=0.$$

In the short-wave limit, the real root of this equation is $\nu_3=2|\beta_1|^2$. The two other roots,

$$\nu_{1,2}=\pm 2ikn^{-1}-|\beta_1|^2+2(\operatorname{Re}\alpha_1)^2-2,$$

have a smaller real part. At large values of z, therefore, the behavior of the expectation values is determined exclusively by the root ν_3.

Under the boundary conditions $I(0)=1$ and $q(0)=0$, the expectation value $\langle I\rangle$ is $2\langle 1/T\rangle-1$. Finally, we give the results for $\langle 1/T\rangle$ for the case of scattering by δ-shaped centers, with $\alpha_1=1+ik_b/k$ and $\beta_1=ik_b/k$ (k_b is a measure of the strength of the potential of the center). Under the condition

$$|k_b+k^2/n|\ll|k_b(k_b/n)^{1/2}|$$

we have

$$2\left\langle\frac{1}{T}\right\rangle-1=\frac{1}{3}e^{z/l}\left[1+\frac{1}{(2kl)^2}\right]+\frac{2}{3}e^{-z/2l}$$
$$\times\left[\cos\left(\frac{\sqrt{3}z}{2l}\right)+\frac{1}{(2kl)^2}\cos\left(\frac{\sqrt{3}z}{2l}-\frac{2\pi}{3}\right)\right],$$

where $1/l=2(k_b{}^2n)^{1/3}$. In the opposite limit,

$$|k_b+k^2/n|\gg|k_b(k_b/n)^{1/2}|,$$

we find

$$2\left\langle\frac{1}{T}\right\rangle-1=\frac{(k_bl-1/2)^2}{k_bl(k_bl-1)}\left\{e^{z/l}-e^{-z/2l}\frac{1}{4(k_bl-1/2)^2}\right.$$
$$\left.\times\left[\cos(\varkappa z)+\frac{1}{(2nl)^{1/2}}\sin(\varkappa z)\right]\right\},$$

where

$$k_bl=1+(k^2/2k_bn), \quad \varkappa=(8k_b^2nl)^{1/2}.$$

Only under the two conditions ($kl\gg 1$ and $|k_b|l\gg 1$) is the following expression[3-7,14] valid:

$$\langle 1/T\rangle=1/2[\exp(z/l)+1].$$

APPENDIX 1

It is not always possible to expand the solution of Eq. (6) in powers of $1/k$. The successive-approximation procedure is non-contradictory and can in principle be pursued to arbitrary order in $1/k$, only under boundary conditions of special form. Specifically, since $W^{(1)}$, $W^{(2)}$,..., are determined unambiguously by the zeroth approximation, $W^{(0)}$, the val-

ues of these functions at $z = 0$ are thus also determined unambiguously by the boundary condition on $W^{(0)}$. The boundary condition for W should thus be

$$W(I,\varphi)_{z=0}=W^{(0)}(I)_{z=0}+\frac{1}{k}W^{(1)}(I,\varphi)_{z=0}+\ldots,$$

where the function $W^{(0)}(I)_{z=0}$ is arbitrary, and all the succeeding terms in the expansion are expressed in terms of it (as it completely determined by the dependence of $W|_{z=0}$ on φ).

Equation (8) could be derived in a different way. If we expand $W(I,\varphi)$ in a Fourier series in φ, we find from (6) a system of coupled equations for the Fourier components. At large values of k, the coupling of the zeroth component with all the others is weak. Ignoring this coupling, we find Eq. (8).

APPENDIX 2

We denote by $w(\gamma,\varphi_\alpha,\varphi_\beta,z)$ the total probability density for transformation matrix (12). We can then obviously write

$$W^{(0)}(I,z)=\int_0^{2\pi}d\varphi_\alpha\int_0^{2\pi}d\varphi_\beta\int_1^{\infty}d\gamma\, w(\gamma,\varphi_\alpha,\varphi_\beta,z)\,g(\gamma,\varphi_\alpha,\varphi_\beta,I),$$

where $g(\gamma,\varphi_\alpha,\varphi_\beta,I)$ is the probability that, for the given values of γ,φ_α, and φ_β, the quantity $|\Psi_+|^2+|\Psi_-|^2$ has the value I:

$$g(\gamma,\varphi_\alpha,\varphi_\beta,I)=\int_0^{2\pi}\frac{d\varphi_0'}{2\pi}\int_0^{\infty}dI_0'W^{(0)}(I_0',0)\,\delta[I-I(\gamma,\varphi_\alpha,\varphi_\beta,\varphi_0',I_0')].$$

Here $I(\gamma,\varphi_\alpha,\varphi_\beta,\varphi_{0'},I_0')$ is determined by (7) with $\varphi_1'\beta_1\to\alpha,\beta$ and with $\tilde{I}\to I_0'$, $\tilde{\varphi}\to\varphi_0'$. We see that g is independent of φ_α and φ_β. Assuming $W^{(0)}(I_0',O)=\delta(I_0'-I_0)$, we find Eq. (14).

[1)] This equation can be written in the form $\langle 1/t\rangle=(1/t_1)^N\exp(-ikz)$. In the short-wave limit the reciprocal of the transmission coefficient is thus multiplicative on the average. However, the same cannot be said of the transmission coefficient, as Thouless has done.[27] In taking an average of (3) over the phase we find information only on $\langle 1/t\rangle$—not on $\langle t\rangle$. The reason is that the averaging in (3) presupposes that the incoming and outgoing fluxes at the beginning of the chain are specified, rather than the fluxes entering the chain at its beginning and end (which are given in Ref. 27).

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