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Transparency of a one-dimensional system with an arbitrary degree of disorder subjected to an electric field

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The effect of an applied electric field on the propagation of an electron in a chain of random scatterers with delta-function potentials is studied. Numerical modeling is used to obtain the dependences of the logarithm of the transmission coefficient (averaged over an ensemble) on the length of a chain, degree of disorder, electron energy, and electric field intensity. The deviations of such dependences from the analytic expressions obtained in the short-wavelength limit are discussed. The results of calculations for "vertical" and "horizontal" types of disorder in the distribution of scatterers are compared. The distribution of the transmission coefficient of a one-dimensional system subjected to an electric field is investigated.

1. The propagation of an electron in a one-dimensional electron system has been studied both analytically[1-5] and numerically.[6-9] An interest in this problem was stimulated, in particular, by the fact that the behavior of the transmission coefficient may be used to investigate changes in one-electron states due to changing parameters of the system and due to external fields. It is assumed in the calculations of the transmission coefficient of a finite chain that a segment with a random static potential is connected to two semiinfinite "perfectly" conducting contacts in which electrons move freely. The proportion of electrons which transmitted from one contact to the other across the "imperfect" region determines the transparency of the system.

In view of the localization of electron states in a one-dimensional system,[1,2] in the absence of an electric field the transmission coefficient decreases exponentially with increasing chain length L. For an ensemble of disordered chains, the transmission coefficient T fluctuates from sample to sample. The distribution function of the values of T is logarithmically normal[3,4] about its geometric mean

$$\tilde{T} = e^{\langle \ln T\rangle} = e^{-L/\xi}, \qquad (1)$$

where ξ is half the localization length of the wave function of a one-electron state. In what follows, the averaging over an ensemble of chains (denoted by the angular brackets) will always refer to ln T.

In an applied electric field, the variation of the transparency with the length of the system depends on the form of the random potential. For a low concentration n of scatterers, we can assume that the electron is scattered at each center independently of the other centers. In this case, the effect of the electric field on the transparency is completely determined by the dependence of the elastic scattering cross section of a center $R_1 = 1 - T_1$ on the electron energy E, which is a function of the position of the center x. In the short-wavelength approximation $k\ell \gg 1$ [where k is the electron momentum and $\ell = (nR_1)^{-1}$ is the mean free path], it was shown in Ref. 4 that

$$\langle \ln T\rangle = n\int_0^L dx \ln[T_1(x)]. \qquad (2)$$

Prigodin[5] considered a chain of centers with delta-function potentials in a homogeneous electric field of intensity F and obtained the following expression in the approximation of a white-noise potential:

$$-\frac{\xi}{L}\langle \ln T\rangle = \frac{\ln(1+FL/E)}{FL/E} \equiv \Phi\left(\frac{FL}{E}\right), \qquad (3)$$

where the electronic charge is unity. It is well known that the transmission coefficient for a potential $V(x) = V_1\delta(x)$ has the form $T_1 = (1 + V_1^2/4E)^{-1}$. We can obtain Eq. (3) from Eq. (2) assuming that the scattering is weak, which is equivalent (for delta-function centers) to the condition of validity of the Born approximation $R_1 \approx V_1^2/4E \ll 1$. It is an important property of a chain of delta-function scatterers that the transmission probability depends on L for arbitrarily long chains, in contrast to potentials for which R_1 tends to zero faster than E^{-1} (see Refs. 4 and 7).

It is of interest to calculate the transmission coefficient without the assumption of weak scattering and also outside the limits of the short-wavelength approximation, which can be accomplished on a computer. The value of T is usually computed using the transfer matrix method.[6-9] In this case, there are two ways of modeling a chain: in the form of delta-function potentials with different amplitudes distributed periodically (vertical disorder)[6-8] or by identical delta-function centers distributed randomly over the chain (horizontal disorder).[9] The dependence of <ln T > on the electric field was studied in Refs. 6 and 7. It was found that in the case of weak scattering the modeling results are in good agreement with Eq. (3).

We shall report the results of numerical calculations of the transmission of an electron by a one-dimensional disordered system of delta-function potentials. In Sec. 2, we shall explain the computational method developed in Refs. 10 and 11. The computed results for an arbitrary degree of disorder, obtained for both zero and nonzero electric fields, are discussed in Sec. 3. In this section, we shall also consider the distribution function of T over various realizations of the random potential in an applied electric field.

2. We shall consider a model in which delta function potentials of arbitrary amplitudes V_j are located at arbitrary points x_j of a chain:

$$V'(x) = \sum_{j=1}^{N} V_j\delta(x - x_j), \quad x_j > x_{j-1}. \qquad (4)$$

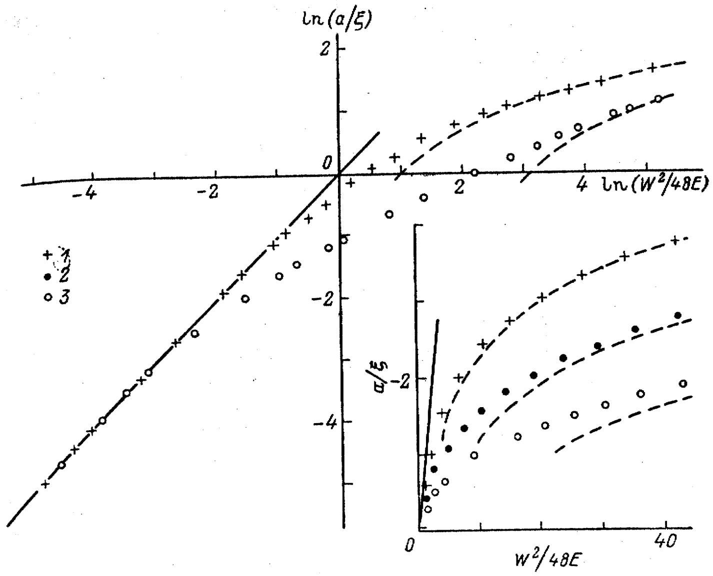

FIG. 1. Dependence of the reciprocal localization radius a/ξ = $\langle \ln T\rangle /N$ on $W^2/48E$ for a problem with a vertical disorder and for electron energies E = 5 (1), 7.13 (2), and 8.21 (3). The solid line represents the weak-scattering asymptote [Eq. (13)] and the broken curve corresponds to the strong-localization limit [Eq. (15)].

We shall assume that there is also a regular potential U(x) such as an applied electric field, a periodic potential, etc. The retarded Green function G(x, x') of an electron traveling in the total potential satisfies the Schrödinger equation

$$[-d^2/dx^2 + U(x) + V(x) - k^2]\, G(x, x') = -\delta(x - x'), \qquad (5)$$

where $k = \sqrt{E + i\varepsilon}$ ($\varepsilon \to 0$); $\hbar = 2m_0 = 1$; and m_0 is the free-electron mass. It was shown in Ref. 11 that the electron Green function satisfying Eq. (5) is related to the bare Green function $G_0(x, x')$ in an external field U(x) by

$$G(x, x') = G_0(x, x') - r_1 \frac{G_0(x, x_1)\, G_0(x_1, x')}{G_0(x_1\, x_1)}, \quad x;\, x' \leqslant x_1, \qquad (6)$$

where $G_0(x, x')$ satisfies the equation

$$[-d^2/dx^2 + U(x) - k^2]\, G_0(x, x') = -\delta(x - x') \qquad (7)$$

and r_1 is the reflection coefficient for the amplitude. The transmission coefficient of a chain of potentials (4) is then given by [10,11]

$$T = 1 - |r_1|^2 = |D_N|^{-2}, \qquad (8)$$

where D_N is the determinant of the matrix

$$D_{jq} = \delta_{jq} + V_j G_0(x_j, x_j)\, z_{jq}^{1/2}. \qquad (9)$$

Here, z_{jq} is the phase an electron acquires during its motion in the field U(x) between the scatterers j and q:

$$z_{jq} = \exp\left[-\int_{\min(j,q)}^{\max(j,q)} \frac{dx}{G_0(x, x)}\right] = z_{qj}. \qquad (10)$$

For $U(x) \equiv 0$, the function $G_0 = i/2k$ is the Green function of a free electron and we have $z_{jq} = \exp(2ik|x_j - x_q|)$.

The determinant D_N of the matrix (9) satisfies the recurrence equations

$$D_N = A_N D_{N-1} - B_N D_{N-2}, \qquad (11)$$

where

$$B_N = z_{N,N-1} \frac{V_N G_0(x_N, x_N)}{V_{N-1} G_0(x_{N-1}, x_{N-1})}, \qquad (12a)$$

$$A_N = 1 + B_N + V_N G_0(x_N, x_N)(1 - z_{N,N-1}), \quad N > 1, \qquad (12b)$$

$$A_1 = 1 + V_1 G_0(x_1, x_1); \quad D_0 = 1, \quad D_{-1} = 0, \qquad (12c)$$

and $D_{N-1(N-2)}$ is the determinant with the N-th [and (N − 1)-th] column and row removed. Making use of the recurrence relationships (11) and (12), we can obtain from Eq. (9) the dependence of $\langle \ln T\rangle$ on the chain length and on the energy of an incident electron for an arbitrary degree of vertical and horizontal disorder of a chain of delta-function potentials. In an applied field, $G_0(x, x)$ in Eqs. (9) and (10) represents the Green function of an electron moving in an electric field.

In our view, it is better to calculate the transmission coefficient from Eqs. (8)-(12) rather than by the method used in Refs. 6-9. We shall first consider the effect of a horizontal disorder on the behavior of $\langle \ln T\rangle$ for both F = 0 and

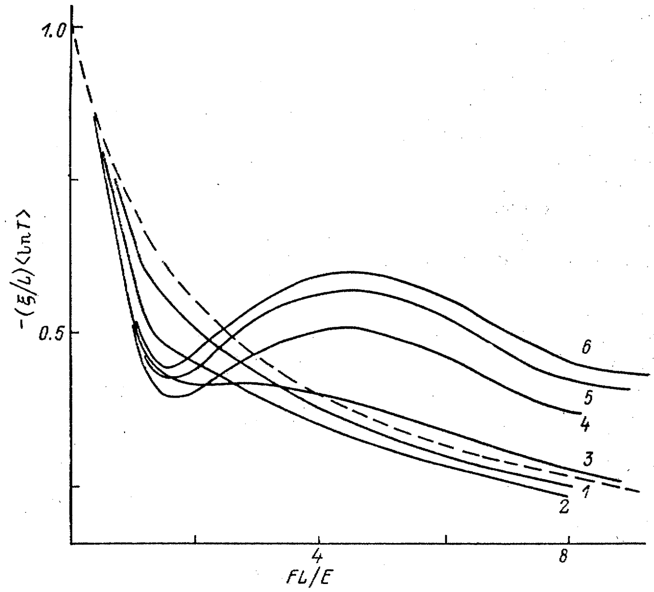

FIG. 2. Dependence of $-(\xi/L)\langle \ln T\rangle$ on the electric field parameter FL/E for an energy E = 5 and a range of values of the vertical disorder W: 1) 4; 2) 7; 3) 14; 4) 50; 5) 80; 6) 100. The broken curve is the field dependence in the weak-scattering limit [Eq. (3)].

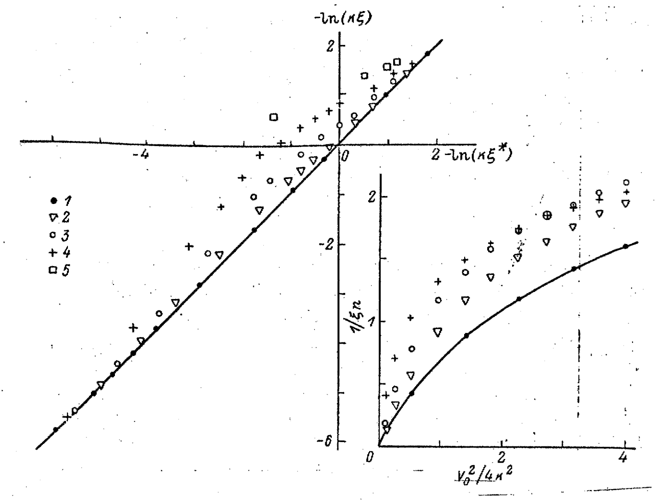

FIG. 3. Dependence of the scattering parameter $k\xi$ on its value in the short-wavelength approximation $k\xi^*$ [Eq. (16)] for a problem with a horizontal disorder and for a range of values of the concentration of delta-function centers n/k: 1) 0.01; 2) 0.45; 3) 1; 4) 2; 5) 4. The inset shows the dependence of the reciprocal localization radius $(\xi n)^{-1}$ on the disorder parameter $V^2/4k^2$. The solid curve is the short-wavelength limit described by Eq. (16).

in an applied field [in a homogeneous field, k in Eqs. (9) and (10) should be replaced by $\sqrt{E + Fx_j}$]. Calculations can then be carried out for an arbitrary magnitude and position dependence of the applied field, provided the electron Green function in such a field is known. Moreover, this method of calculating T can be generalized, for example, to scattering potentials in the form of rectangular barriers.

3. We first computed the transmission coefficient for a chain with a vertical disorder where the amplitudes of the delta-function potentials V_j were distributed uniformly in an interval [$-W/2$, $W/2$]. The transparency of such chain in the ensemble was calculated using the recurrence equations (11) and (12) for a range of energies E of an incident electrons and different degrees of disorder W. The length of a chain with a period a was as much as $N = L/a \approx 20{,}000$ sites. Averaging was carried out over ∿3000 realizations of the random potential. It can be seen from Eq. (1) that we can use the result that $\langle \ln T \rangle$ is proportional to the chain length L to determine the localization length ξ. In the weak scattering limit $R_1 \to 1$, the localization length is given by[6,7]

$$a/\xi = \langle V_j^2 \rangle / 4E = W^2/48E, \tag{13}$$

provided the energy does not correspond to the resonance points $ka = m\pi$ (the scattering amplitude is in this case imaginary $iV_1/2k$ and, therefore, there are no singularities at the center of the zone $ka = m\pi/2$; see Ref. 12). In the other limiting case of strong scattering $\xi \ll a$, it was found in in Ref. 10 that

$$\frac{a}{\xi} = \left\langle \ln \frac{V_j^2 \sin^2 ka}{E} \right\rangle. \tag{14}$$

For uniformly distributed amplitudes V_j, we can easily evaluate the average logarithm and, therefore, the localization radius using Eq. (14):

$$\frac{a}{\xi} = \ln\left[\frac{W^2 \sin^2 ka}{4E}\right] - 2. \tag{15}$$

Figure 1 shows the dependence of the reciprocal localization radius $a/\xi = \langle \ln T \rangle / N$ on $W^2/48E$ for momenta in the first Brillouin zone $ka < \pi$. It can be seen that in the two scattering limits the calculated values of a/ξ agree well with the asymptotic equations (13) and (14). We note that the short-wavelength approximation $k\ell = kaR^{-1} \sim R^{-1} \gg 1$ energies in the first zone is violated when the scattering ceases to be weak. Moreover, as the energy approaches the edge of the zone, the disorder required for the validity of the strong-scattering approximation becomes greater.

In an applied electric field $F > 0$, the ensemble average $\langle \ln T \rangle$ increases with increasing L more slowly than for $F = 0$, which corresponds to the transition from an exponential localization to a localization "power law" described by Eq. (3). Since the static field enters the expression for the transmission coefficient T only in the combination Fx_j/E, we selected a fixed value of the field $F = 2\cdot 10^{-3}$ and varied only the length of the system. For convenience, we used the atomic units, i.e., the lengths were measured in units of the Bohr radius $a_B = 5.29\cdot 10^{-11}$ m, the energy in rydbergs Ry = 13.6 eV, and the electric field strength in units of $Ry/ea_B = 2.57\cdot 10^9$ V·cm^{-1}.

Figure 2 shows the dependences of the ratio $(\xi/L)\langle \ln T \rangle$ on the parameter FL/E for a given energy E = 5 and for different magnitudes of the scatter of the amplitudes W. It can be seen that, in the short-wavelength region $W \lesssim 4$ ($\xi/a \gtrsim 15$, $k\xi \gtrsim 33.5$), the transmission coefficient $\langle \ln T \rangle$ is practically identical with that described by Eq. (3). A similar result was obtained in Ref. 6 where the potential applied to a chain was not linear Fx, but a "step-like" function in the form of a sum of θ functions

$$U(x) = F \sum_{j=1}^{N} \theta(x - ja).$$

When the degree of disorder is increased $W = 7$, $k\xi \sim 10$, the dependence gradually deviates from that described by Eq. (3) as the short-wavelength limit ceases to be applicable. The deviation reaches its maximum in the vicinity of $FL/E \sim 1$ which is, clearly, due to the periodicity in the impurity distribution. However, for large $FL/E \gtrsim 5$, the asymptotic behavior described by Eq. (3) is again satisfied because an electron acquires high enough energies over large distances so that $k\ell \gg 1$. In the case of strong scattering $W \gtrsim 50$ ($k\xi \lesssim 0.2$) when $\xi \lesssim a$, the behavior of $\langle \ln T \rangle$ becomes nonmonotonic and very different from that in the short-wavelength limit [Eq. (3)].

To reveal the causes of the nonmonotonic dependence of the transmission coefficient on the field for a vertical disorder, we also carried out calculations for a chain with a horizontal disorder of the delta-function potentials. In this case, the amplitudes of all the delta-function potentials are constant equal to $V_0 > 0$. Moreover, the number of scatterers N and their concentration n are fixed.

The distribution of the centers in a chain is determined as follows. The first impurity is placed at the origin $x_1 = 0$. The position of the next impurity $x_2 > x_1$ is chosen in accordance with the Poisson distribution $P \propto \exp[-n(x_2 - x_1)]$, etc. This procedure is carried out $N - 1$ times. The length of a system in the ensemble of such

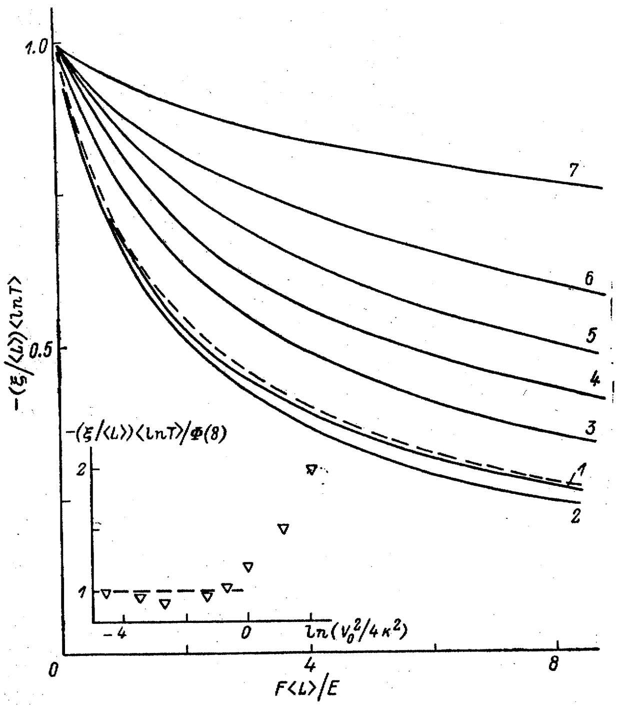

FIG. 4. Dependence of $(-\xi/\langle L\rangle)\langle \ln T\rangle$ on $F\langle L\rangle/E$ for a chain with a horizontal disorder, a concentration $n/k = 0.45$, and an energy $E = 5$ for a range of amplitudes V_0: 1) 0.2; 2) 1.2; 3) 4.4; 4) 8; 5) 13; 6) 20; 7) 80. The broken curves represent the dependence described by Eq. (3). The inset shows the dependence of $(-\xi/\Phi(8))$ $(\langle \ln T\rangle/\langle L\rangle)$ on the disorder parameter $V_0^2/4k^2$ for a single point $FL/E = 8$.

chains is not fixed and its average value is equal to $\langle L\rangle = N/n$.

It follows from the recurrence equations (11) and (12) that the parameters of a horizontal disorder in the absence of an external field $U(x) = 0$ are the average number of impurities per electron wavelength n/k and the Born scattering cross section of a single delta-function center $V_0^2/4k^2$. It was shown in Ref. 4 that in the short-wavelength limit the localization radius ξ for such a chain is given by

$$1/\xi n = -\langle \ln T\rangle/N = \ln(1 + V_0^2/4k^2) \equiv 1/\xi^* n. \tag{16}$$

It is obvious that at low concentrations $n \ll k$ the short-wavelength approximation is valid for arbitrary scattering: $k\ell \sim k/(nR_1) \gg 1$ (see Ref. 9). For $n \gtrsim k$, the expression (16) holds provided the scattering is weak. For increasing disorder, the calculated value of $(k\xi)^{-1}$ is greater than the value $(k\xi^*)^{-1}$ obtained from Eq. (16) (see Fig. 3). Equations (11) and (12) can be used to obtain an asymptotic expression for the reciprocal localization radius when $V \gg k$ which is independent of the energy $(\xi n)^{-1} \propto \ln(V^2/n^2)$.

In an applied static electric field and at low concentrations the transmission coefficient can be evaluated by integrating Eq. (2) after the substitution $T_1 = [1 + V_1^2/4\,(E + Fx)]^{-1}$. Figure 4 shows the dependences of $(\xi/\langle L\rangle)\langle \ln T\rangle$ on $F\langle L\rangle/E$ for a horizontal disorder with a concentration of the delta-function centers $n = 1.0$ and an incident electron energy $E = 5$ for a range of values of the disorder parameter $V_0/4k^2$. It can be seen that the deviation from the weak-scattering limit described by Eq. (3) increases with increasing disorder. Since the spectrum contains no singular points, the transmission coefficient is monotonic, in contrast to a chain with a vertical disorder (Fig. 2).

It is of interest to consider the distribution function of the transmission coefficient of a one-dimensional system of delta-function potentials.[13] It is well known that the variance σ^2 of the logarithm of the transmission coefficient under weak-scattering conditions is twice the value of its mean[3,9]

$$\sigma^2 = \langle(\ln T - \langle \ln T\rangle)^2\rangle = -2\langle \ln T\rangle = 2L/\xi, \tag{17}$$

but the ratio in the region of strong scattering decreases with increasing disorder. In fact, it can be seen from Eqs. (11) and (12) that in the $\xi \ll a$ case the variance for a problem with vertical disorder of the amplitudes of delta-function potentials distributed uniformly within a finite interval of width W is equal to $\sigma^2 = 4N$ for $F = 0$ and, therefore,

$$\frac{2\langle \ln T\rangle}{\sigma^2} = \ln\left(\frac{W}{2}\frac{|\sin ka|}{k}\right) - 1. \tag{18}$$

Figure 5 shows the dependences of $2\langle \ln T\rangle/\sigma^2$ on the variance in the absence of an external field (1) and for $F = 2\cdot 10^{-3}$ (2). The transition from the asymptotic behavior (17) to the dependence (18) can be clearly seen for $F = 0$. The application of an electric field for strong scattering $\xi \lesssim a$ leads to a deviation of σ^2 from the dependence (18).

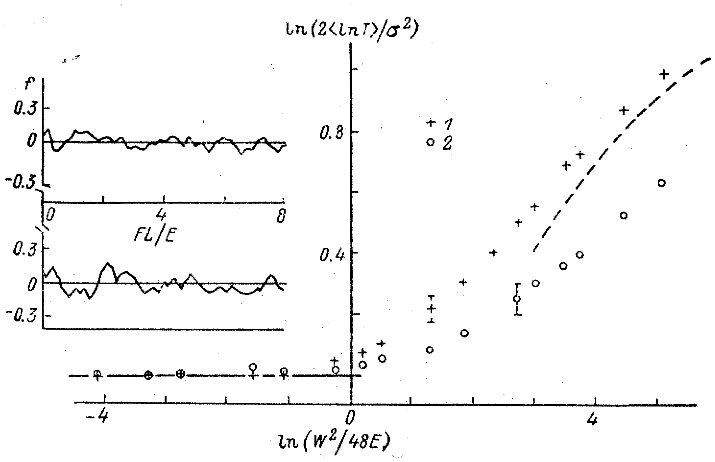

FIG. 5. Dependence of the ratio of the mean to the variance $2\langle \ln T\rangle/\sigma^2$ on the parameter $W^2/48E$. The solid curve corresponds to Eq. (17) and the broken curve to Eq. (18).

We verified that the distribution of the logarithms of the transmission probability T is Gaussian by checking that the odd central moments, beginning from the third, vanish and that the equality

$$M_p = \langle(\ln T - \langle \ln T\rangle)^p\rangle = 1 \cdot 3 \cdot \ldots \cdot (p-1)\,\sigma^p \qquad (19)$$

is satisfied for the even p-th moments, where p = 2-10. The field dependences of the quantities characterizing the distribution function, i.e., of the asymmetry f and excess g

$$f = M_3/\sigma^3, \quad g = M_4/\sigma^4 - 3 \qquad (20)$$

are shown in the inset in Fig. 5 for a chain with a vertical disorder, $W^2 = 12$ and $F = 2\cdot 10^{-3}$. For arbitrary scattering strengths, the computed values of the asymmetry f and excess g are mainly concentrated around zero, which indicates that the logarithmically normal distribution law of T about its typical value $\tilde{T}$ [Eq. (1)] is conserved even in an electric field. For comparison, we should mention that the excess of a uniform distribution is equal to −1, 2.

4. It follows that there are essentially two regimes for one-dimensional disordered systems of delta-function potentials, i.e., the weak-scattering limit $\xi \gg a$ when the Born approximation is applicable and the strong-scattering limit $\xi \ll a$; the intermediate case can be investigated only numerically. In an applied electric field, the transparency of a system with strong scattering and high concentration of centers has a different field dependence than that obtained in the short-wavelength approximation. The quantity ln T has a Gaussian distribution near its average value both in the absence of a field and in an applied field. We note that the same distribution law applies also to the relaxation times of the electron density in a one-dimensional insulator,[14] which is also related to a normal distribution of the reciprocal localizations radii $(a/\xi)(E/FL)\ln(1 + FL/E)$. There is clearly a direct relationship between the transmission coefficient and the lifetime of a wave packet in a one-dimensional disordered sample of finite length.

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Characteristics of point-contact spectra of heterojunctions between simple metals

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An experimental investigation was made of point-contact spectra of K–Na, K–Li, and Au–Al heterojunctions. The spectra of alkali metals were in reasonable qualitative agreement with the available theoretical calculations allowing for the refraction and reflection of electrons at the interface between two metals. In the case of Au–Al heterojunctions there were two spectra attributed to the characteristics of the passage of electrons across clean and dirty contacts.

Point-contact spectroscopy has become an effective method for the investigation of the electron–phonon interaction (EPI) in metals.[1] This method is based on a study of small deviations from Ohm's law describing the conductance of point contacts formed, for example, when a sharp point is in contact with a flat surface of the same material. A theoretical analysis[2] of the conductance of contacts of size less than the mean free path of electrons has shown that the second derivative d^2V/dI^2 of the current-voltage characteristic is proportional to the EPI function $G(\varepsilon)$. This function can be represented by a product of the density of the phonon states $F(\varepsilon)$ and another function $\alpha^2(\varepsilon)$ which depends less strongly on energy and allows for the "force" of the interaction of electrons

