

Boundary conditions, phase distribution and hidden symmetry in 1D localization

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One-dimensional disordered systems with a random potential of a small amplitude and short-range correlations are considered near the initial band edge. The evolution equation is obtained for the mutual distribution $P(\rho, \psi)$ of the Landauer resistance ρ and the phase variable $\psi = \theta - \varphi$ (θ and φ are phases entering the transfer matrix), when the system length L is increased. In large L limit, the equation allows separation of variables, which provides the existence of the stationary distribution $P(\psi)$, determinative the coefficients in the evolution equation for $P(\rho)$. The limiting distribution $P(\rho)$ for $L \rightarrow \infty$ is log-normal and does not depend on boundary conditions. It is determined by the 'internal' phase distribution, whose form is established in the whole energy range including the forbidden band of the initial crystal. The random phase approximation is valid in the deep of the allowed band, but strongly violated for other energies. The phase ψ appears to be the 'bad' variable, while the 'correct' variable is $\omega = -\text{ctg } \psi/2$. The form of the stationary distribution $P(\omega)$ is determined by the internal properties of the system and is independent of boundary conditions. Variation of the boundary conditions leads to the scale transformation $\omega \rightarrow s\omega$ and translations $\omega \rightarrow \omega + \omega_0$ and $\psi \rightarrow \psi + \psi_0$, which determinates the 'external' phase distribution, entering the evolution equations. Independence of the limiting distribution $P(\rho)$ on the external distribution $P(\psi)$ allows to say on the hidden symmetry, whose character is revealed below.

1. Introduction

For description of 1D disordered systems it is convenient to use the transfer matrix T , relating the amplitudes of plane waves on the left ($Ae^{ikx} + Be^{-ikx}$) and on the right ($Ce^{ikx} + De^{-ikx}$) of a scatterer,

$$\begin{pmatrix} A \\ B \end{pmatrix} = T \begin{pmatrix} C \\ D \end{pmatrix}. \quad (1)$$

In the presence time-reversal invariance, the matrix T can be parametrized in the form [1]

$$T = \begin{pmatrix} 1/t & -r/t \\ -r^*/t^* & 1/t^* \end{pmatrix} = \begin{pmatrix} \sqrt{\rho+1} e^{i\varphi} & \sqrt{\rho} e^{i\theta} \\ \sqrt{\rho} e^{-i\theta} & \sqrt{\rho+1} e^{-i\varphi} \end{pmatrix}, \quad (2)$$

where t and r are the amplitudes of transmission and reflection, while $\rho = |r/t|^2$ is the dimensionless Landauer resistance [2]. For the successive arrangement of scatterers their transfer matrices are multiplied. For a weak scatterer its transfer matrix T is close to the unit one, which allows to derive the differential evolution equations for its parameters, and in particular for the Landauer resistance ρ .

In the random phase approximation (when distributions of φ and θ are considered as uniform) such equation for the distribution $P(\rho)$ has a form [3]–[8]

$$\frac{\partial P(\rho)}{\partial L} = D \frac{\partial}{\partial \rho} \left[\rho(1+\rho) \frac{\partial P(\rho)}{\partial \rho} \right] \quad (3)$$

(where D is of the order of the inverse mean free path) and describes evolution of the initial distribution $P_0(\rho) = \delta(\rho)$ at zero length L to the log-normal distribution in the large L limit.

As shown in the paper [9], the distributions of phases φ and θ ceased be uniform, if semi-transparent boundaries are introduced between the disordered system and the ideal leads connected to it, even if they were uniform in the initial system. In the latter case, the more general equation arises

$$\frac{\partial P(\rho)}{\partial L} = D \frac{\partial}{\partial \rho} \left[-\gamma(1+2\rho)P(\rho) + \rho(1+\rho) \frac{\partial P(\rho)}{\partial \rho} \right], \quad (4)$$

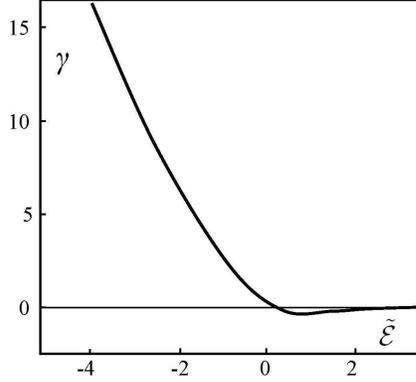


Figure 1: Parameter γ in equation (4), as a function of the reduced energy $\tilde{\mathcal{E}} = \mathcal{E}/W^{4/3}$. Parameter γ is close to zero in the deep of the allowed band, in correspondence with the random phase approximation.

which reduces to (3) in the random phase approximation. The latter approximation is working sufficiently good in the deep of the allowed band for the "natural" ideal leads (made from the same material as a disordered system, but without impurities), as it is usually accepted in the theoretical papers (see references in [10, 11, 12]); the fluctuation states in the forbidden band are considered infrequently [13, 14, 15] and only on the level of the wave functions. To study the evolution of $P(\rho)$ for the arbitrary Fermi level position (including the forbidden band of the initial crystal), one should explicitly introduce the foreign ideal leads made from the good metal¹, which automatically brings to the nontrivial boundary conditions. As a result, the still more general equation arises [16],

$$\frac{\partial P(\rho)}{\partial L} = D \frac{\partial}{\partial \rho} \left[-\gamma_1(1+2\rho)P(\rho) - 2\gamma_2\sqrt{\rho(1+\rho)}P(\rho) + \rho(1+\rho) \frac{\partial P(\rho)}{\partial \rho} \right], \quad (5)$$

whose coefficients are determined by the stationary phase distribution (see Eq. 34 below) in the large L limit. Equation (5) reduces to (4) with $\gamma = \gamma_1 + \gamma_2$ in the region of large L , when typical values of ρ are large. Fig.1 illustrates the dependence of the parameter γ on the quantity $\tilde{\mathcal{E}} = \mathcal{E}/W^{4/3}$, where \mathcal{E} is the Fermi energy counted from the lower edge of the initial band, and W is the amplitude of a random potential; all energies are measured in the units of the hopping integral for the 1D Anderson model (see below Eq.13). Parameter γ is close to zero in the deep of the allowed band in correspondence with the random phase approximation, while violation of the latter in the whole energy interval is surely not a small effect. This violation occurs due to internal reasons and incorporation of semi-transparent boundaries is not necessary for it. Moreover, the limiting log-normal distribution $P(\rho)$ in the large L region,

$$P(\rho) = \frac{1}{\rho\sqrt{4\pi DL}} \exp \left\{ -\frac{[\ln \rho - vL]^2}{4DL} \right\}, \quad (6)$$

where $v = (2\gamma+1)D$, is determined by the internal properties of the disordered system (Fig.2) and does not depend on the boundary conditions [16].

The dependence of γ on $\tilde{\mathcal{E}}$ (Fig.1) clearly demonstrates violation of the random phase approximation, but was obtained in [16] by analysis of the moments of the transfer matrix elements (see below), in which the problem of phase distribution was completely avoided. Clarification of a situation with phase distribution is necessary for the logical completeness of theory of 1D localization and is the main purpose of the present

¹It is easy to understand, that for energies in the forbidden band of the initial crystal the 'natural' ideal leads will be non-conducting, while the fluctuational states are present in the disordered system under consideration.

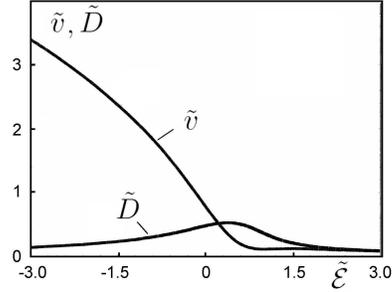


Figure 2: Parameters $\tilde{v} = v/W^{2/3}$ and $\tilde{D} = D/W^{2/3}$ versus the reduced energy $\tilde{\mathcal{E}} = \mathcal{E}/W^{4/3}$. The equality $v = D$, followed from the random phase approximation, is realized only in the deep of the allowed band.

paper. It is closely related with elucidation of the role of boundary conditions and needs resolution of visible contradictions.

Indeed, in the papers [9, 16] we have made two statements, which look hardly compatible. On one hand, variation of the boundary conditions essentially affects the distribution of phases, which generally changes the parameters of the evolution equations (3–5) and even its structure. On the other hand, these changes have no influence on the form of the limiting distribution (6) in the large L region. Validity of these two statements means that the system obeys a hidden symmetry, i.e. invariance of the physical quantities respective to a certain class of transformations. From the theoretical viewpoint, revelation of the hidden symmetry is of the evident interest, indicating the possibility of essential simplifications. From the practical point, one cannot differ the real physical effects from the fictive ones, if the nature of hidden invariance is not clarified. Revelation of this invariance appears to be very nontrivial and demands derivation of the evolution equations in the most general form.

Let explain the origin of two indicated statements. Under a change of the boundary conditions, the transfer matrix T transforms to $\tilde{T} = T_l T T_r$, where T_l and T_r are the edge matrices, related amplitudes of waves on the left and on the right of the corresponding interface. Thereby, the change of the boundary conditions leads to the linear transformation of the transfer matrix elements. The linear transformation does not affect the growth exponents for the second and fourth moments of the matrix elements, which can be found for a given matrix T and hence are determined by internal properties of the system. Knowledge of these two exponents allows to establish the 'diffusion constant' D and the 'drift velocity' v in the limiting distribution (6) (Fig.2), which consequently does not depend on the boundary conditions [16]; after that there is no problem to obtain the behavior of the parameter γ (Fig.1).

Influence of boundary conditions on the distribution of phases can be easily demonstrated by introducing the point scatterers on the system boundaries, when

$$\tilde{T} = T_l T T_r, \quad T_l = T_r = \begin{pmatrix} 1 - i\chi & -i\chi \\ i\chi & 1 + i\chi \end{pmatrix}. \quad (7)$$

Accepting the parametrization (1) for \tilde{T} , one has in the main order for large χ

$$\begin{aligned} \sqrt{1 + \rho} e^{i\varphi} &= -\chi^2 T', & \sqrt{\rho} e^{i\theta} &= -\chi^2 T', \\ \sqrt{\rho} e^{-i\theta} &= \chi^2 T', & \sqrt{1 + \rho} e^{-i\varphi} &= \chi^2 T', \end{aligned} \quad (8)$$

where $T' = T_{11} - T_{12} + T_{21} - T_{22}$ and T_{ij} are the elements of the T -matrix. For large χ we have $\rho \sim \chi^4$ and $1 + \rho \approx \rho$, so it is easy to see that

$$\varphi = \pm\pi/2, \quad \theta = \pm\pi/2 \quad \text{for } \chi \rightarrow \infty. \quad (9)$$

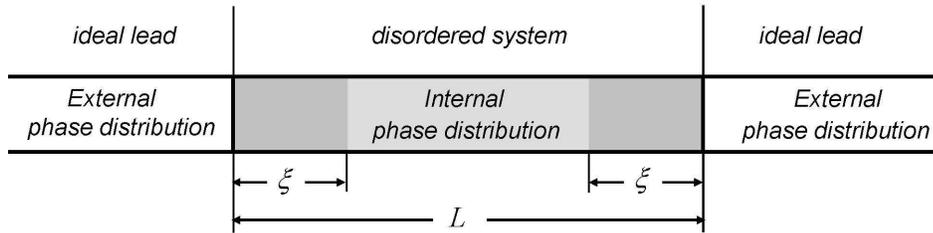


Figure 3: External and internal phase distribution.

Thereby, for large χ the phase variables φ and θ are localized near values $\pm\pi/2$ independently of their distributions in the initial system.

From the physical viewpoint, the situation looks as follows (Fig.3). In the deep of the sufficiently long disordered system, a certain 'internal' phase distribution is realized, which does not depend on the boundary conditions. If the system is considered from the side of the ideal leads, one observes the 'external' phase distribution, which is determined by the boundary conditions; namely these phases are entered in the transfer matrix. Influence of interfaces extends till the length scale of the order of the localization length ξ , which determined the transient region, where the internal phase distribution continuously transforms to the external one. In the large L limit, the distribution $P(\rho)$ is determined by the internal phase distribution, which provides its independence on the boundary conditions. However, the evolution equations contain namely the external phase distribution², and there is a problem to understand, why it does not affect the limiting distribution $P(\rho)$. The second question, related with the first one, is as follows: how can we find the internal phase distribution, if it is not entering the evolution equations?

Let discuss the character of invariance mentioned above. The change of the matrix T with a system length L is determined by relation

$$T_{L+\Delta L} = T_L T_{\Delta L}, \quad (10)$$

where the matrix $T_{\Delta L}$ is close to the unit one; it allows to derive the differential evolution equations. For the change of boundary conditions, let multiply Eq.10 by T_l and T_r , introducing the product $T_r T_r^{-1} = 1$ between two multipliers:

$$T_l T_{L+\Delta L} T_r = T_l T_L T_r \cdot T_r^{-1} T_{\Delta L} T_r. \quad (11)$$

Then for the matrix $\tilde{T}_L = T_l T_L T_r$ one has the relation, analogous to (10)

$$\tilde{T}_{L+\Delta L} = \tilde{T}_L T'_{\Delta L}, \quad (12)$$

where the matrix $T'_{\Delta L} = T_r^{-1} T_{\Delta L} T_r$ is again close to the unit one. A passage from $T_{\Delta L}$ to $T'_{\Delta L}$ changes the form of the evolution equations, determined by the parameters $\alpha, \beta, \gamma, \Delta, \epsilon^2$ (see Secs. 2, 3), while a passage

² It is quite natural, since for small L the internal phase distribution is not manifested at all, and the boundary conditions essentially affect the distribution $P(\rho)$, as was extensively discussed in [16].

from T_L to \tilde{T}_L changes the stationary phase distribution, which determines the coefficients in Eq. 5 for $P(\rho)$. These two factors should compensate each other, in order the limiting distribution $P(\rho)$ remains invariant.

However, such invariance is not evident from the evolution equations, and its revelation needs essential efforts. Resolution of these difficulties is closely related with solution of the question on the internal phase distribution.

2. Succession of point scatterers

As clear from experience of the paper [16], it is convenient to consider the energies inside the forbidden band of the initial crystal, while the description of the allowed band can be obtained by analytical continuation. For definiteness, we have in mind the 1D Anderson model

$$\Psi_{n+1} + \Psi_{n-1} + V_n \Psi_n = E \Psi_n \quad (13)$$

near the band edge, where it corresponds to discretization of the usual continuous Schroedinger equation; E is the energy counted from the band center.

A scatterer in the forbidden band is described by the pseudo-transfer matrix t , relating solutions on the left ($Ae^{\kappa x} + Be^{-\kappa x}$) and on the right ($Ce^{\kappa x} + De^{-\kappa x}$) of the scatterer. Succession of scatterers with amplitudes $V_0, V_1, V_2, \dots, V_n$, arranged at the points $0, L_1, L_1 + L_2, \dots, L_1 + L_2 + \dots + L_n$, is described by the matrix

$$t^{(n)} = t_{\epsilon_0} t_{\delta_1} t_{\epsilon_1} t_{\delta_2} t_{\epsilon_2} \dots t_{\delta_n} t_{\epsilon_n}, \quad (14)$$

where

$$t_{\epsilon_n} = \begin{pmatrix} 1 + \bar{\epsilon}_n & \bar{\epsilon}_n \\ -\bar{\epsilon}_n & 1 - \bar{\epsilon}_n \end{pmatrix}, \quad \bar{\epsilon}_n = \frac{V_n}{2\kappa a_0}, \quad (15)$$

$$t_{\delta_n} = \begin{pmatrix} e^{-\delta_n} & 0 \\ 0 & e^{\delta_n} \end{pmatrix}, \quad \delta_n = \kappa L_n$$

and a_0 is the lattice constant. The passage to the true transfer matrix $T^{(n)} = T_l t^{(n)} T_r$ is realized with the help of the edge matrices, describing the attachment of the ideal leads made from the good metal with the Fermi momentum k . Introducing the product $T_r T_l = 1$ between any two multipliers in Eq.14, we have ³

$$T^{(n)} = T_{\epsilon_0} T_{\delta_1} T_{\epsilon_1} T_{\delta_2} T_{\epsilon_2} \dots T_{\delta_n} T_{\epsilon_n}, \quad (16)$$

where

$$T_{\epsilon_n} = T_l t_{\epsilon_n} T_r, \quad T_{\delta_n} = T_l t_{\delta_n} T_r. \quad (17)$$

In the Anderson model all δ_n are equal, $\delta_n = \kappa a_0$, since the scatterers are present at each site of the lattice. Examples of the edge matrices are given below, and in the most general case lead to the following structure of the matrices T_{ϵ_n} and T_{δ}

$$T_{\epsilon_n} = \begin{pmatrix} 1 - i\epsilon_n & \epsilon_n e^{i\gamma} \\ \epsilon_n e^{-i\gamma} & 1 + i\epsilon_n \end{pmatrix}, \quad \epsilon_n = K \bar{\epsilon}_n, \quad (18)$$

$$T_{\delta} = \begin{pmatrix} \mathcal{A} & \mathcal{B} \\ \mathcal{B}^* & \mathcal{A}^* \end{pmatrix} = \begin{pmatrix} \sqrt{1 + \Delta^2} e^{i\alpha} & \Delta e^{i\beta} \\ \Delta e^{-i\beta} & \sqrt{1 + \Delta^2} e^{-i\alpha} \end{pmatrix}.$$

The matrix T_{δ} is the transfer matrix of the general form, while for T_{ϵ_n} the given form is sufficient. As usual, we accept that all V_n are statistically independent, and $\langle V_n \rangle = 0$, $\langle V_n^2 \rangle = W^2$. Then the evolution equations will be determined by parameters $\alpha, \beta, \gamma, \Delta$ and the quantity

$$\epsilon^2 = \langle \epsilon_n^2 \rangle = \text{const } W^2. \quad (19)$$

In the allowed band for the 'natural' ideal leads, the succession of point scatterers is described not by product (14), but the product (16), where

$$T_{\epsilon_n} = \begin{pmatrix} 1 - i\epsilon_n & -i\epsilon_n \\ i\epsilon_n & 1 + i\epsilon_n \end{pmatrix}, \quad \epsilon_n = \frac{V_n}{2\kappa a_0},$$

³ The condition $T_r T_l = 1$ can be accepted without the loss of generality. If it is not so, then we can set $T_l = T_l' T_l''$ with $T_r T_l'' = 1$, and use the matrix T_l'' instead of T_l . The role of the matrix T_l' reduces to the change of the initial conditions to the evolution equation, while the form of the latter is not changed.

$$T_{\delta_n} = \begin{pmatrix} e^{-i\delta_n} & 0 \\ 0 & e^{i\delta_n} \end{pmatrix}, \quad \delta_n = \bar{k}L_n, \quad (20)$$

and \bar{k} is the Fermi momentum in our disordered system, which corresponds to the change $\kappa \rightarrow i\bar{k}$ in the previous relations. Such change corresponds to the smooth transition from the energy $\mathcal{E} = -\kappa^2$ in the forbidden band to the energy $\mathcal{E} = \bar{k}^2$ in the allowed band. The change of the boundary conditions leads to the matrices $\tilde{T}_{\epsilon_n} = T_l T_{\epsilon_n} T_r$ and $\tilde{T}_{\delta_n} = T_l T_{\delta_n} T_r$, having the structure (18).

3. Evolution equations

Let us use the recurrence relation

$$T^{(n+1)} = T^{(n)} T_\delta T_\epsilon, \quad (21)$$

where matrices $T^{(n)}$ and T_ϵ are statistically independent, and T_δ is not random. Accepting parametrization (2) for $T^{(n)}$, and designating parameters of the matrix $T^{(n+1)}$ as $\tilde{\rho}$, $\tilde{\varphi}$, $\tilde{\theta}$, we have

$$\begin{aligned} \sqrt{1+\tilde{\rho}} e^{i\tilde{\varphi}} &= \sqrt{1+\rho} e^{i\varphi} (\mathcal{A} + \epsilon\mathcal{C}) + \sqrt{\rho} e^{i\theta} (\mathcal{B}^* + \epsilon\mathcal{D}^*), \\ \sqrt{\tilde{\rho}} e^{i\tilde{\theta}} &= \sqrt{1+\rho} e^{i\varphi} (\mathcal{B} + \epsilon\mathcal{D}) + \sqrt{\rho} e^{i\theta} (\mathcal{A}^* + \epsilon\mathcal{C}^*), \end{aligned} \quad (22)$$

where we introduced notations

$$\mathcal{C} = \mathcal{B} e^{-i\gamma} - i\mathcal{A} \quad \mathcal{D} = \mathcal{A} e^{i\gamma} + i\mathcal{B}. \quad (23)$$

In what follows we consider the limit

$$\delta \rightarrow 0, \quad \epsilon \rightarrow 0, \quad \delta/\epsilon^2 = \text{const} \quad (24)$$

and retain the terms of the first order in δ and the second order in ϵ . Squaring the modulus of one of equations (22), we have

$$\tilde{\rho} = \rho + \mathcal{K} \sqrt{\rho(1+\rho)} + \epsilon^2(1+2\rho), \quad (25)$$

where

$$\mathcal{K} = 2\Delta \cos(\psi-\beta) + 2\epsilon \cos(\psi-\gamma) - 2\epsilon^2 \sin(\psi-\gamma) \quad (26)$$

and the combined phase variable is introduced

$$\psi = \theta - \varphi. \quad (27)$$

Now let us take the product of the second equation (22) with the complex conjugated first equation

$$\begin{aligned} \sqrt{\tilde{\rho}(1+\tilde{\rho})} e^{i\tilde{\psi}} &= (1+2\rho) [\Delta e^{i\beta} + \epsilon e^{i\gamma} + i\epsilon^2 e^{i\gamma}] + \\ &+ \sqrt{\rho(1+\rho)} [(e^{-2i\alpha} + 2i\epsilon - \epsilon^2) e^{i\psi} + \epsilon^2 e^{2i\gamma - i\psi}]. \end{aligned} \quad (28)$$

Excluding $\tilde{\rho}$ using equation (25), we obtain the relation between $\tilde{\psi}$ and ψ

$$\begin{aligned} \tilde{\psi} &= \psi + 2(\epsilon - \alpha) + (R^2/2 - 1)\epsilon^2 \sin 2(\psi - \gamma) - \\ &- R [\Delta \sin(\psi - \beta) + \epsilon \sin(\psi - \gamma) + \epsilon^2 \cos(\psi - \gamma)], \end{aligned} \quad (29)$$

where

$$R = \frac{1+2\rho}{\sqrt{\rho(1+\rho)}}. \quad (30)$$

Using (22), (26) and following the scheme of the papers [9, 16, 17], we come to the evolution equation for $P(\rho, \psi)$

$$\begin{aligned} \frac{\partial P}{\partial L} &= \left\{ \epsilon^2 [1 - 2\cos^2(\psi - \gamma)] (1+2\rho) P - \right. \\ &- 2 [\Delta \cos(\psi - \beta) + \epsilon^2 \sin(\psi - \gamma)] \sqrt{\rho(1+\rho)} P + \\ &\left. + 2\epsilon^2 \cos^2(\psi - \gamma) \rho(1+\rho) P'_\rho + \right. \end{aligned}$$

$$\begin{aligned}
& +2\epsilon^2 \cos(\psi-\gamma) [2-R \sin(\psi-\gamma)] \sqrt{\rho(1+\rho)} P'_\psi \Big\}'_\rho + \\
& + \left\{ \epsilon^2 \cos(\psi-\gamma) [2 \sin(\psi-\gamma) - R] P + \right. \\
& \quad + [2\alpha + R\Delta \sin(\psi-\beta)] P + \\
& \quad \left. + \frac{1}{2} \epsilon^2 [2 - R \sin(\psi-\gamma)]^2 P'_\psi \right\}'_\psi .
\end{aligned} \tag{31}$$

The right-hand side is a sum of full derivatives, which provides the conservation of probability. Relation between distributions of ρ and ψ is determined by the quantity R , which tends to 2 in the limit of large L , when the typical values of ρ are large. Then the solution of Eq.31 is factorized, $P(\rho, \psi) = P(\rho)P(\psi)$, though the situation is somewhat unusual for separation of variables (see Appendix 1); the equation for $P(\psi)$ is splitted off,

$$\begin{aligned}
\frac{\partial P(\psi)}{\partial L} = & \left\{ [2\alpha + 2\Delta \sin(\psi-\beta) - 2\epsilon^2 \cos(\psi-\gamma) + \right. \\
& \quad \left. + \epsilon^2 \sin 2(\psi-\gamma)] P(\psi) + \right. \\
& \quad \left. + 2\epsilon^2 [1 - \sin(\psi-\gamma)]^2 P'_\psi(\psi) \right\}'_\psi
\end{aligned} \tag{32}$$

giving the condition for the stationary distribution of the phase ψ

$$\begin{aligned}
& \epsilon^2 [1 - \sin(\psi-\gamma)]^2 P'_\psi - \\
& - \epsilon^2 [1 - \sin(\psi-\gamma)] \cos(\psi-\gamma) P + \\
& + [\alpha + \Delta \sin(\psi-\beta)] P = C_0,
\end{aligned} \tag{33}$$

where the constant C_0 is fixed by normalization.⁴

Averaging over ψ leads to equation (5) with parameters

$$\begin{aligned}
D & = 2\epsilon^2 \langle \cos^2(\psi-\gamma) \rangle, \\
\gamma_1 D & = \epsilon^2 \langle 1 - 2 \cos^2(\psi-\gamma) \rangle, \\
\gamma_2 D & = \Delta \langle \cos(\psi-\beta) \rangle - \epsilon^2 \langle \sin(\psi-\gamma) \rangle,
\end{aligned} \tag{34}$$

while for the 'drift velocity' in (6) one has

$$\begin{aligned}
v & = 2\Delta \langle \cos(\psi-\beta) \rangle + \\
& + 2\epsilon^2 \langle \sin^2(\psi-\gamma) - \sin(\psi-\gamma) \rangle.
\end{aligned} \tag{35}$$

The averaging in Eqs.(34, 35) is produced over the stationary distribution $P(\psi)$.

4. Dependence on the properties of the ideal leads

Let the Fermi momentum k in the ideal leads is different from the Fermi momentum \bar{k} in the disordered system, while the boundary between them is abrupt. Then the edge matrices in the forbidden band can be chosen in the form

$$\begin{aligned}
T_l & = \begin{pmatrix} l & l^* \\ l^* & l \end{pmatrix}, & T_r & = \begin{pmatrix} r & r^* \\ r^* & r \end{pmatrix}, \\
l & = \frac{1}{2} \left(1 + \frac{\kappa}{ik} \right), & r & = \frac{1}{2} \left(1 + \frac{ik}{\kappa} \right),
\end{aligned} \tag{36}$$

⁴ Equations (31, 32) are analogous to Eqs.(10.27), (10.28) in the book [10], derived in the framework of the different formalism, so the quantities entering them are not related clearly with the transfer matrix parameters. The same is valid relative equations (39, 40) in the paper [18].

leading to the results (18) for matrices T_{ϵ_n} and T_δ with parameters

$$\begin{aligned}\alpha &= -\frac{1}{2} \left(\frac{k}{\kappa} - \frac{\kappa}{k} \right) \delta = \frac{\kappa^2 - k^2}{2k} a_0, \\ \beta &= \frac{\pi}{2}, \quad \gamma = -\frac{\pi}{2}, \quad \epsilon^2 = \tilde{\epsilon}^2 \left(\frac{\kappa}{k} \right)^2 = \frac{W^2}{4k^2 a_0^2}, \\ \Delta &= \frac{1}{2} \left(\frac{k}{\kappa} + \frac{\kappa}{k} \right) \delta = \frac{\kappa^2 + k^2}{2k} a_0,\end{aligned}\tag{37}$$

which are the regular functions of the energy $\mathcal{E} = -\kappa^2$ and can be analytically continued to the allowed band. Then for parameters D and v one has

$$D = 2\epsilon^2 \langle \sin^2 \psi \rangle,\tag{38}$$

$$v = 2\Delta \langle \sin \psi \rangle + 2\epsilon^2 \langle 1 - \cos \psi \rangle - 2\epsilon^2 \langle \sin^2 \psi \rangle,$$

while the equation for the stationary distribution $P(\psi)$ accepts the form

$$\begin{aligned}\epsilon^2 (1 - \cos \psi)^2 P'_\psi + \epsilon^2 \sin \psi (1 - \cos \psi) P + \\ + (\alpha - \Delta \cos \psi) P = C_0.\end{aligned}\tag{39}$$

The change of variables in Eq.39

$$\omega = -\text{ctg } \psi/2\tag{40}$$

and renormalization of probability $P \rightarrow P(1 + \omega^2)/2$, following from $P(\psi)d\psi = P(\omega)d\omega$, reduce it to the simple form

$$P'_\omega + P(b + a\omega^2) = C_0,\tag{41}$$

where

$$a = \frac{\alpha - \Delta}{2\epsilon^2}, \quad b = \frac{\alpha + \Delta}{2\epsilon^2}\tag{42}$$

or inversely

$$\alpha = \epsilon^2(b + a), \quad \Delta = \epsilon^2(b - a).\tag{43}$$

Equation (41) can be integrated in quadratures, but this quadrature is practically useless. It is more effective to investigate the transformation properties. If $P_{a,b}(\omega)$ is a solution of Eq.41, then the following relation is valid

$$P_{a,b}(\omega) = s^{-1} P_{as^3, bs}(\omega/s).\tag{44}$$

It can be established, making the change $\omega = s\tilde{\omega}$ and reducing the obtained equation to the initial form by redefinition of parameters $\tilde{a} = as^3$, $\tilde{b} = bs$; then $P_{a,b}(\omega)$ coincides with $P_{\tilde{a}, \tilde{b}}(\tilde{\omega})$ to the constant factor, which is established from normalization. Using the relation

$$ab = \frac{\alpha^2 - \Delta^2}{4\epsilon^4} = -\frac{\delta^2}{4\epsilon^4},\tag{45}$$

one can see that the scale transformation $a \rightarrow as^3$, $b \rightarrow bs$ leads to renormalization $\epsilon \rightarrow \tilde{\epsilon}$, where

$$\tilde{\epsilon} = \epsilon s^{-1} = \tilde{\epsilon} \frac{\kappa}{k} s^{-1}.\tag{46}$$

Substitution of (37) to (43) gives the initial values of the parameters a and b

$$a = -\frac{k}{\kappa} \frac{\delta}{2\epsilon^2}, \quad b = \frac{\kappa}{k} \frac{\delta}{2\epsilon^2},\tag{47}$$

while the relations (33) allow to establish the change of parameters $\alpha \rightarrow \tilde{\alpha}$, $\Delta \rightarrow \tilde{\Delta}$ in the result of the scale transformation

$$\tilde{\alpha} = \frac{1}{2} \left(\frac{\kappa}{k} s^{-1} - \frac{k}{\kappa} s \right) \delta, \quad \tilde{\Delta} = \frac{1}{2} \left(\frac{\kappa}{k} s^{-1} + \frac{k}{\kappa} s \right) \delta.\tag{48}$$

Relations (46) and (48) show that transformation of all parameters α , Δ , ϵ^2 entering the evolution equations reduces to the change

$$\frac{k}{\kappa} \rightarrow \frac{k}{\kappa} s, \quad (49)$$

which is equivalent to renormalization of the Fermi momentum in the ideal leads. Inversely, variation of the properties of the ideal leads results in the scale transformation of the distribution $P(\omega)$.

5. Influence of the delta potential on interfaces

If there is the delta potential on interfaces between the disordered system and the ideal leads, then the edge matrices (36) transform to the form

$$T_l = \begin{pmatrix} l & l_1^* \\ l^* & l_1 \end{pmatrix}, \quad l = \frac{ik + \kappa - \kappa_1}{2ik}, \quad l_1 = \frac{ik + \kappa + \kappa_1}{2ik}, \quad (50)$$

$$T_r = \begin{pmatrix} r & r^* \\ r_1^* & r_1 \end{pmatrix}, \quad r = \frac{ik + \kappa - \kappa_2}{2\kappa}, \quad r_1 = \frac{ik + \kappa + \kappa_2}{2\kappa},$$

where κ_1 and κ_2 corresponds to the jumps of the logarithmic derivative of the wave function on the left and right interfaces. The condition $T_r T_l = 1$ is realized for $\kappa_2 = -\kappa_1$, and can be accepted without the loss of generality (see Footnote 3). Then the matrix T_{ϵ_n} remains unchangeable, while T_δ accept the form (18) with parameters

$$\alpha = -\frac{k^2 - \kappa^2 + \kappa_1^2}{2\kappa k} \delta, \quad \Delta \cos \beta = -\frac{\kappa_1}{\kappa} \delta, \quad (51)$$

$$\Delta \sin \beta = \frac{k^2 + \kappa^2 - \kappa_1^2}{2\kappa k} \delta,$$

which, as previously, are the regular functions of the energy $\mathcal{E} = -\kappa^2$ (due to $\delta = \kappa a_0$). Thereby, we again have $\gamma = -\pi/2$, while the parameter β becomes different from the value $\pi/2$. The change of variables (40) transforms equation (33) to the form

$$P'_\omega + P(b + c\omega + a\omega^2) = C_0, \quad (52)$$

with parameters

$$a = \frac{\alpha - \Delta \sin \beta}{2\epsilon^2}, \quad b = \frac{\alpha + \Delta \sin \beta}{2\epsilon^2}, \quad c = -\frac{\Delta \cos \beta}{\epsilon^2}, \quad (53)$$

which accept the following form after substitution of the physical values (51):

$$a = -\frac{k}{\kappa} \frac{\delta}{2\epsilon^2}, \quad b = \frac{\kappa^2 - \kappa_1^2}{\kappa k} \frac{\delta}{2\epsilon^2}, \quad c = \frac{\kappa_1}{\kappa} \frac{\delta}{2\epsilon^2}. \quad (54)$$

A solution of Eq. 52 satisfies to relation

$$P_{a,b,c}(\omega) = s^{-1} P_{as^3, bs, cs^2}(\omega/s), \quad (55)$$

and the scale transformation of $P(\omega)$ as previously corresponds to a change of the Fermi momentum k in the ideal leads.

It is easy to see, that the shift $\omega \rightarrow \omega - \omega_0$ of the variable ω allows to reduce Eq. 52 to the form (41), which is expressed by the relation

$$P_{a,b,c}(\omega) = P_{\tilde{a}, \tilde{b}, 0}(\omega + \omega_0), \quad (56)$$

$$\omega_0 = -\frac{\kappa_1}{k}, \quad \tilde{a} = a = -\frac{k}{\kappa} \frac{\delta}{2\epsilon^2}, \quad \tilde{b} = \frac{\kappa}{k} \frac{\delta}{2\epsilon^2},$$

where the values of parameters \tilde{a} and \tilde{b} corresponds to the situation with $\kappa_1 = 0$. As a result, the appearance of the delta potential on interfaces leads to translation of the distribution $P(\omega)$ to the quantity ω_0 , proportional to the amplitude of the delta potential.

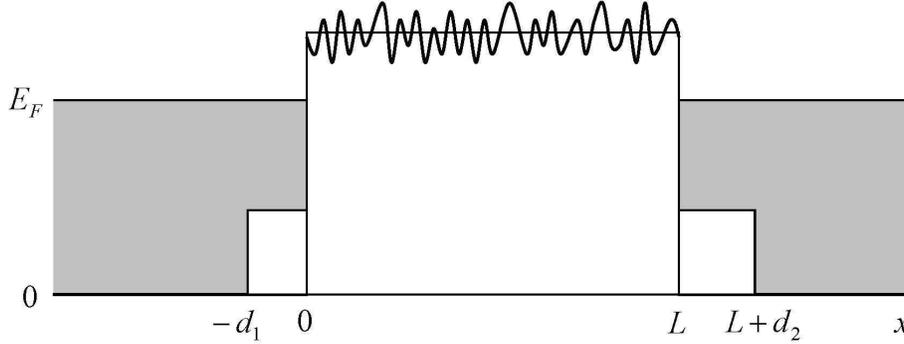


Figure 4: The model to describe the smearing of interfaces.

6. Smearing of interfaces

For energies in the forbidden band, the disordered system in the absence of impurities reduces to the potential barrier. The smearing of interfaces can be simulated by incorporating the layers of a metal with the Fermi momentum k_1 and thickness d_1 and d_2 on the boundaries of the system (Fig.4). The edge matrices T_l and T_r for such model are given in Appendix 2. The condition $T_r T_l = 1$ is satisfied, if the following constraints are imposed on d_1 and d_2

$$k_1(d_1 + d_2) = 2\pi m, \quad k(d_1 + d_2) = 2\pi n, \quad (57)$$

where m and n are integers. The matrix T_δ is the transfer matrix of the general form, and its calculation is not very actual. For the matrix T_{ϵ_n} one obtains the expression (18) with parameters

$$K = \frac{\kappa \mathcal{R}}{k_1}, \quad \gamma = \arcsin\left(\frac{\sin \alpha}{\mathcal{R}}\right) - \frac{k}{k_1} \alpha - \frac{\pi}{2}, \quad (58)$$

where

$$\begin{aligned} \mathcal{R} &= \mathcal{P} + \mathcal{Q} \cos \alpha, \quad \alpha = k_1(d_2 - d_1), \\ \mathcal{P} &= \frac{k_1^2 + k^2}{2kk_1}, \quad \mathcal{Q} = \frac{k_1^2 - k^2}{2kk_1}. \end{aligned} \quad (59)$$

The value of γ , different from $-\pi/2$, is obtained for $d_1 \neq d_2$. Since the parameter γ enters both in expressions (34,35) for D and v , and in Eq.33 for the stationary distribution $P(\psi)$, it can be excluded from equations by the shift $\psi \rightarrow \psi + \psi_0$, which reduces it to the value $-\pi/2$; only the corresponding redefinition of β is necessary. After it, the change of variables (40) leads to equation (52) of the previous section.

If the Fermi momentum k_1 is chosen to be proportional to k , then the parameters \mathcal{P} and \mathcal{Q} are independent of k , and the scale transformation of $P(\omega)$ as previously corresponds to renormalization (49) of the Fermi

momentum k . In general, the proportionality $k_1 \propto k$ is not realized, but the change of the properties of the ideal leads corresponds to the scale transformation of $P(\omega)$ with the more complicated relation of the momentum k with the scale factor s .

7. General approach to the edge matrices

Let discuss the general approach to analysis of the role of the boundary conditions, not related with the model assumptions. We try to find out the degree of arbitrariness, permissible in the edge matrices.

As was indicated in Sec.2, the condition $T_r T_l = 1$ can be accepted without the loss of generality. According to (16,17), we are interested in expressions containing the equal number of matrices T_r and T_l , and so the common factors can be easily extracted from one matrix and include into another. Hence, without the loss of generality the matrices T_r and T_l can be chosen in the form

$$T_l = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad T_r = \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}, \quad ad - bc = 1, \quad (60)$$

accepting the unit value for their determinants. The role of the edge matrices is the most essential in the forbidden band: they allow to transform the pseudo-transfer matrix t to the true transfer matrix $T = T_l t T_r$. The condition for a matrix T to be the true transfer matrix is expressed by the following relations between its matrix elements T_{ij} [19]⁵

$$\begin{aligned} T_{11} T_{11}^+ - T_{12} T_{12}^+ &= 1, \\ T_{22} T_{22}^+ - T_{21} T_{21}^+ &= 1, \\ T_{11} T_{21}^+ - T_{12} T_{22}^+ &= 0, \end{aligned} \quad (61)$$

which follows from the flux conservation.

Let demand that matrices T_δ and T_ϵ , entering (16,17) were true transfer matrices. Then (see Appendix 3) the admissible edge matrices form the free parameter family

$$T_l = \begin{pmatrix} |r_1| e^{i\alpha_1} & |r_2| e^{i\alpha_2} \\ \pm i |r_1| e^{-i\alpha_1} & \pm i |r_2| e^{-i\alpha_2} \end{pmatrix}, \quad 1 = 2|r_1 r_2| \sin(\alpha_2 - \alpha_1), \quad (62)$$

where the upper sign is chosen for $\sin(\alpha_2 - \alpha_1) > 0$, and the lower sign in the opposite case. Then for the matrices T_δ and T_ϵ we have the expressions (18) with parameters

$$\begin{aligned} \alpha &= -2\delta |r_1| |r_2| \cos(\alpha_2 - \alpha_1), \\ \beta &= \alpha_1 + \alpha_2, \\ \gamma &= 2\alpha_1 - 2 \arcsin \frac{|r_2| \cos(\alpha_2 - \alpha_1)}{r}, \\ \Delta &= 2\delta |r_1| |r_2|, \\ K &= r^2 = |r_1|^2 + |r_2|^2 - 2|r_1| |r_2| \cos(\alpha_2 - \alpha_1). \end{aligned} \quad (63)$$

Analogous research in the allowed band leads to the physically evident result: the edge matrices are the true transfer matrices of the general form

$$T_l = \begin{pmatrix} |r_1| e^{i\alpha_1} & |r_2| e^{i\alpha_2} \\ |r_2| e^{-i\alpha_2} & |r_1| e^{-i\alpha_1} \end{pmatrix}, \quad |r_1|^2 - |r_2|^2 = 1. \quad (64)$$

In this case, we have the following parameters in the expressions (18) for T_δ and T_ϵ

$$\begin{aligned} \alpha &= -\delta (|r_1|^2 + |r_2|^2), \\ \beta &= \pi/2 + \alpha_1 + \alpha_2, \\ \gamma &= -\frac{\pi}{2} + 2\alpha_1 - 2 \arcsin \frac{|r_2| \cos(\alpha_1 - \alpha_2)}{r}, \\ \Delta &= 2\delta |r_1| |r_2|, \end{aligned} \quad (65)$$

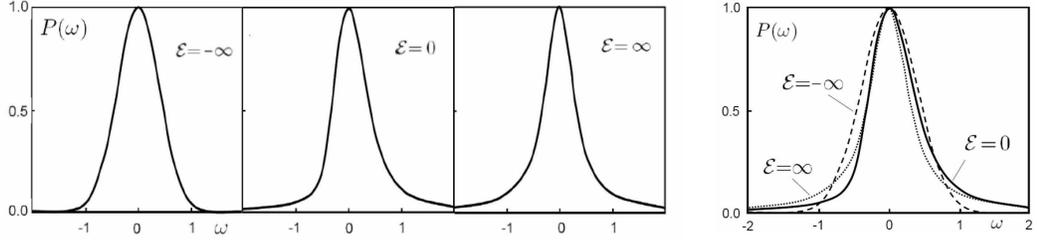


Figure 5: Distributions $P(\omega)$ for different energies differ only slightly.

$$K = r^2 = |r_1|^2 + |r_2|^2 - 2|r_1||r_2|\cos(\alpha_2 - \alpha_1).$$

It should be clear from the preceding sections, that the whole free parameter arbitrariness of the edge matrices can be realized physically, while the evolution equations derived in Sec.3 have the most general form.

8. Distribution $P(\omega)$

As clear from preceding, the most general results for the parameters of the evolution equation (5) and the limiting distribution (6) are given by relations (34, 35), where averaging over ψ is carried out over the stationary distribution $P(\psi)$, determined by equation (33). The shift $\psi \rightarrow \psi + \psi_0$ allows to reduce the parameter γ to the value $-\pi/2$, and after it the change of variables $\omega = -\text{ctg}\psi/2$ leads to equation (52). Then translation $\omega \rightarrow \omega + \omega_0$ allows to transfer (52) to equation (41), which by the scale transformation $\omega \rightarrow s\omega$ can be reduced to one of the canonical form, either with $|a| = |b|$, or with $a = -1$, depending on the single parameter; this one-parameter freedom is associated with the dependence on the reduced energy $\tilde{\mathcal{E}}$. Thereby, the form of the distribution $P(\omega)$ with $\omega = -\text{ctg}\psi/2$ is determined by the internal properties of the system, while the change of the boundary conditions transfers it to the distribution $P(\tilde{\omega})$, where the variable

$$\tilde{\omega} = \omega_0 - s \text{ctg} \frac{\psi + \psi_0}{2} \quad (66)$$

is related with ω by the homographic transformation

$$\tilde{\omega} = \frac{A\omega + B}{C\omega + D}. \quad (67)$$

⁵ We give these relations in the form applicable to quasi-1D systems, when the elements T_{ij} are in fact matrices.

According to [16], the situation $|a|=|b|$ is distinguished by the fact, that in the deep of the allowed and forbidden bands parameters of the evolution equation (5) remain constant till very small length scales⁶. The case $a=b$, which is realized in the allowed band, corresponds to the 'natural' ideal leads (Sec.1). Under condition $-a=-b \gg 1$ (in the deep of the allowed band) one can omit the term P'_ω in Eq.41, and obtain

$$P(\omega) = \frac{1}{\pi} \frac{1}{1 + \omega^2}, \quad (68)$$

which correspond to $P(\psi) = \text{const}$, i.e. the random phase approximation. For $-a=b \gg 1$ (in the deep of the forbidden band) one can neglect the constant C_0 in Eq.41 near the maximum of distribution and, setting $\omega = -1 + \tilde{\omega}$, obtain $P'_\omega \approx -2|a|\tilde{\omega}P$, which gives the Gaussian distribution

$$P(\omega) = \sqrt{\frac{|a|}{\pi}} \exp\{-|a|\tilde{\omega}^2\}, \quad (69)$$

localized near $\omega=-1$; it corresponds to the Gaussian distribution $P(\psi)$, localized near $\pi/2$ [16]. If the condition $|a|=|b|$ is violated in the allowed band, it leads to appearance of the oscillations of distribution $P(\rho, \psi)$, related with the fact that the matrix T in the absence of impurities reduces to the transfer matrix of the potential barrier, which becomes transparent, if its width L corresponds to the semi-integer number of the de Broglie waves (analogously to blooming in optics) [16]. If the condition $|a|=|b|$ is violated in the deep of the forbidden band, then the distribution $P(\rho, \psi)$ is localized near the value of ψ , different from $\pi/2$, which leads to its slow relaxation to the latter value.

Near the edge of the initial band, it is convenient to reduce equation (41) to the canonical form with $a=-1$. Its solution with $b=0$ corresponds to the 'critical' region for the smoothed Anderson transition [16] and can be presented in the form (see Appendix 4)

$$P(\omega) = A_0 \int_0^\infty dt e^{-t} t^{-1/3} \frac{\omega}{\omega^3 + 3t}, \quad (70)$$

where A_0 is determined from normalization. For large ω we have $P(\omega) \sim \omega^{-2}$, which is the general property (see Appendix 4) and corresponds to the finite values of $P(\psi)$ on the boundaries of the interval $(0, 2\pi)$.

If by the scale transformation and translation we provide the maximum of the distribution $P(\omega)$ at $\omega=0$ with the unit value in it, then distributions (68-70) differ not very essentially (Fig.5), witnessing on the weak dependence of $P(\omega)$ on the reduced energy $\tilde{\mathcal{E}}$.

9. External phase distribution

If the distribution $P(\omega)$ is known, then its change under variation of the boundary condition reduces to the scale transformation and translations. The corresponding change of the external phase distribution $P(\psi)$ is easily predictable on the qualitative level and illustrated in Fig.6. The distribution $P(\psi)$ is uniform (Fig.6,a), if $P(\omega)$ has a form (68) and corresponds to the random phase approximation. Widening of the distribution $P(\omega)$ leads to localization of $P(\psi)$ near the edges of the interval $(0, 2\pi)$ (Fig.6,b), while narrowing leads to localization of $P(\psi)$ in the middle of the interval $(0, 2\pi)$. (Fig.6,c). A shift of $P(\omega)$ to right or to left leads to appearance of the maximum of $P(\psi)$ in the right or left part of the interval $(0, 2\pi)$ (Fig.6,d,e). If the parameter γ is different from $-\pi/2$, it leads to translation $\psi \rightarrow \psi + \psi_0$ and the presented dependences are valid not in the interval $(0, 2\pi)$, but in the interval $(\psi_0, 2\pi + \psi_0)$.

If the distribution $P(\omega)$ is accepted not in the form (68), but in the Gaussian form (69), then Fig.6 does not change qualitatively, but $P(\psi)$ will not be constant in Fig.6,a. The asymmetrical form of the function $P(\omega)$ for $\mathcal{E}=0$, corresponding to the critical distribution (Fig.5), leads to a new qualitative effect: its translations $\omega \rightarrow \omega + \omega_0$ leads to appearance of the two-humped distribution $P(\psi)$ in a certain interval of the ω_0 values (Fig.7).

10. Internal phase distribution

⁶ For sufficiently large L these parameters are always constant, since they are determined by the stationary distribution $P(\psi)$.

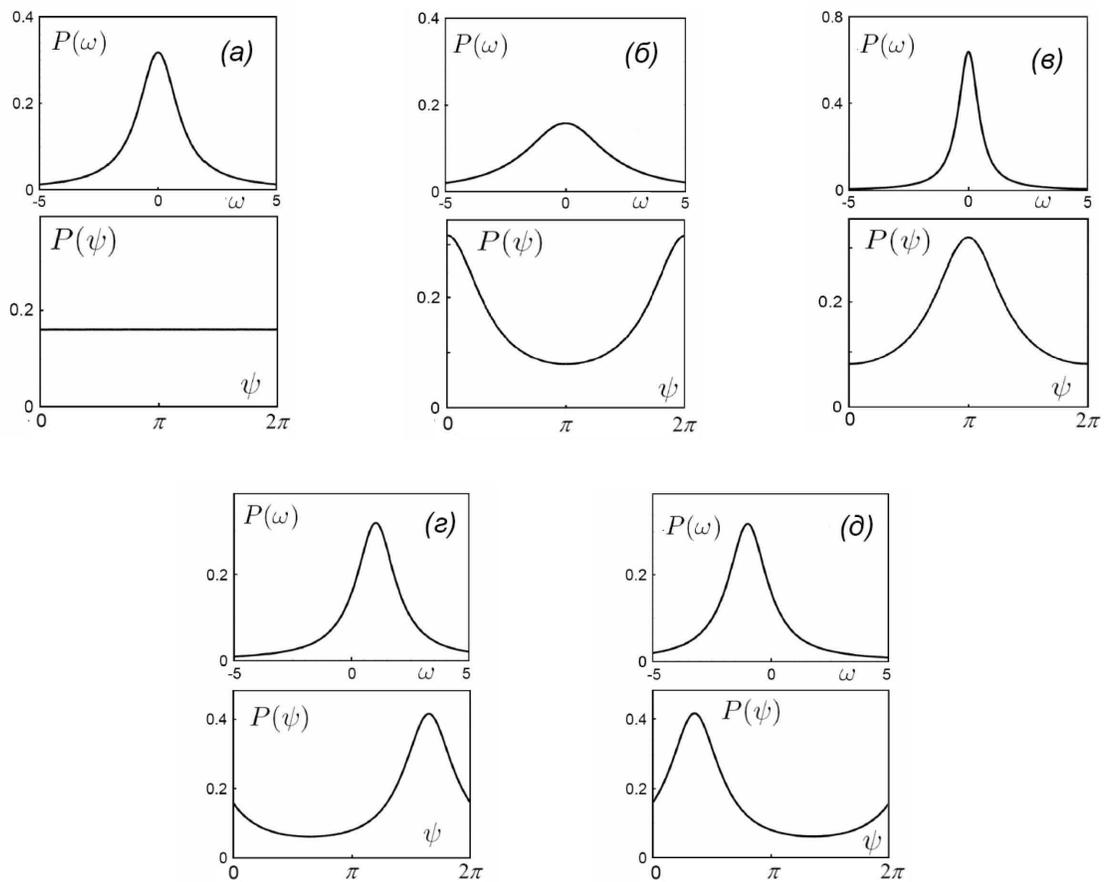


Figure 6: The change of the distribution $P(\psi)$ under the scale transformation and translation of the function $P(\omega)$, if the form of the latter corresponds to the random phase approximation.

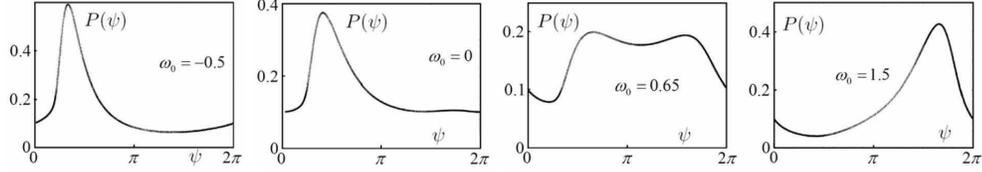


Figure 7: The change of the distribution $P(\psi)$ under translations of the critical distribution $P(\omega)$.

Let return to the case $\beta = \pi/2$, $\gamma = -\pi/2$, considered in Sec.4, and produce the change of variables $\omega = -\text{ctg } \psi/2$ in the complete evolution equation (31). If the typical values of ρ are sufficiently large, then the evolution equation for $P(\rho, \omega)$ accepts the form

$$\begin{aligned} \frac{\partial P}{2\partial L} = & \left\{ \epsilon^2 \frac{4\omega^2}{(1+\omega^2)^2} \rho^2 P'_\rho - \Delta \frac{2\omega}{1+\omega^2} \rho P + \right. \\ & \left. + \epsilon^2 \frac{2}{1+\omega^2} \rho P + \dots \right\}'_\rho + \epsilon^2 \left\{ P'_\omega + (b + a\omega^2) P \right\}'_\omega. \end{aligned} \quad (71)$$

Making the change $\omega = s\tilde{\omega}$ and redefinition of parameters $\tilde{a} = as^3$, $\tilde{b} = bs$, $\tilde{\epsilon}^2 = \epsilon^2 s^{-2}$, we have

$$\begin{aligned} \frac{\partial P}{2\partial L} = & \left\{ \tilde{\epsilon}^2 s^2 \frac{4s^2 \tilde{\omega}^2}{(1+s^2 \tilde{\omega}^2)^2} \rho^2 P'_\rho - \tilde{\Delta} \frac{2s\tilde{\omega}}{1+s^2 \tilde{\omega}^2} \rho P + \right. \\ & \left. + \tilde{\epsilon}^2 s^2 \frac{2}{1+s^2 \tilde{\omega}^2} \rho P + \dots \right\}'_\rho + \tilde{\epsilon}^2 \left\{ P'_\omega + (\tilde{b} + \tilde{a}\tilde{\omega}^2) P \right\}'_\omega. \end{aligned} \quad (72)$$

The latter term in Eq. 72 has the same form as in Eq. 71, but the other terms are not invariant. According to Eq.5, the parameter D is determined by the coefficient before $\rho^2 P'_\rho$, and equations (71, 72) lead to two expressions

$$D = 2\epsilon^2 \left\langle \frac{4\omega^2}{(1+\omega^2)^2} \right\rangle_{a,b}, \quad (73)$$

$$D = 2\tilde{\epsilon}^2 s^2 \left\langle \frac{4s^2 \omega^2}{(1+s^2 \omega^2)^2} \right\rangle_{\tilde{a}, \tilde{b}}, \quad (74)$$

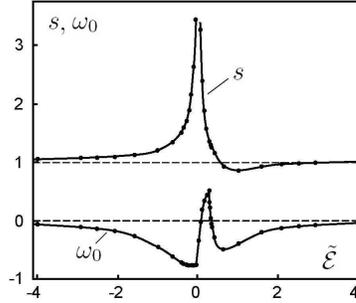


Figure 8: Behavior of the scale factors s and the translational shift ω_0 as functions of the reduced energy $\tilde{\mathcal{E}}$.

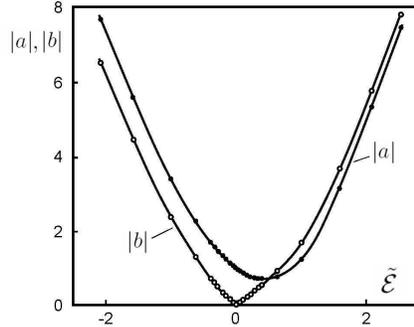


Figure 9: Parameters a and b for the internal phase distribution as functions of the reduced energy $\tilde{\mathcal{E}}$.

which are equivalent due to relation (44). If Eq.74 is accepted as a definition of the diffusion coefficient D , then its invariance in respect to the change of the boundary conditions is fulfilled automatically. However, the change of a, b, ϵ to $\tilde{a}, \tilde{b}, \tilde{\epsilon}$ in Eq. 71 leads to the analogous changes in Eq. 73, which together with Eq. 74 gives the relation

$$\left\langle \frac{4\omega^2}{(1+\omega^2)^2} \right\rangle_{\tilde{a}, \tilde{b}} = s^2 \left\langle \frac{4s^2\omega^2}{(1+s^2\omega^2)^2} \right\rangle_{\tilde{a}, \tilde{b}}, \quad (75)$$

which is not fulfilled for arbitrary s , and valid only for a certain 'correct' choice of the scale factor. It is easy to understand that this 'correct' choice corresponds to the 'internal' phase distribution. Analogous considerations can be given in respect to the parameter v in the distribution (6), which is determined by the coefficient before ρP .

Let the initial values a_0, b_0 of the parameters a, b are chosen from the condition $|a_0| = |b_0|$, which is 'natural' beyond the vicinity of the initial band edge [16]. If $P(\omega)$ is the solution of equation (41) with parameters a_0, b_0 , then replacement $\omega \rightarrow s(\tilde{\omega} + \omega_0)$ allows to provide the correct values of D and v , following from analysis of moments, by the proper choice of s and ω_0 . The obtained distribution $P(\tilde{\omega})$ after return to the variable ψ will determine the internal phase distribution. Behavior of s and ω_0 as a function of the reduced energy $\tilde{\mathcal{E}}$ is shown in Fig.8. The scale factor s is diverging at $\tilde{\mathcal{E}} \rightarrow 0$, and the renormalized parameters

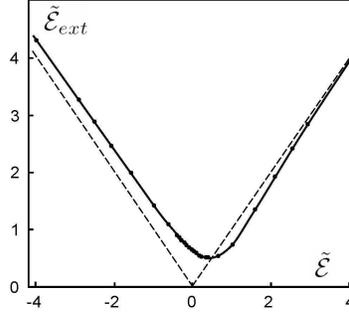


Figure 10: Dependence of the Fermi energy $\tilde{\mathcal{E}}_{ext}$ in the ideal leads on the Fermi energy in the disordered system $\tilde{\mathcal{E}}$ for the internal phase distribution. The dashed line corresponds to the dependence $\tilde{\mathcal{E}}_{ext} = |\tilde{\mathcal{E}}|$.

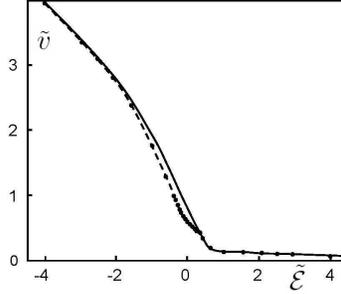


Figure 11: The best fit of the parameter v for the real values of the translational shift ω_0 .

$a = a_0 s^3$ and $b = b_0 s$ become not be bounded by the relation $|a| = |b|$ (Fig.9), which is realized only for large $|\tilde{\mathcal{E}}|$, i.e. in the deep of the allowed and forbidden bands. The physical meaning of this fact is more explicit from Fig.10, demonstrating the dependence of the Fermi energy $\tilde{\mathcal{E}}_{ext}$ in the ideal leads against the Fermi energy $\tilde{\mathcal{E}}$ in the disordered system. The minimum of $\tilde{\mathcal{E}}_{ext}$ is reached at the value $\tilde{\mathcal{E}} = \tilde{\mathcal{E}}_0 = 0.28$, which can be interpreted as a renormalized band edge, shifted due to fluctuations of a random potential. This conclusion is confirmed by the fact, that for $\tilde{\mathcal{E}} < \tilde{\mathcal{E}}_0$ the translational shift ω_0 moves to the complex plane, which has a simple physical sense. For $\tilde{\mathcal{E}} = \tilde{\mathcal{E}}_0$ we have $\tilde{\mathcal{E}}_{ext} = \tilde{\mathcal{E}}_0$ (Fig.10) and the shifted band edge is below the Fermi level in the ideal leads for $\tilde{\mathcal{E}} > \tilde{\mathcal{E}}_0$ and upper it for $\tilde{\mathcal{E}} < \tilde{\mathcal{E}}_0$. In the latter case the internal properties of the system are described not by true, but the pseudo-transfer matrix, and the distribution $P(\psi)$ becomes complex-valued. The detailed study of the latter is not very actual, and the 'internal' distribution $P(\psi)$, presented below for $\tilde{\mathcal{E}} < \tilde{\mathcal{E}}_0$, is in fact the external distribution, which is closest to internal; it practically coincides with the modulus of the complex distribution $P(\psi)$. The latter follows from the fact, that the shift of the parameter ω_0 to the complex plane is comparatively small and allows analytical investigation (see Appendix 5): it is illustrated by Fig.11, which shows the best fit of the parameter v (with exact fitting of D), possible for real values of ω_0 .

Evolution of the internal distribution $P(\psi)$ (with a given reservation) under variation of the reduced

energy $\tilde{\mathcal{E}}$ is shown in Fig.12. The first row of figures corresponds to variation of $\tilde{\mathcal{E}}$ from large positive values till the value $\tilde{\mathcal{E}} = 0.63$, corresponding to the right minimum of ω_0 in Fig.8; here the distribution $P(\omega)$ is close to the Lorentz form (68), while the change of $P(\psi)$ is mainly related with translation of $P(\omega)$ to the left direction (Fig.6,e). The third row of Fig.12 corresponds to variation of $\tilde{\mathcal{E}}$ from large negative values till the value $\tilde{\mathcal{E}} = -0.10$, corresponding to the left minimum of ω_0 in Fig.8; here the distribution $P(\psi)$ is localized near $\pi/2$ and gradually spreads with growth of $\tilde{\mathcal{E}}$, while $P(\omega)$ changes from the Gaussian form (69) to the critical form (70). The second row of Fig.12 corresponds to variation of $\tilde{\mathcal{E}}$ between two minima of ω_0 in Fig.8; here the distribution $P(\omega)$ is close to the critical form (70), while the change of $P(\psi)$ is mainly related with translational shift of $P(\omega)$ and corresponds to Fig.7. The fourth and ninth dependences of Fig.12 are close to each other, since the form of $P(\omega)$ is close to critical, while the translational shifts ω_0 are approximately equal.

Let discuss the mechanism of realization of the internal phase distribution. As was discussed in papers [16, 20, 21], the distribution $P(\rho)$ of the Landauer resistance undergoes aperiodic oscillations, related with the fact that the form of $P(\rho)$ depends essentially on the several first moments, while the moments $\langle \rho^n \rangle$ are oscillating functions of L : the n th moment is determined by a superposition of n discrete harmonics. The relative amplitude of oscillations decays exponentially on the scale $L \sim \xi$, and they become inessential for large L . The analogous situation takes place for the complete distribution $P(\rho, \omega)$; correspondingly, both the mean of ω and its dispersion are oscillating. The latter are directly related with the translational shift ω_0 and the scale factor s , which become oscillating on the scale $L \lesssim \xi$, tending to 'correct' constant values at large L : these 'correct' values correspond to the internal phase distribution.

11. Conclusion

In the present paper we have derived the evolution equation for the mutual distribution $P(\rho, \psi)$ of the Landauer resistance ρ and the phase variable ψ . For large L , this equation allows the separation of variables, which provides the existence of the stationary distribution $P(\psi)$, determining the coefficients in the evolution equation (5) for $P(\rho)$.

In the result of the present analysis we come to a very simple picture. The phase ψ appears to be a "bad" variable, while the "correct" variable is $\omega = -\text{ctg } \psi/2$. The form of the stationary distribution $P(\omega)$ is determined by the internal properties of the system and does not depend on the boundary conditions. Variation of the boundary conditions leads to three effects: (a) the scale transformation $\omega \rightarrow s\omega$, which is mainly related with the change of properties of the ideal leads, attached to the system; (b) translation $\omega \rightarrow \omega + \omega_0$, which is mainly determined by existence of the delta-potential on the boundaries of the system; (c) translation $\psi \rightarrow \psi + \psi_0$, related with smearing of interfaces. The boundary conditions essentially affect the 'external' phase distribution, which enters the evolution equations, but do not affect the limiting distribution $P(\rho)$ in the region of large L , which allows to say on existence of the hidden symmetry in the evolution equations. The limiting distribution $P(\rho)$ has the log-normal form, which can be established under the most general conditions⁸. The limiting distribution $P(\rho)$ is determined by the 'internal' distribution $P(\psi)$, which is obtained from the stationary distribution $P(\omega)$ with the proper choice of the scale factor s and translational shifts ω_0 and ψ_0 .

The discussed problems are not restricted by 1D systems, and analogous difficulties arise in the studies of the Lyapunov exponents in the framework of the generalized version [17] of the Dorokhov–Mello–Peyrera–Kumar equation [28, 29]. The minimal Lyapunov exponent determines the critical properties of the Anderson transition (it is clear from the well-known numerical algorithm, see references in [17]), and the analogous hidden symmetry can be essential in the studies of the latter.

Appendix 1. To separation of variables in the equation (31).

For separation of variables in the eigenvalue problem

$$\hat{L} P(\rho, \psi) = \lambda P(\rho, \psi) \tag{A.1}$$

⁷ The distribution $P(\rho)$ is determined by the even moments of the transfer matrix elements T_{ij} . The odd moments should be taken into account in the analysis of $P(\rho, \omega)$.

⁸ More precisely, we consider a random potential of small amplitude with short-ranged correlations for energies near the edge of the initial band. If the energy is comparable with the bandwidth, there arise the effects of commensurability of the Fermi momentum \bar{k} with the lattice constant a_0 [22, 23], which can result in complication of the situation [24, 25].

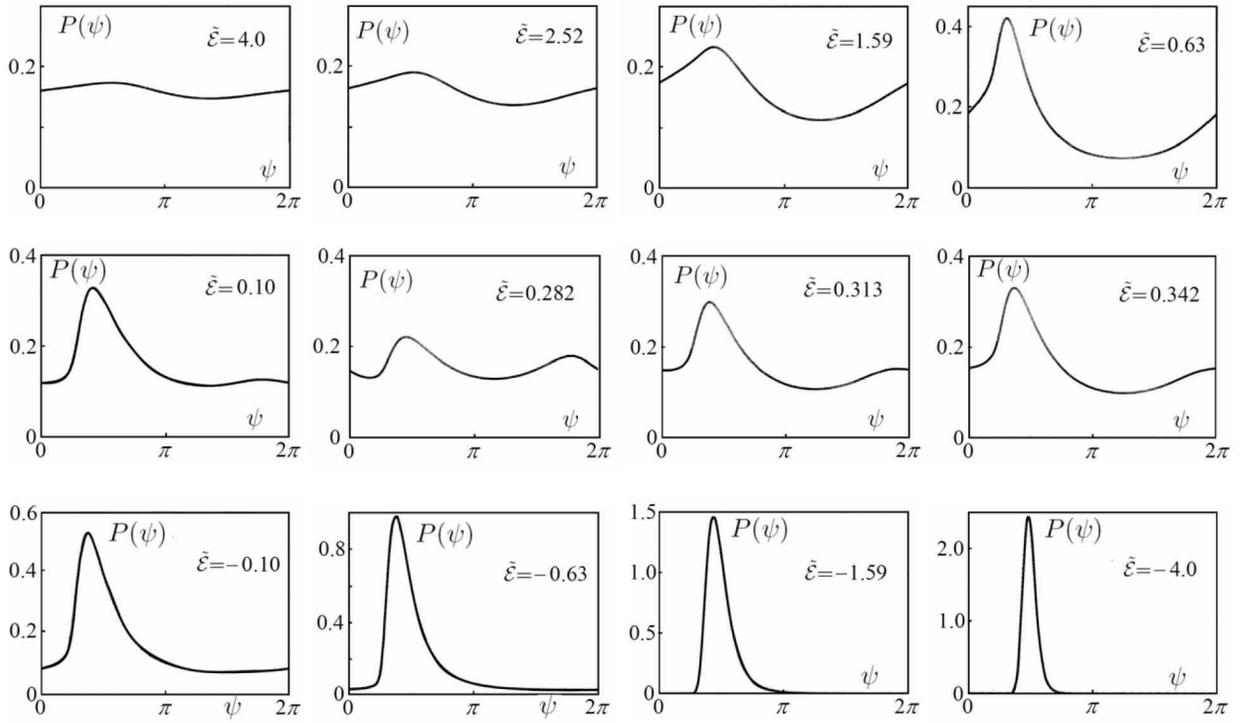


Figure 12: Evolution of the internal phase distribution under variation of the reduced energy $\tilde{\mathcal{E}}$.

the operator \hat{L} should be represented as a sum of two operators $\hat{L}_\rho + \hat{M}_\psi$, depending only on ρ and ψ correspondingly.

Conditions for separation of variables in the equation (31) appear to be essentially weaker. In the limit of large L , when the typical values of ρ are sufficiently large, one can set $R = 2$ to have the following structure for equation (31)

$$\frac{\partial P}{\partial L} = \left\{ \hat{L}_{\rho, \psi} P \right\}'_\rho + \left\{ \hat{M}_\psi P \right\}'_\psi. \quad (\text{A.2})$$

Setting $P = P(\rho)P(\psi)$ and dividing by $P(\rho)$, one has

$$\begin{aligned} -\frac{\partial P(\psi)}{\partial L} + \left\{ \hat{M}_\psi P(\psi) \right\}'_\psi &= \\ &= \frac{P(\psi)}{P(\rho)} \frac{\partial P(\rho)}{\partial L} - \frac{1}{P(\rho)} \left\{ \hat{L}_{\rho, \psi} P \right\}'_\rho. \end{aligned} \quad (\text{A.3})$$

The left-hand side is independent of ρ , and can be considered as a certain function $F(\psi)$. Then

$$P(\psi) \frac{\partial P(\rho)}{\partial L} - \left\{ \hat{L}_{\rho, \psi} P \right\}'_\rho = F(\psi) P(\rho) \quad (\text{A.4})$$

and integration over ρ gives $F(\psi) \equiv 0$, since the left-hand side turns to zero, while the integral over $P(\rho)$ is equal to unity due to normalization. As a result, the left-hand side and right-hand side of Eq. (A.3) turn to zero independently, and the equation for $P(\psi)$ is splitted off. Correspondingly, the averages of function of ψ , entering (34, 35), are determined by the stationary distribution $P(\psi)$, satisfying to equation (33).

Appendix 2. Edge matrices for the smeared interfaces

The edge matrices for the model represented in Fig.4 can be chosen in the form

$$T_l = \begin{pmatrix} e^{ikd_1} & 0 \\ 0 & e^{-ikd_1} \end{pmatrix} T_a \begin{pmatrix} e^{-ik_1 d_1} & 0 \\ 0 & e^{ik_1 d_1} \end{pmatrix} T_c \quad (\text{A.5})$$

$$T_r = T_{\tilde{c}} \begin{pmatrix} e^{-ik_1 d_2} & 0 \\ 0 & e^{ik_1 d_2} \end{pmatrix} T_{\tilde{a}} \begin{pmatrix} e^{ikd_2} & 0 \\ 0 & e^{-ikd_2} \end{pmatrix},$$

where

$$\begin{aligned} T_a &= \begin{pmatrix} a_1 & a_2 \\ a_2 & a_1 \end{pmatrix}, & a_1 &= \frac{k + k_1}{2k}, & a_2 &= \frac{k - k_1}{2k}, \\ T_c &= \begin{pmatrix} c & c^* \\ c^* & c \end{pmatrix}, & c &= \frac{ik_1 + \kappa}{2ik_1}, \\ T_{\tilde{a}} &= \begin{pmatrix} \tilde{a}_1 & \tilde{a}_2 \\ \tilde{a}_2 & \tilde{a}_1 \end{pmatrix}, & \tilde{a}_1 &= \frac{k_1 + k}{2k_1}, & \tilde{a}_2 &= \frac{k_1 - k}{2k_1}, \\ T_{\tilde{c}} &= \begin{pmatrix} \tilde{c} & \tilde{c}^* \\ \tilde{c}^* & \tilde{c} \end{pmatrix}, & \tilde{c} &= \frac{\kappa + ik_1}{2\kappa}, \end{aligned} \quad (\text{A.6})$$

Comparison with [16] shows that T_a and $T_{\tilde{a}}$ are the edge matrices for the boundary between two metals, while T_c and $T_{\tilde{c}}$ are the edge matrices for the boundary between a metal and a dielectric.

Composing the product $T_l T_r$, we find that relations $T_c T_{\tilde{c}} = 1$ and $T_a T_{\tilde{a}} = 1$ leads to essential simplifications, and under condition (57) this product reduces to the unit matrix.

For calculation of T_ϵ we can write

$$T_\epsilon = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \epsilon T_l \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} T_r \quad (\text{A.7})$$

and use the relations

$$T_c \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} T_{\tilde{c}} = \frac{\kappa}{ik_1} \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix},$$

$$\begin{aligned} & \begin{pmatrix} e^{-ik_1 d_1} & 0 \\ 0 & e^{ik_1 d_1} \end{pmatrix} \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \begin{pmatrix} e^{-ik_1 d_2} & 0 \\ 0 & e^{ik_1 d_2} \end{pmatrix} \\ & = \begin{pmatrix} 1 & e^{i\alpha} \\ -e^{-i\alpha} & -1 \end{pmatrix} \end{aligned} \quad (\text{A.8})$$

$$T_a \begin{pmatrix} 1 & e^{i\alpha} \\ -e^{-i\alpha} & -1 \end{pmatrix} T_{\bar{a}} = \begin{pmatrix} \mathcal{P} + \mathcal{Q} \cos \alpha & \mathcal{Q} + \mathcal{P} \cos \alpha + i \sin \alpha \\ -\mathcal{Q} - \mathcal{P} \cos \alpha + i \sin \alpha & -\mathcal{P} - \mathcal{Q} \cos \alpha \end{pmatrix},$$

which with the use of equality $\mathcal{P}^2 = \mathcal{Q}^2 + 1$ allow to reduce T_ϵ to the form (18).

Appendix 3. Degree of arbitrariness for the edge matrices

Let accept the form (60) for the edge matrices T_l and T_r , and demand that the matrix $T_\delta = T_l t_\delta T_r$ was the true transfer matrix, satisfying conditions (61); it is sufficient to impose the latter for small δ and obtain the relations

$$ad + bc + a^* d^* + b^* c^* = 0, \quad ab + c^* d^* = 0. \quad (\text{A.9})$$

The first relation together with the unit condition for the determinant leads to more simple relations

$$2 \operatorname{Re} ad = 1, \quad 2 \operatorname{Re} bc = -1. \quad (\text{A.10})$$

Setting

$$a = |a|e^{i\alpha}, \quad b = |b|e^{i\beta}, \quad c = |c|e^{i\gamma}, \quad d = |d|e^{i\delta}, \quad (\text{A.11})$$

we have the complete set of conditions

$$\begin{aligned} 2|b||c| \cos(\beta + \gamma) &= -1, \\ 2|a||d| \cos(\alpha + \delta) &= 1, \\ |a||b| &= |c||d|, \\ e^{i\alpha + i\beta + i\gamma + i\delta} &= -1, \\ |a||d| \sin(\alpha + \delta) - |b||c| \sin(\beta + \gamma) &= 0. \end{aligned} \quad (\text{A.12})$$

It is easy to see that $\sin(\alpha + \delta) = \sin(\beta + \gamma)$, $\cos(\alpha + \delta) = -\cos(\beta + \gamma)$; then from the last relation (A.12) we have $|a||d| = |b||c|$, which gives $|a| = |c|$, $|b| = |d|$ together with the third relation (A.12). As a result, the condition for T_δ to be the true transfer matrix determines 4-parameter family for the matrix T_l ,

$$\begin{aligned} T_l &= \begin{pmatrix} |a|e^{i\alpha} & |b|e^{i\beta} \\ |a|e^{i\gamma} & |b|e^{i\delta} \end{pmatrix}, \\ e^{i\alpha + i\beta + i\gamma + i\delta} &= -1, \quad 1 = -2|a||b| \cos(\beta + \gamma). \end{aligned} \quad (\text{A.13})$$

Calculating the matrix T_ϵ

$$T_\epsilon = \begin{pmatrix} 1 - \bar{\epsilon}(a-b)(c-d) & \bar{\epsilon}(a-b)^2 \\ -\bar{\epsilon}(c-d)^2 & 1 + \bar{\epsilon}(a-b)(c-d) \end{pmatrix}, \quad (\text{A.14})$$

and demanding that it was the true transfer matrix, we obtain

$$\begin{aligned} (a-b)(c-d) + (a^* - b^*)(c^* - d^*) &= 0, \\ (a-b)^2 + (c^* - d^*)^2 &= 0, \end{aligned} \quad (\text{A.15})$$

Introducing the parametrization

$$(a-b) = r e^{i\theta/2}, \quad (c-d) = r_1 e^{i\varphi/2}, \quad (\text{A.16})$$

we have $r = r_1$, $\varphi = \pi - \theta + 2\pi n$, so

$$T_\epsilon = \begin{pmatrix} 1 - i\bar{\epsilon}r^2(-1)^n & \bar{\epsilon}r^2 e^{i\theta} \\ \bar{\epsilon}r^2 e^{-i\theta} & 1 + i\bar{\epsilon}r^2(-1)^n \end{pmatrix}, \quad (\text{A.17})$$

where n is integer. Taking into account relations

$$\begin{aligned} r^2 &= |a-b|^2 = |a|^2 + |b|^2 - 2|a||b| \cos(\alpha-\beta), \\ r^2 &= |c-d|^2 = |a|^2 + |b|^2 - 2|a||b| \cos(\gamma-\delta), \end{aligned} \quad (\text{A.18})$$

we have $(\alpha-\beta) = \pm(\gamma-\delta) + 2\pi k$. The upper sign leads to contradiction, since $\beta+\gamma = \pi/2 + \pi k$ and the left-hand side of (A.12) turns to zero. For the lower sign we have $\gamma = \pi/2 - \alpha + \pi k$, $\delta = \pi/2 - \beta + \pi k'$, where k and k' should be chosen even for $\sin(\beta-\alpha) > 0$ and odd in the opposite case. As a result, we come to representation (62) for the matrix T_l with 3-parameter arbitrariness. For even k, k' we have even n in the expression (A.17) for T_ε , and it reduces to (18) with parameters K and γ , given by Eq.63. For odd k, k' we have odd n in (A.17), and to reduce it to the form (18) we need to make the inessential change of sign for $\bar{\varepsilon}$.

Appendix 4. Distribution $P(\omega)$ for $\mathcal{E} = 0$

Differentiating (41) and suggesting the power-law asymptotics $P(\omega) \sim \omega^{-\alpha}$ for $\omega \rightarrow \infty$, we obtain $\alpha = 2$. Considering corrections to the asymptotics in the form of a series over inverse powers of ω ,

$$P(\omega) = \omega^{-2} \sum_{n=0}^{\infty} A_n \omega^{-n}, \quad (\text{A.19})$$

we have the recurrence relations

$$\begin{aligned} A_0 &= 1, \quad A_1 = 0, \quad A_2 = -b/a, \\ aA_{n+1} &= -bA_{n-1} + nA_{n-2}, \quad n \geq 2. \end{aligned} \quad (\text{A.20})$$

For the critical distribution ($\mathcal{E} = 0$) we have $b = 0$, and the coefficients of the series can be found explicitly

$$P(\omega) = \frac{1}{\omega^2} \sum_{k=0}^{\infty} \frac{\Gamma(k+2/3)}{\Gamma(2/3)} \left(\frac{3}{a\omega^3} \right)^k. \quad (\text{A.21})$$

The divergent series can be summed in the Borel sense [26], if one write the gamma function $\Gamma(k+2/3)$ in the form of the defining integral and summing the arising geometrical progression. Setting $a = -1$ and including the normalization factor, we obtain (70).

Expressions (A.19), (A.20) are useful for numerical integration of equation (41) for arbitrary b . For $|\omega| > 5$ the function $P(\omega)$ is well approximated by the series (A.19), interpreted in the asymptotical sense and summed till the minimal term. Such approximation can be used as an initial condition at large positive ω for integration in the direction of diminishing of ω .⁹ If the standard procedures with the accuracy control [27] are used, the solution automatically comes to the correct asymptotics at $\omega \rightarrow -\infty$.

Appendix 5. Behavior of s and ω_0 in the forbidden band

In the deep of the forbidden band, the constant C_0 in (41) is exponentially small, and the distribution $P(\omega)$ can be accepted in the form

$$P(\omega) = \text{const} \exp \{ -b\omega - a\omega^3/3 \}. \quad (\text{A.22})$$

In the case $-a = b \gg 1$ the distribution has a maximum at $\omega = -1$, in whose vicinity it reduces to the Gaussian form (69). Calculation of averages in (38) gives the results

$$\begin{aligned} \langle \sin \psi \rangle &= \left\langle -\frac{2\omega}{1+\omega^2} \right\rangle \approx \left\langle 1 - \frac{\tilde{\omega}^2}{2} \right\rangle = 1 - \frac{1}{4|a|}, \\ \langle \sin^2 \psi \rangle &= \left\langle \frac{4\omega^2}{(1+\omega^2)^2} \right\rangle \approx \langle 1 - \tilde{\omega}^2 \rangle \approx 1, \end{aligned}$$

⁹ Attempts to integrate in the direction of increasing of ω meet instabilities, relating with existence of the growing exponent, being a solution of equation (41) for $C_0 = 0$.

$$\langle \cos \psi \rangle = \left\langle \frac{\omega^2 - 1}{1 + \omega^2} \right\rangle \approx \langle -\tilde{\omega} \rangle \approx 0, \quad (\text{A.23})$$

and for parameters D and v one has

$$D = 2\bar{\epsilon}^2, \quad v = 2\delta - \bar{\epsilon}^2, \quad (\text{A.24})$$

which agree with results from the analysis of moments [16] within accuracy; here $\tilde{\omega}$ is deviation from the maximum, and the fact is used that ϵ reduces to $\bar{\epsilon}$ for $|a| = |b|$.

To reproduce D and v with higher accuracy, let make the scale transformation and translation of the distribution (A.22) with $-a = b$; then for $s = 1 - \bar{s}$, $\omega_0 = \bar{s} + \tilde{\omega}_0$ and $\bar{s}, \tilde{\omega}_0 \ll 1$ one has

$$D = 2\bar{\epsilon}^2 (1 + 2\bar{s} - \bar{\epsilon}^2/\delta), \quad (\text{A.25})$$

$$v = 2\delta - \bar{\epsilon}^2 + (\bar{s}^2 - \tilde{\omega}_0^2) \delta - \bar{\epsilon}^2 (2\tilde{\omega}_0 + 2\bar{s} + 9\bar{\epsilon}^2/4\delta),$$

where the shift of the maximum and small deviations from the Gaussian form are taken into account. Comparison with values from the analysis of moments [16]

$$D = 2\bar{\epsilon}^2 - \frac{15}{2} \frac{\bar{\epsilon}^2}{\delta}, \quad v = 2\delta - \bar{\epsilon}^2 + \frac{27}{4} \frac{\bar{\epsilon}^2}{\delta} \quad (\text{A.26})$$

leads to the following results, if the relation $\delta/\bar{\epsilon}^2 = 4|\tilde{\mathcal{E}}|^{3/2}$ is taken into account,

$$s = 1 + \frac{11}{32} \frac{1}{|\tilde{\mathcal{E}}|^{3/2}}, \quad \omega_0 = \frac{-19 \pm i\sqrt{215}}{32|\tilde{\mathcal{E}}|^{3/2}}, \quad (\text{A.27})$$

which explains the behavior of curves in the left-hand part of Fig.8. The translational shift ω_0 appears to be complex-valued; one can easily verify for the Gaussian distribution, that neglect of the small imaginary part of ω_0 is equivalent to taking the modulus of the complex distribution $P(\omega)$.

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