Spectral Dependence of Degree of Localization of Eigenfunctions of the 1D Schrodinger Equation with a Peacewise-Constant Random Potential

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Abstract

The perturbation theory is developed for joint statistics of the advanced and retarded Green’s functions of the 1D Schrodinger equation with a piecewise-constant random potential. Using this method, analytical expressions are obtained for spectral dependence of the degree of localization and for the limiting (at $t \to \infty$) probability to find the particle at the point it was located at $t = 0$ (Andeson criterion). Definition of the localization length is introduced. The computer experiments confirming correctness of the calculations are described.

1 Introduction, Formulation of the Problem, and Main Results

Mathematical problems arising in the physics of solid-state random systems are characterized by a complexity and absence of universal methods of analysis. In searching for such methods, an important role is played by strongly simplified models of disordered systems, with the 1D single-particle ones being the most important among them. The heuristic significance of the 1D models is, however, not the only one. The physical systems like J-aggregates, quantum wells, optical fibers, Bragg layered structures, etc. can be directly described by the 1D models. In such systems, one may expect strong effects of disorder, which makes studying of the disordered 1D models especially topical.

In the theory of the simplest solid-state disordered models, one can distinguish the continuous and discrete models\cite{1}. The continuous models employ the Schrodinger equation
$[-d^2/dx^2 + U(x)]\psi = E\psi$ with one or another potential $U(x)$, while the discrete models use random matrices of a model Hamiltonian. In spite of similarity of these two models, each of them has its own specificity. For example, when analyzing vibrations of disordered chains [2, 3], the discrete model is used, whereas when studying propagation of electromagnetic waves in disordered layered structures, the continuous model looks more convincing.

For the 1D models, in a number of cases, mathematically correct methods of theoretical analysis can be proposed [4, 5, 1]. Of particular interest are the cases, when one and the same method appears to be suitable for analysis of several different model problems, and the method proves to be, to a certain extent, universal. It is noteworthy, in this connection, that the perturbation theory for the joint statistics of the advanced and retarded Green’s functions used in this paper for analysis of the continuous disordered model, has been successfully used previously for studying the discrete models [6, 7].

Let us pass to the problem studied in this paper. Consider a 1D continuous disordered model with a piecewise-constant random potential $U(x)$ equal to $u$ inside the intervals $x \in [b(n-1), bn], n = 1, 2, ..., N$. Here, $\varepsilon_n$ are the independent limited random quantities with a known distribution function $P(\varepsilon)$, and $u < 0$ is the negative number sufficiently big to make $U(x) < 0$ at $x \in [0, Nb]$. The length $b$ is a specified parameter of the potential $U(x)$. For $x \in [0, Nb]$, we assume that $U(x) = 0$. The distribution function $P(\varepsilon)$ is taken in the following, fairly general, form

$$P(\varepsilon) = \frac{1}{\Delta} p\left(\frac{\varepsilon}{\Delta}\right), \quad p(\varepsilon) > 0, \quad M_n \equiv \int p(\varepsilon)\varepsilon^n d\varepsilon, \quad M_0 = 1, \quad M_1 = 0$$

(1)

The parameter $\Delta$ is the measure of disorder and, at $\Delta = 0$, the function $U(x)$ represents a potential box with a flat bottom with the depth $u$ and length $Nb$. At $\Delta > 0$, we can say that the function $U(x)$ corresponds to a potential box with a fluctuating bottom. Hereafter, we imply the thermodynamic limit $N \to \infty$.

Consider the motion of a particle in such a random potential and formulate the following problem. Let the particle, at $t = 0$, to be located in the point $r = Nb$, (i.e., at the right side of the potential box with the fluctuating bottom), and we are seeking for the density of probability that the particle will remain in this point at $t \to \infty$. From the mathematical viewpoint, it means that, at $t = 0$, the wave function of the particle had the form $\Psi(t = 0, x) = \delta(x - r)$, and we have to find $D = \lim_{t \to \infty} \langle |\Psi(t, r)|^2 \rangle$. The angle brackets here and below indicate averaging over realizations of the random potential $U(x)$. This problem is well known in the theory of Anderson localization [1, 8] and it can be shown [6] that, if $\psi_n(x)$ are the eigenfunctions of the Hamiltonian $H = -d^2/dx^2 + U(x)$, then $D = \langle \sum_n |\psi_n(r)|^4 \rangle$. Nonzero value of $D$ indicates that there exist localized functions (i.e., functions essentially nonzero in some finite region, with its
size independent of \( N \), at \( N \to \infty \) among eigenfunctions of the Hamiltonian \( H \) \[6, 1, 8\]. To judge about the presence or absence of the localized states in the energy interval \([U, U + dU]\), in \[6\] there has been introduced the participation function \( W(U) \) defined by the relationship

\[
W(U)\,dU = \langle \sum_{n, E_n \in [U, U + dU]} |\psi_n(r)|^4 \rangle,
\]

where \( E_n \) is the eigenenergy of the Hamiltonian \( H \). If the eigenfunctions of the Hamiltonian \( H \) with energy \( U \) are delocalized, then \( W(U) = 0 \). Otherwise, \( W(U) \) is nonzero. For this reason, the participation function will be below referred to as *spectral dependence of the degree of localization*. The main results of this paper are the following expressions for the function \( W \) and the quantity \( D \):

\[
W(U) = \Theta(-U)\Theta(U - u) \left( \frac{\Delta}{u} \right)^2 \frac{M_2}{2\pi} \sin^2 b\sqrt{U - u} \cdot O(\Delta^3), \quad u < 0 \tag{2}
\]

\[
D = \int_u^0 W(U)\,dU = \left( \frac{\Delta}{u} \right)^2 \frac{M_2}{2\pi b} \left( \sqrt{-u} - \frac{\sin[2b\sqrt{-u}]}{2b} \right) + O(\Delta^3), \tag{3}
\]

These formulas are applicable to the above 1D continuous model with a piecewise-constant random potential.

Concluding the introduction, note that the Helmholtz equation describing propagation of electromagnetic waves in a layered system, in fact, coincides with the Schrodinger equation studied in this paper. This gives the grounds to assert that the results obtained in this paper can be used in studies of propagation of electromagnetic waves in 1D photonic crystals in the presence of disorder.

## 2 Continuous model. General properties of the Schrodinger equation Green’s function.

To solve the above typical problem of the theory of disordered systems, we will apply the method of joint statistics of the advanced and retarded edge Green’s function (EGF) used in \[6,7\] for analysis of the discrete 1D disordered models. A crucial point of the above method is the fact that, in the discrete 1D model, the EGF of a chain with a single structural unit added can be expressed algebraically through the EGF of the initial chain \[4,1,7\]. In this section, we will briefly remind the properties of Green’s function of the differential Schrodinger equation with the Hamiltonian

\[
H \equiv -d^2/dx^2 + U(x) \tag{4}
\]

and, in the next one, we will present a similar relation for the EGF, valid for the case of the continuous model with the piecewise-constant potential \( U(x) \).
Green’s function of operator (4) is defined by the formula

\[ G_{xx'}(\Omega) \equiv \sum_n \frac{\psi_n(x)\psi_n^*(x')}{\Omega - E_n} + \int dp \frac{\phi_p(x)\phi_p^*(x')}{\Omega - E_p} \]  

(5)

where \( \psi_n(\phi_p) \) and \( E_n(E_p) \) are, respectively, the eigenfunctions and eigenvalues of operator (4), corresponding to the discrete (continuous) spectrum. Here, \( n(p) \) is the discrete (continuous) number of the eigenfunction. The energy argument \( \Omega \) of the Green’s function is, generally, a complex number \( \Omega = U - iV \) (with \( U \) and \( V \) being real). Using Eq. (5), one can show that the solution \( \Psi(t, x) \) of the time-dependent Schrödinger equation, with the initial condition \( \Psi(0, x) = \Psi_0(x) \), can be expressed in terms of the Green’s function (5), as follows

\[ \Psi(t, x) = \lim_{V \to +0} \frac{1}{2\pi i} \int dU dU' e^{U't} G_{xx'}(U - iV) \Psi_0(x'), \quad t > 0 \]  

(6)

It can be easily shown that the Green’s function (5) satisfies the differential equation

\[ \left[ \Omega + \frac{d^2}{dx^2} - \mathcal{U}(x) \right] G_{xx'}(\Omega) = \delta(x - x') \]  

(7)

where only solutions vanishing at \( x \to \pm \infty \) should be taken to provide convergence of integrals [6]. Taking into account the above properties of the Green’s function, one can see that the quantity \( D \), introduced in Sect.1, is expressed through the product of diagonal elements of the advanced and retarded EGF in the following way

\[ D = \lim_{t \to \infty} \left\langle |\Psi(t, r)|^2 \right\rangle = \lim_{l \to \infty} \lim_{V_{1,2} \to 0} \frac{1}{4\pi^2} \int dU_1 dU_2 \ e^{\left(U_1 - U_2\right)t} \left\langle G_{rr}(U_1 - iV_1)G_{rr}(U_2 + iV_2) \right\rangle, \]  

(8)

Hear \( r \) is the coordinate of the right side of the potential box with a fluctuating bottom described in Introduction. Using spectral expansion (5), one can show that the quantity \( D \) is determined only by discrete states of the Hamiltonian (4), with the following formula being valid [6]

\[ D = \lim_{t \to \infty} \left\langle |\Psi(t, r)|^2 \right\rangle = \left\langle \sum_n |\psi_n(r)|^4 \right\rangle \]  

(9)

By limiting the region of integration in (8) so that \( U_{1,2} \in [U, U + dU] \), we can obtain the participation function \( W(U) \), introduced in [6]

\[ W(U)dU = \left\langle \sum_{E_n \in [U, U + dU]} |\psi_n(r)|^4 \right\rangle \]  

(10)

As was already mentioned, nonzero value of \( W(U) \) indicates presence of localized states in the energy interval \([U, U + dU]\). In the opposite case, \( W(U) = 0 \).
3 Case of the peacewise-constant potential. Recurrent relations for the EGF.

Consider the following family of random potentials constant within the intervals of length $b$:

$$U_m(x) = \begin{cases} u + \varepsilon_n, & x \in [b(n-1), bn], \quad x \leq mb \quad (u < 0, n-) \\ 0, & x > mb \end{cases}$$  \hspace{1cm} (11)

Here $\varepsilon_n$ are the independent bounded random quantities with the distribution function $P(\varepsilon)$, and $u$ is the negative number sufficiently large to meet the condition $u + \varepsilon_n < 0$. Assume the EGF $G_{mb,mb}^m(\Omega) \equiv \gamma_m(\Omega)$ of the Schrodinger equation (4) with the potential $U_m(x)$ to be known.

Let us pass to the potential $U_{m+1}(x)$ and consider the EGF $G_{mb+1,mb+1}^{m+1}(\Omega) \equiv \gamma_{m+1}(\Omega)$ of Eq. (4) corresponding to this potential $U_{m+1}(x)$. In this section, we will express the EGF $\gamma_{m+1}(\Omega)$ through $\gamma_m(\Omega)$ using the fact that, at $x < mb$, these potentials are the same.

Note, first of all, that the discrete spectrum of operator (4) with potential (11), we are interested in, is positioned on the negative semiaxis. For this reason, in what follows, we will consider real part $U$ of the energy argument of the Green’s function to be negative $\Omega = U - iV, U < 0$. The Green’s function $G_{x,mb}^m(\Omega)$ meets the equations

$$\begin{cases} \left[\Omega + \frac{d^2}{dx^2} - U_m(x)\right]G_{x,mb}^m(\Omega) = 0, & \text{at } x < mb \\ \left[\Omega + \frac{d^2}{dx^2}\right]G_{x,mb}^m(\Omega) = 0, & \text{at } x > mb \end{cases}$$

Let us introduce the functions $\Psi_\pm(x)$, so that

$$\begin{cases} \left[\Omega + \frac{d^2}{dx^2} - U_m(x)\right]\Psi_-(x) = 0, & \text{with } \Psi_-(\infty) = 0 \quad \Psi_-(mb) = 1 \\ \left[\Omega + \frac{d^2}{dx^2}\right]\Psi_+(x) = 0, & \text{with } \Psi_+(\infty) = 0 \quad \Psi_+(bm) = 1 \end{cases}$$  \hspace{1cm} (13)  \hspace{1cm} (14)

Equations and conditions (13) and (14) determine the functions $\Psi_\pm(x)$ in a unique way. It follows from Eq. (14) that

$$\Psi_+(x) = e^{\sqrt{\Omega}x - bm}, \quad \Omega = U - iV, \quad V > 0, \quad U < 0$$  \hspace{1cm} (15)

The Green’s function we are interested in can be expressed in terms of the functions $\Psi_\pm(x)$ as follows

$$G_{x,mb}^m(\Omega) = \begin{cases} A\Psi_-(x), & \text{at } x < mb \\ B\Psi_+(x), & \text{at } x > mb \end{cases}$$  \hspace{1cm} (16)

The continuity of the function $G_{x,mb}^m(\Omega)$ at $x = mb$ together with a unit jump of its derivative in this point lead to the system of equations for the constants $A$ and $B$. Solving this system and
taking into consideration that \( \Psi_\pm(mb) = 1 \), we obtained for the EGF \( G_{bm,bm}^m(\Omega) \) the following relation
\[
\gamma_m(\Omega) \equiv G_{bm,bm}^m(\Omega) = \frac{1}{\Psi_+(bm) - \Psi_-(bm)} \tag{17}
\]
Note that the function \( \Psi_+(x) \), entering this relation, is known in the explicit form \([15]\).

Now, let us pass from the potential \( U_m(x) \) to the potential \( U_{m+1}(x) \) and consider the Green’s function \( G_{x,b(m+1)}^{m+1}(\Omega) \). It satisfies the equations similar to \([12]\)
\[
\begin{aligned}
\Omega + \frac{d^2}{dx^2} - U_{m}(x) G_{x,b(m+1)}^{m+1}(\Omega) & = 0, \text{ at } x < bm \\
\Omega + \frac{d^2}{dx^2} - \eta G_{x,b(m+1)}^{m+1}(\Omega) & = 0, \text{ at } bm < x < b(m+1), \quad \eta \equiv u + \varepsilon_{m+1} \\
\Omega + \frac{d^2}{dx^2} G_{x,b(m+1)}^{m+1}(\Omega) & = 0, \text{ at } x > b(m+1)
\end{aligned}
\tag{18}
\]
By analogy with \([16]\), we can write the following expressions for \( G_{x,b(m+1)}^{m+1}(\Omega) \)
\[
\begin{aligned}
G_{x,b(m+1)}^{m+1}(\Omega) & = \hat{A} \Psi_-(x), \text{ at } x < bm \\
G_{x,b(m+1)}^{m+1}(\Omega) & = Ce^{i\sqrt{\Omega-\eta}x} + Fe^{-i\sqrt{\Omega-\eta}x}, \text{ at } bm < x < b(m+1) \\
G_{x,b(m+1)}^{m+1}(\Omega) & = \hat{B} \Psi_+(x), \text{ at } x > b(m+1)
\end{aligned}
\tag{19}
\]
At \( x = mb \), the Green’s function \( G_{x,b(m+1)}^{m+1}(\Omega) \) should be continuous together with its first derivative, while, at \( x = (m+1)b \), the function \( G_{x,b(m+1)}^{m+1}(\Omega) \) should be continuous, and its derivative should experience a unit jump. This yields four equations for the constants \( \hat{A}, C, F, \) and \( \hat{B} \) entering \([19]\). The EGF \( \gamma_{m+1}(\Omega) \) of interest, corresponding to the potential \( U_{m+1}(x) \), can be obtained from \([19]\)
\[
\gamma_{m+1}(\Omega) \equiv G_{b(m+1),b(m+1)}^{m+1}(\Omega) = \hat{B} \Psi_+(b(m+1)) \tag{20}
\]
Finding the constant \( \hat{B} \) from the above system of equations for \( \hat{A}, C, F, \) and \( \hat{B} \) and using Eq. \([15]\) for the function \( \Psi_+(x) \), we obtain for the EGF \( \gamma_{m+1}(\Omega) \) the following relation
\[
\frac{t \sqrt{\Omega - \eta} - \Psi_-'(mb)}{\sqrt{\Omega - \eta} + t \Psi_-'(mb)} = -i \sqrt{\frac{\Omega}{\Omega - \eta}} + \frac{1}{\gamma_{m+1}(\Omega) \sqrt{\Omega - \eta}} \quad t \equiv \tan [b \sqrt{\Omega - \eta}] \tag{21}
\]
Now, using \([17]\) we can express \( \Psi_-'(mb) \) through the EGF \( \gamma_m(\Omega) \)
\[
\Psi_-'(mb) = i \sqrt{\Omega} - \frac{1}{\gamma_m(\Omega)} \tag{22}
\]
Here, we took into consideration that \( \Psi_+'(bm) = i \sqrt{\Omega} \) at \( U < 0 \). With the use of Eqs. \([21]\) and \([22]\), we can obtain the sought relation between EGF \( \gamma_{m+1}(\Omega) \) and EGF \( \gamma_m(\Omega) \) (the corresponding operation will be further referred to as \( \mathcal{R}^{-1} \))
\[
\gamma_{m+1} = \frac{h + \gamma_m}{q + v\gamma_m} \equiv \mathcal{R}_{\Omega,b}^{-1}(\gamma_m) \tag{23}
\]
where
\[ h \equiv -\frac{t}{\sqrt{\Omega - \eta + it\sqrt{\Omega}}}, \quad q \equiv \frac{\sqrt{\Omega - \eta - it\sqrt{\Omega}}}{\sqrt{\Omega - \eta + it\sqrt{\Omega}}} \quad v \equiv -\frac{t\eta}{\sqrt{\Omega - \eta + it\sqrt{\Omega}}} \]
\[ t = \tan[b\sqrt{\Omega - \eta}], \quad \Omega = U \pm iV, \quad U < 0, V = +0, \quad \eta \equiv u + \varepsilon_{m+1} \]

Below, we will need the operation \( R \) inverse to (23), which has the following form
\[ \gamma_m = \gamma_{m+1} + \frac{h}{1 - v\gamma_{m+1}} \equiv R_{\Omega, \eta}(\gamma_{m+1}) \] (24)

Thus, the whole method of analysis of the joint statistics of the EGF, developed in [6, 7] for discrete models, can be applied to the considered case of a continuous model, corresponding to Schrödinger equation (4) with the piecewise-constant potential [11]. Relevant calculations are presented in the following sections.

4 Calculating spectral dependence of the degree of localization

4.1 Joint statistics of the Green’s functions

Spectral dependence of the degree of localization \( W(U) \) and the probability \( D \) to find the particle at the edge of the random 1D system under consideration are given, respectively, by Eqs. (10) and (9). These formulas are identical to those for similar quantities of the discrete model [6, 7]. For this reason, for realization of Eqs. (10) and (9), one can use the method based on calculation of joint statistics of the advanced and retarded Green’s functions developed in [6, 7]. Let us remind briefly this method. In the integrals entering Eq. (8), we make the following substitution \( \omega \equiv U_2 - U_1, U \equiv U_1 \) and change the notations \( G_{rr} \to \gamma \). Then, for the value \( D \) (9), we can write the following expression
\[ D = \frac{1}{4\pi^2} \lim_{\epsilon \to 0} \lim_{V_1, V_2 \to +0} \int d\omega dU e^{-\epsilon t}(\gamma(U - iV_1)\gamma(U + \omega + iV_2)) \] (25)

If the function \( \rho(x_1 y_1 x_2 y_2) \) is the joint statistics of the advanced and retarded Green’s functions entering (25) (here, the arguments \( x_i \) and \( y_i, i = 1, 2 \) correspond to real and imaginary parts of these functions), then the averaged value of their product can be represented in the form
\[ \langle \gamma(U - iV_1)\gamma(U + \omega + iV_2) \rangle = \int dx_1 dy_1 dx_2 dy_2 \rho(x_1 y_1 x_2 y_2)\langle x_1 x_2 - y_1 y_2 + i(x_1 y_2 + x_2 y_1) \rangle \equiv \langle x_1 x_2 \rangle - \langle y_1 y_2 \rangle + i\langle x_1 y_2 \rangle + i\langle y_1 x_2 \rangle, \] (26)
It was shown in [6] that it suffices to calculate only $i\langle x_1y_2 \rangle$ and to multiply the result by 4. In accordance with [7], calculation of this contribution at $V_{1,2} \to +0$ can be performed using the formula

$$\langle x_1y_2 \rangle = \int d\varepsilon d\tilde{x}_1 d\tilde{x}_2 P(\varepsilon) \sigma_{U,U+\omega}(\tilde{x}_1, \tilde{x}_2) x_1(\tilde{x}_1) y_2(\tilde{x}_2),$$  

(27)

with the form of the dependences $x_1(\tilde{x}_1)$ and $y_2(\tilde{x}_2)$ being determined by the fractional-linear function $\mathcal{R}_{\Omega,\eta}^{-1}(x)$ (23),

$$\mathcal{R}_{\Omega,\eta}^{-1}(x) = \frac{h + x}{q + vx} \equiv \frac{a_{\Omega,\eta} + b_{\Omega,\eta}x}{c_{\Omega,\eta} + g_{\Omega,\eta}x},$$  

(28)

which looks like this

$$x_1 = \text{Re} \left[ \mathcal{R}_{\Omega,\eta}^{-1}(\tilde{x}_1) \right], \quad y_2 = \text{Im} \left[ \mathcal{R}_{\Omega,\eta}^{-1}(\tilde{x}_2) \right], \quad \eta = u + \varepsilon, \quad \Omega_1 = U - iV_1, \quad \Omega_2 = U + \omega + iV_2$$  

(29)

Function $\sigma_{U,U+\omega}(x_1x_2)$ in Eq. (27) represents the joint statistics of the real Green’s functions with the energy arguments $U$ and $U + \omega$, respectively. In [7], it has been shown that this function satisfies the following equation

$$\sigma_{U_1U_2}(x_1x_2) = \int d\varepsilon \ P(\varepsilon) \sigma_{U_1U_2} \left[ \mathcal{R}_{U_1\eta}(x_1), \mathcal{R}_{U_2\eta}(x_2) \right] \left| \frac{d\mathcal{R}_{U_1\eta}(x_1)}{dx_1} \right| \left| \frac{d\mathcal{R}_{U_2\eta}(x_2)}{dx_2} \right|, \quad \eta = u + \varepsilon$$  

(30)

with the operation $\mathcal{R}_{U_\eta}(x)$, in this case, being determined by Eq. (24). As shown in [7], at $V_{1,2} \to +0$, the relations (29) lead to the following expressions for $y_2(\tilde{x}_2)$ and $x_1(\tilde{x}_1)$:

$$y_2(\tilde{x}_2) \bigg|_{V_2 \to +0} = \pi \frac{a_{U+\omega,\eta}g_{U+\omega,\eta} - b_{U+\omega,\eta}c_{U+\omega,\eta}}{g_{U+\omega,\eta}^2} \delta \left( \tilde{x}_2 + \frac{c_{U+\omega,\eta}}{g_{U+\omega,\eta}} \right),$$   

(31)

$$x_1(\tilde{x}_1) \bigg|_{V_1 \to +0} = \frac{a_{U,\eta} + b_{U,\eta}\tilde{x}}{c_{U,\eta} + g_{U,\eta}\tilde{x}}$$  

(32)

Substitution of these expressions into (27), allows us to obtain, for the quantity $\langle x_1y_2 \rangle$ of interest the following relationship [7]

$$\langle x_1y_2 \rangle = \pi \lim_{a \to 0} a^2 \int \sigma_{U,U+\omega}(x,a)xdx$$  

(33)

When deriving this relationship, we took into account that the function $\sigma_{U,U+\omega}(x_1x_2)$ meets Eq. (30). It follows from the above formulas that the quantity $D$, we are interested in, may be represented in the form

$$D = \frac{1}{\pi^2} \lim_{V_{1,2} \to 0, t \to \infty} \int e^{\omega t} \langle x_1y_2 \rangle d\omega dU = \frac{1}{\pi} \lim_{a \to 0, t \to \infty} \int e^{\omega t} a^2 \sigma_{U,U+\omega}(x,a)xdxd\omega dU$$  

(34)
As shown in [6], the participation function $W(U)$ can be obtained from Eq. (34) by omitting the integration over $U$:

$$W(U) = \frac{1}{\pi} \lim_{a \to \infty, t \to \infty} \int e^{i\omega t} a^2 \sigma_{U,U+a}(x,a) x dx d\omega$$

(35)

In this way, the problem is reduced to solving Eq. (30). The perturbative approach to equations of the type (30), proposed in [6], is the power expansion in $\Delta$ (see Eq. (1)), with the first nonzero correction being of the order of $\Delta^2$. It was also shown in [6] that, to calculate the quantities $D$ and $W(U)$, only the part of the solution of the equation for the joint statistics (in our case, Eq. (30)), singular in $\omega$, is needed, with the singularity being of the pole type. Thus, the needed singular part (referred to as sing) can be represented in the form

$$\text{sing } \sigma_{U\omega}(x_1 x_2) = \frac{\Delta^2}{\omega} F_U(x_1 x_2) + O(\Delta^3)$$

(36)

Now, using Eq. (35), for the function $W(U)$ and quantity $D$, we obtain the following formulas

$$W(U) = -\Delta^2 \lim_{a \to \infty} a^2 \int F_U(x,a) x dx + O(\Delta^3), \quad D = \int W(U) dU$$

(37)

In the following section, we will present the perturbative approach to Eq. (30) and will derive an explicit expression for the function $F_U(x_1 x_2)$ entering Eq. (36).

4.2 Perturbative approach to Eq. (30)

To solve the functional equations arising in the perturbation theory described below one has to find the eigenfunctions and eigenvalues of the functional operator $\mathcal{H}_{\Omega,\eta}$, which acts upon an arbitrary function $f(x)$ as follows:

$$\mathcal{H}_{\Omega,\eta} f(x) \equiv \frac{dR_{\Omega,\eta}}{dx} f[R_{\Omega,\eta}(x)]$$

(38)

where $R_{\Omega,\eta}$ is given by (24). We assume the parameter $\Delta$ to be small and represent the sought function $\sigma_{U_1 U_2}(x_1 x_2)$ as a power series in $\Delta$.

$$\sigma_{U_1 U_2}(x_1 x_2) = \sum_{n=0}^{\infty} Q_n(x_1, x_2) \Delta^n$$

(39)

Let us expand the function $\sigma_{U_1 U_2}[R_{U_1,\eta}(x_1), R_{U_2,\eta}(x_2)] \frac{dR_{U_1,\eta}(x_1)}{dx_1} \frac{dR_{U_2,\eta}(x_2)}{dx_2}$, in the right-hand side of (30) into a power series in $\varepsilon$. Then, Eq. (30) yields

$$\sum_{n=0}^{\infty} Q_n(x_1, x_2) \Delta^n =$$

(40)

$^2$This problem is solved in Appendix, and, in what follows, we will use the results obtained in it.
\[
\sum_{n,l=0}^{\infty} \frac{M_n \Delta^{n+l}}{n!} \frac{\partial^n}{\partial \varepsilon^n} \left\{ Q_l \left[ \mathcal{R}_{U_1,\eta}(x_1), \mathcal{R}_{U_2,\eta}(x_2) \right] \right\} \left[ \frac{d\mathcal{R}_{U_1,\eta}(x_1)}{dx_1} \right] \left[ \frac{d\mathcal{R}_{U_2,\eta}(x_2)}{dx_2} \right] \bigg|_{\varepsilon=0}
\]

Remind that the dependence on \( \varepsilon \) in this equation is provided by the quantity \( \eta = u + \varepsilon \). By equating the coefficients at the same powers of \( \Delta \) in the right- and left-hand sides of Eq. \( \text{(40)} \), we obtain the recurrent relations for the function \( Q_0 \)

\[ \Delta^0 : \quad Q_0(x_1 x_2) - Q_0 \left[ \mathcal{R}_{U_1,u}(x_1), \mathcal{R}_{U_2,u}(x_2) \right] \left| \frac{d\mathcal{R}_{U_1,u}(x_1)}{dx_1} \right| \left| \frac{d\mathcal{R}_{U_2,u}(x_2)}{dx_2} \right| = 0 \quad (41) \]

Since the first moment of the function \( P(\varepsilon) \) [1] is zero, the quantity \( Q_1 \) vanishes,

\[ \Delta^2 : \quad Q_2(x_1 x_2) - Q_2 \left[ \mathcal{R}_{U_1,u}(x_1), \mathcal{R}_{U_2,u}(x_2) \right] \left| \frac{d\mathcal{R}_{U_1,u}(x_1)}{dx_1} \right| \left| \frac{d\mathcal{R}_{U_2,u}(x_2)}{dx_2} \right| = \quad (42) \]

\[ = \frac{M_2}{2} \frac{\partial^2}{\partial \varepsilon^2} \left\{ Q_0 \left[ \mathcal{R}_{U_1,\eta}(x_1), \mathcal{R}_{U_2,\eta}(x_2) \right] \left| \frac{d\mathcal{R}_{U_1,\eta}(x_1)}{dx_1} \right| \left| \frac{d\mathcal{R}_{U_2,\eta}(x_2)}{dx_2} \right| \right\} \bigg|_{\varepsilon=0} \quad \eta = u + \varepsilon \]

and so on. From Eqs. [41] and [42], we see that they contain the functional operator \( \mathcal{H}_{U_i,u,i = 1,2} \) [38]. Taking into account its properties, described in Appendix, we can immediately write the solution of Eq. (41) for \( Q_0 \):

\[ Q_0(x_1 x_2) = \mathcal{L}_{U_1,u}(x_1) \mathcal{L}_{U_2,u}(x_2) \quad (43) \]

To solve Eq. (42), we will present the sought function \( Q_2(x_1 x_2) \) in the form of expansion over eigenfunctions [76] of operator [38]:

\[ Q_2(x_1 x_2) = \sum_{|n|+|l| \neq 0} C_{nl} s_n^{U_1,u}(x_1) s_l^{U_2,u}(x_2) \quad (44) \]

By substituting this series into the left-hand side of Eq. (42) and by expanding its right-hand side using [75], we obtain, for the coefficients \( C_{nl} \), the following formulas:

\[ C_{nl} = \frac{1}{1 - \lambda_n(U_1,u)\lambda_l(U_2,u)} \frac{M_2}{2} \frac{\partial^2}{\partial \varepsilon^2} \left[ J_n(U_1 \varepsilon) J_l(U_2 \varepsilon) \right] \bigg|_{\varepsilon=0} \quad (45) \]

where the quantities \( J_n(U \varepsilon) \) are defined as

\[ J_n(U \varepsilon) \equiv \int \frac{\mathcal{L}_{U,u}(\mathcal{R}_{U,n}(x)) \mathcal{R}_{U,n}(x)}{\mathcal{G}_{U,u}(x)} \ dx = \int \frac{\mathcal{L}_{U,u}(z)}{\mathcal{G}_{U,u}(\mathcal{R}_{U,n}^{-1}(z))} \ dz = J^*_n(U \varepsilon), \quad \eta = u + \varepsilon \quad (46) \]

Definitions of the functions \( \mathcal{L} \) and \( \mathcal{G} \) entering these expressions are given in Appendix. When expanding the right-hand side of [42], we used expression [43] for the function \( Q_0(x_1 x_2) \). As was pointed out above, we are interested only in the part of \( Q_2(x_1 x_2) \) singular in \( \omega = U_2 - U_1 \). To extract this part, one has to retain, in [44], only the terms with \( n = -l \) [6], since only for these terms the denominator \( 1 - \lambda_n(U_1,u)\lambda_l(U_2,u) \) in [45] turns into zero at \( \omega = U_2 - U_1 = 0 \).
Finally, using expressions for the moments and limiting values of the functions \( \sigma \), we can obtain the following expressions for the integrals \( (46) \):

\[
\int s_n^{U,u}(x)dx = \frac{n}{\pi} \frac{\sqrt{U-u}}{u} \frac{|t|}{t} \quad \text{lim}_{a \to \infty} a^2 s_n^{U,u}(a) = \frac{1}{\pi} \frac{\sqrt{U-u}}{u} \frac{|t|}{t}
\]

Then, using Eq. \( (37) \), we obtain, for the participation function \( W(U) \) and the quantity \( D \), expressions \( (2) \) and \( (3) \).
5 Numerical experiment. Localization length.

The most convincing way to verify theoretical results related to 1D solid-state disordered models is, nowadays, to compare them with a numerical experiment. Below, we present the results of numerical verification of Eq. (2) for the participation function $W(U)$ (spectral dependence of the degree of localization), which is considered to be the main result of this paper. In this verification, we used definition (10) at $dU \ll |u|$. The wave functions entering Eq. (10) were obtained by solving numerically the edge problem for Schrodinger equation (4) with the random potential (11) using the transfer matrix technique. In the calculations, we assumed $p(\varepsilon) = \Theta(\varepsilon + 1/2) - \Theta(\varepsilon - 1/2)$ (see Eq. (1)) and the number of regions of constant potential $N \sim 200 - 900$. The final function $W(U)$ was obtained by averaging over $N_r \sim 2000 - 4000$ realizations of the random potential. When performing the above calculations, one should keep in mind the following: (i) As far as formula (2) obtained in this paper is valid in the thermodynamic limit, the number $N$ should be sufficiently large. However, at $N > 800 - 900$, in the calculations of the wave functions, the errors arising at multiplications of a great number of the transfer matrices rapidly increase; (ii) For a given length $bN$ of a random system, the degree of its disorder $\Delta$, on the one hand, should be large enough for the localization length to be smaller than $bN$, and, on the other, should be small enough not to come out of the range of applicability of Eq. (2); (iii) In these calculations, one has to check quadratic character of the dependence of the computed function $W(U)$ and independence of the results on $N$.

The results of numerical calculations for different values of the parameters $b$ and $\Delta$ are presented in Fig.1 (the values of all the parameters are given in the figure), the smooth curves being calculated using Eq. (2) with no fitting. Figure 1b demonstrates better agreement between the theory and experiment than Fig.1a, because, the above conditions were satisfied much better for the case of numerical dependence for Fig.1b.

In the numerical calculations, it is useful to be able to evaluate the localization length $l$ of the wave functions for the random system with a given energy $U$. For such evaluations, one can use the participation function $W(U)$ (2) obtained in this paper. Consider the states of the random system with the energies lying within the interval $[U, U + dU]$. The number of such states will be $\rho(U)dU$, where $\rho(U)$ is the density of states. In virtue of spatial uniformity of statistical properties of the random potential $U(x)$, we can say that the "centers of gravity" of these localized states are distributed more or less uniformly along the $x$ axis. Therefore, the number of states in the energy interval $[U, U + dU]$, whose centers of gravity fall into the spatial interval $dL$ of the $x$-axis, can be estimated as $[\rho(U)/L]dUdL$, where $L = Nb$ – is the length of the potential box with a fluctuating bottom. Note that the participation function (10) is
mainly contributed by the states whose centers of gravity are separated from the edge of the potential box by the distance not exceeding their localization length \( l \). The number \( dn \) of such states is estimated to be \( dn = [\rho(U)/L]dU \). By denoting the mean amplitude of these states at \( x = 0 \) as \( \psi_U(0) \), we can write, for the participation function \([10]\), the following approximate expression:

\[
W(U)dU = |\psi_U(0)|^4dn \\
W(U) = \frac{\rho(U)}{L}|\psi_U(0)|^4.
\]  

(54)

With the accuracy acceptable for our purposes, we may assume that the density of states \( \rho(U) \) entering this equation does not strongly differ from that \( \rho_0(U) \) for the potential box with the length \( L \) and depth \( u \) with no disorder:

\[
\rho(U) \approx \rho_0(U) = \frac{L}{2\pi\sqrt{U} - u}
\]  

(55)

Then, formula (54) yields

\[
W(U) = \frac{l}{2\pi\sqrt{U} - u}|\psi_U(0)|^4
\]  

(56)

The localization length \( l \) entering this formula and the amplitude of the wave function \( \psi_U(0) \) can be connected by the normalization condition, which will provide a second relationship for their calculation. If the quantity \( \psi_U(0) \) were close to a typical amplitude of the wave function, the above connection would have a simple form \( |\psi_U(0)|^2l = 1 \). However, the arguments presented below show that the amplitude of the wave function at \( x = 0 \) can be much smaller than its typical value, which we denote as \( \bar{\psi}_U \). Let us evaluate \( \bar{\psi}_U \) based on the following reasoning. At \( x < 0 \), (i.e., outside the potential box), the wave function has the form \( \psi_U(x) = \psi_U(0)\exp[\sqrt{-U}x] \). At \( 0 < x < l \), scattering in the random potential is weak, and the wave function, within this interval, approximately corresponds to free motion of the particle with the energy \( U \). For this reason, for the wave function near the edge of the random system we can write the following expressions

\[
\begin{cases}
\psi_U(x) = \psi_U(0)\exp[\sqrt{-U}] & x < 0 \\
\psi_U(x) = A\sin[x\sqrt{U} - u + \varphi] & 0 < x < l
\end{cases}
\]  

(57)

The energy \( U \) is assumed here to be sufficiently high, so that the motion of the particle has a ballistic, rather than tunnel, character \( U - u - \varepsilon_i > 0 \). In the case of small disorder, when \( U - u - \varepsilon_i \approx U - u \), this requirement does not essentially restrict our consideration. The conditions of continuity of the wave function and its first derivative at \( x = 0 \) allow one to find the constants \( A \) and \( \varphi \):

\[
\begin{cases}
\psi_U(0) = A\sin\varphi \\
\psi_U(0)\sqrt{-U} = A\sqrt{U} - u \cos\varphi
\end{cases} \Rightarrow \begin{cases}
A^2 = |\psi_U(0)|^2\frac{u}{u-U} \\
tg\varphi = \sqrt{\frac{U-u}{U}}
\end{cases}
\]  

(58)
The typical values of the wave function module squared in the region of localization $l$, we are interested in, can be estimated as a half of its peak value within $[0, l]$:

$$|\bar{\psi}_U|^2 = \frac{A^2}{2} \max_{x \in [0,l]} \sin^2[x\sqrt{U - u} + \varphi]$$  \hspace{1cm} (59)

Using Eq. (58), we can obtain for $|\bar{\psi}_U|^2$ the following expressions

$$|\bar{\psi}_U|^2 = \frac{|\psi_U(0)|^2}{2} \frac{u}{u - U}, \quad \text{when} \quad l\sqrt{U - u + \varphi} > \frac{\pi}{2}$$  \hspace{1cm} (60)

$$|\bar{\psi}_U|^2 = \frac{|\psi_U(0)|^2}{2} \frac{u}{u - U} \sin^2[l\sqrt{U - u + \varphi}], \quad \text{when} \quad l\sqrt{U - u + \varphi} < \frac{\pi}{2}$$

Now we can apply the normalization condition mentioned above $|\bar{\psi}_U|^2 l = 1$:

$$\frac{|\psi_U(0)|^2}{2} \frac{l}{u - U} = 1, \quad \text{when} \quad l\sqrt{U - u + \varphi} > \frac{\pi}{2}$$  \hspace{1cm} (61)

$$\frac{|\psi_U(0)|^2}{2} \frac{l}{u - U} \sin^2[l\sqrt{U - u + \varphi}] = 1, \quad \text{when} \quad l\sqrt{U - u + \varphi} < \frac{\pi}{2}$$  \hspace{1cm} (62)

Equations (61), (62) and (56) allow us to express the localization length $l$ through the participation function $W(U)$ obtained in this paper. For instance, Eqs. (61) and (56) give the following expression for the localization length:

$$l = \frac{2|U - u|^{3/2}}{\pi W(U) u^2} \equiv l_0(U)$$  \hspace{1cm} (63)

For algebraic consistency, we retained here the numerical factor $2/\pi$. This formula is applicable provided that the localization length $l$, obtained with its aid, meets condition (61): $l\sqrt{U - u + \varphi} > \frac{\pi}{2}$. Combining Eqs. (62) and (56), we obtain equations for determination of the localization length in the case when $l\sqrt{U - u + \varphi} < \frac{\pi}{2}$:

$$\frac{l_0(U)}{l} = \sin^4 \left[l\sqrt{U - u + \arctg\frac{u - U}{U}}\right]$$  \hspace{1cm} (64)

In the topical case when $U - u > \Delta$, formula (63) appears to be the main one. This is why we will not analyze the transcendent equation (64). Figure 2 shows a typical form of wave functions of the random system at different energies. Horizontal thick lines show the localization lengths obtained using (63) and (2). It is seen from Fig. 2 that these formulas may be used to evaluate spectral dependence of the localization length for the states of the random system considered in this paper.
6 Conclusions

The perturbative approach to the joint statistics of the advanced and retarded Green’s functions, developed previously for the discrete random 1D models [6, 7], is applied to analysis of the continuous disordered model described by the Schrödinger equation with a piecewise-constant random potential. Using the developed approach, we derived the expression for spectral dependence of the degree of localization in the sense of the Anderson criterion. Numerical verification of the results obtained is presented. In conformity with the commonly accepted opinion, the states with negative energies of the considered random system prove to be, generally speaking, localized, because the participation function [2], at these energies, is nonzero. Exceptions are the points of delocalization arising at $b\sqrt{-u} > \pi$ (see Eq. [2]). Unfortunately, we have not managed to study behavior of the participation function at large values of the parameter $b$ (when these points appear), because the used algorithm of numerical solution of the Schrödinger equation became unstable. In this connection, it makes sense to pay attention to similarity between the continuous model described in this paper and the discrete model with a complex structural unit [7]. There are strong grounds for believing that the behavior of the participation function $W(U)$ of the continuous model under consideration qualitatively coincides with that for the discrete model [7], for which the numerical analysis appears to be feasible. In conclusion, emphasize once again that the developed approach and the results obtained can be useful for analysis of propagation of the electromagnetic waves in structures of the type of 1D photonic crystals in the presence of disorder.

7 Appendix

Solution of the spectral problem for the operator $\mathcal{H}_{\Omega, \eta}$

To solve this problem, we use the system of eigenfunctions $\sigma_C(x)$ for the operator $H_C f(x) \equiv f(C - 1/x)/x^2$, obtained in [9] in explicit form. Consider some of these functions $\sigma(x)$ and denote the corresponding eigenvalue of the operator $H_C$ by $\lambda$. Then, the following relationship should be valid

$$\frac{1}{x^2} \sigma(C - 1/x) = \lambda \sigma(x) \quad (65)$$

Let us pass, in this equation, to a new variable $y = |x - A|/B, \quad x = A + By$, where the parameters $A$ and $B$ are supposed to be defined later. If we now introduce a function $\Phi(y) \equiv C - 1/x = C - 1/[A + By]$, then we can easily see that, by passing to the variable $y$ in Eq.
we come to the following relationship

$$\frac{1}{B} \frac{d\Phi}{dy} \sigma(\Phi(y)) = \lambda \sigma(A + By) \quad (66)$$

Now, we introduce the function $s(y)$ defined as

$$s(y) \equiv B \sigma(A + By) \quad \text{and, consequently,} \quad \sigma(z) = \frac{1}{B} s\left(\frac{z - A}{B}\right) \quad (67)$$

It follows from (66) that

$$\frac{1}{B} \frac{d\Phi}{dy} s\left(\frac{\Phi(y) - A}{B}\right) = \lambda s(y) \quad (68)$$

If we define a function $R$ by the relation

$$R(y) \equiv \Phi(y) - A = \left[\frac{(C - A)A - 1}{AB} + \frac{C - A}{A - y}\right] / \left[1 + \frac{B}{A}y\right], \quad (69)$$

then Eq. (68) can be rewritten in the form

$$\frac{dR}{dy} s[R(y)] = \lambda s(y) \quad (70)$$

Let us now choose the parameters $A, B,$ and $C$ to make operation (69) coincident with (24). This gives rise to a system of equations for these parameters. Solving this system we have

$$A = \sqrt{\Omega - \eta + it\sqrt{\Omega}} \quad B = \frac{t\eta}{\sqrt{(\Omega - \eta)(1 + t^2)}} \quad C = \frac{2}{\sqrt{1 + t^2}}, \quad t = \tan\left[\theta^{2} \sqrt{\Omega - \eta}\right] \quad (71)$$

Thus, the function $s(y)$ (67) constructed with the aid of the eigenfunction $\sigma(x)$ of the operator $H_C$, for the parameters $A, B, \text{and } C$ determined by Eq. (71) is the eigenfunction of the operator $H_{\Omega, \eta}$ (38), with the appropriate eigenvalue $\lambda$ being coincident with that of the operator $H_C$. Below, we present a compact expression for the $s$-functions.

As shown in [9], an arbitrary function $f(x)$ may be expanded in series in terms of the functions $\sigma^n_C(x)$. Remind the explicit form of the functions $\sigma^n_C(x)$ and expressions for the eigenvalues $\lambda_n$ of the operator $H_C$ at $C < 2$:

$$\sigma^n_C(x) = L_C(x)G^n(x), \quad L_C(x) \equiv \frac{1}{2\pi i} \left[\frac{1}{x - R} - \frac{1}{x - R^*}\right], \quad G(x) \equiv \left[\frac{R^* - x}{R - x}\right] \quad (72)$$

$$\lambda_n = \left(\frac{C + i\sqrt{4 - C^2}}{C - i\sqrt{4 - C^2}}\right)^n \quad R \equiv \frac{C + i\sqrt{4 - C^2}}{2}, \quad R^* \equiv \frac{C - i\sqrt{4 - C^2}}{2}, \quad |C| < 2$$

as well as the rules of expansion of an arbitrary function $f(x)$ in series in terms of the above functions:

$$f(x) = \sum_{n=-\infty}^{+\infty} K_n \sigma^n_C(x), \quad K_n = \int \frac{f(x)}{G^n(x)} dx \quad (73)$$
Using these relationships, we can obtain similar rules for the eigenfunctions \((67)\) of the operator\((38)\) (called by \(s\)-functions)

\[
\mathcal{H}_{\Omega,\eta} s_n^{\Omega,\eta}(y) = \lambda_n(\Omega, \eta) s_n^{\Omega,\eta}(y), \quad s_n^{\Omega,\eta}(y) = B \sigma_C^n(A + By), \quad \lambda_n(\Omega, \eta) = \exp[2mb\sqrt{\Omega - \eta}]
\]

(74)

Here, the parameters \(A, B,\) and \(C\) are defined by formulas \((71)\). The superscript of the \(s\)-functions indicates their dependence on the energy argument \(\Omega\).

The arbitrary function \(f(x)\) can be represented as the series

\[
f(y) = \sum_{n=-\infty}^{+\infty} \mathcal{K}_n s_n(y), \quad \mathcal{K}_n = \int \frac{f(y)}{G_n(A + By)} \, dy \equiv \int \frac{f(y)}{G_{\Omega,\eta}^n(y)} \, dy,
\]

with

\[
G_{\Omega,\eta}(y) \equiv \frac{r^* - y}{r^* - y}, \quad \text{where} \quad r \equiv \frac{\sqrt{\Omega} - \sqrt{\Omega - \eta}}{\eta} \quad \quad r^* \equiv \frac{\sqrt{\Omega} + \sqrt{\Omega - \eta}}{\eta}
\]

Using the quantities introduced in this way, we may write the following compact expressions for the \(s_n^{\Omega,\eta}(y)\) \(s\)-functions:

\[
s_n^{\Omega,\eta}(y) = \mathcal{L}_{\Omega,\eta}(y) G_{\Omega,\eta}^n(y), \quad \mathcal{L}_{\Omega,\eta}(y) \equiv \frac{1}{2\pi i} \left[ \frac{1}{y - r} - \frac{1}{y - r^*} \right]
\]

(76)

Here, the subscripts of the Lorentzian \(\mathcal{L}\) indicate dependence of this function on the energy parameters \(\Omega\) and \(\eta = u + \varepsilon\). One can easily make sure that

\[
G_{\Omega,\eta}^n(\mathcal{R}_{\Omega,\eta}(x)) = \lambda_n(\Omega, \eta) G_{\Omega,\eta}^n(x)
\]

(77)

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Figure 1: Spectral dependence of the degree of localization of the states for the 1D disordered system with a piecewise-constant random potential. The noisy curves are obtained by computer simulation and the smooth ones are computed using Eq. (2).
Figure 2: Wave function of the 1D disordered system with a piecewise-constant random potential for different values of the energy $U$. Thick horizontal lines show the localization length calculated using Eq. (63).