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Theory of resonant tunneling of charge carriers within the framework of the Green's function method and the biorthogonal formalism

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A general approach to the analysis of resonant tunneling and scattering effects is developed within the framework of the Green's functions method. The proposed mathematical apparatus is based on the biorthogonal formalism of quantum theory that allows one to describe systems with non-Hermitian Hamiltonians. Such operators are typical for problems wherein particle is supposed to leave the physical system and go to infinity. The stationary Schrodinger equation with a particle source is considered in abstract operator form. The solution of that problem is expressed in a general form in terms of the corresponding Green's operator. Transmission coefficients and their dependences on the particle energy are determined for a single rectangular potential barrier and a double Gaussian barrier. The result of numerical calculation for a single rectangular barrier is compared with the well-known analytical solution of this problem. The proposed method makes it possible to analyze the particles tunneling and scattering in structures with an arbitrary number and shape of potential barriers with high accuracy.

Keywords: resonant tunneling, resonant scattering, potential barrier, Green's function, biorthogonal quantum mechanics.

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Introduction

The effects of resonant tunneling and scattering of charge carriers in semiconductor heterostructures have become widely used in recent years for the development of various optical and quantum electronics devices [1–3]. In particular, new communication devices, detectors, and compact emitters currently being developed, operating in the terahertz wavelength range are based on them [4–6]. For this reason there is an urgent need to develop simple numerical methods that allow analyzing the effects of tunneling of charge carriers through single and multiple potential barriers of arbitrary shape within the framework of single-particle quantum mechanics.

Usually, the analysis of tunneling and scattering processes is reduced to solving the stationary Schrodinger equation in a coordinate representation with a Hamiltonian containing potential barriers in a limited area of space. It is assumed in this case that there is a source of particles away from the barriers, to the left or right. The corresponding equation in the operator form can be generally presented as follows :

$$(\hat{H} - E)|\Psi(E)\rangle = |g\rangle. \qquad (1)$$

Here $\hat{H}$ — the Hamiltonian of the system under consideration, $|\Psi(E)\rangle$ — a vector describing the stationary state of a particle with energy E, $|g\rangle$ — a vector characterizing the particle source. In this equation, energy can take any values and is a parameter of the problem. In the simplest case, the Hamiltonian of such a system has the form

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m_0} + U(\hat{\mathbf{x}}), \qquad (2)$$

where $\hat{\mathbf{p}}$ is the momentum operator, $U(\hat{\mathbf{x}})$ is the potential energy operator.

Equation (1) is usually solved in the basis of states $|\mathbf{x}\rangle$ corresponding to a certain value of the particle coordinate $\mathbf{x}$. The wave function in this coordinate representation $\Psi(\mathbf{x}; E) = \langle \mathbf{x}|\Psi(E)\rangle$ allows calculating the probability flux density for a particle passing through a region with a potential localized in space. The transmission coefficient T defining as the ratio of the flux densities of passing and falling particles is of interest for one-dimensional systems. The scattering cross section plays a similar role in two-dimensional and three-dimensional systems. It is assumed that the particle goes to infinity as a result of the processes under consideration. It should be noted that the kinetic energy operator in the Hamiltonian in these cases is non-Hermitian. This is due to the fact that the proof of hermiticity of the momentum operator in the coordinate representation is based on integration by parts and neglect of the non-integral summand, which vanishes only for damped functions. For this reason, when searching for solutions for particles going to infinity, in principle, it is necessary to consider non-Hermitian operators with complex eigenvalues, whose stationary wave functions fade with time [7–10]. In this case, the imaginary part of the energy eigenvalues determines the characteristic time of the particle's departure from the system.

A new approach to solving this problem is proposed in this paper, in which a large but limited volume of V is considered instead of an infinite space. At the same time, it is assumed that potential barriers are located near the center of the region under consideration, and a dissipative purely imaginary potential smoothly varying in space is additionally introduced into the system, providing attenuation of wave functions near the boundaries. The form of the wave function of the particle in the central region practically does not differ from the case of unlimited space if the attenuation is small enough. Thus, it turns out to be possible to approximate the solution of the problem of the motion of a particle going to infinity by considering a region of finite size.

The introduction of a spatial constraint in the **x**-representation, taking into account the attenuation of wave functions $\Psi(\mathbf{x};E)$ near the boundaries of the region under consideration, allows introducing a periodic continuation of the studied quantum system. This technique is similar to the introduction of cyclic Born-Karman boundary conditions. In this case, it is convenient to solve the problem in the basis of states $|\mathbf{k}\rangle$ corresponding to certain values of the momentum $\mathbf{p} = \hbar\mathbf{k}$ or, what is the same, the wave vector of the particle **k**. This representation is related to the **x**-representation by the Fourier transform. It is essential that we get the opportunity to describe the system with discrete variables instead of continuous ones in the **k**-representation, and the operator equation (1) has the form of a system of linear algebraic equations. The proposed approach is significantly more convenient from the point of view of numerical calculation. It allows studying the effects of tunneling in quantum systems with any number of potential barriers having an arbitrary shape, as well as an arbitrary distribution in space. As an example, this method is used to calculate the transmission coefficient and its dependence on the energy of an incident particle in two one-dimensional systems containing, respectively, a single rectangular barrier and two closely spaced Gaussian barriers.

1. Solving the problem using the method of Green's functions in a biorthogonal formulation

The solution of the problem with a non-Hermitian Hamiltonian is most naturally studied within the framework of biorthogonal formalism in quantum theory [11]. In general case, for non-Hermitian operators, it is necessary to consider two eigenvalue problems, which will be written as follows

$$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle,$$

$$\hat{H}^\dagger|\varphi_n\rangle = E_n^*|\varphi_n\rangle. \tag{3}$$

Index n establishes a correspondence between the eigenvalues E_n, E_n^* and the eigenvectors $|\psi_n\rangle$, $|\varphi_n\rangle$ here. According to (3), the conjugate vectors $\langle\psi_n|$, $\langle\varphi_n|$ are the solution of conjugate equations

$$\langle\psi_n|\hat{H}^\dagger = E_n^*\langle\psi_n|,$$

$$\langle\varphi_n|\hat{H} = E_n\langle\varphi_n|.$$

In this notation, the vectors $\langle\varphi_n|$ and $|\psi_n\rangle$ acquire the meaning of the „left" and the „right" eigenvectors of the non-Hermitian operator $\hat{H}$ corresponding to one complex eigenvalue E_n. The eigenstates of the operators $\hat{H}$ and $\hat{H}^\dagger$ defined in this way are bound by the following conditions of biorthonormality and completeness

$$\langle\varphi_n|\psi_{n'}\rangle = \delta_{nn'},$$

$$\sum_n |\psi_n\rangle\langle\varphi_n| = 1. \tag{4}$$

Using two sets $|\psi_n\rangle$ and $\langle\varphi_n|$ allows bringing both non-Hermitian operators in the equations (3) to a diagonal form:

$$\langle\varphi_n|\hat{H}|\psi_{n'}\rangle = E_n\delta_{nn'},$$

$$\langle\psi_n|\hat{H}^\dagger|\varphi_{n'}\rangle = E_n^*\delta_{nn'}.$$

Thus, the operators $\hat{H}$ and $\hat{H}^\dagger$ can be represented by the following expansions in biorthogonal eigenstates

$$\hat{H} = \sum_n |\psi_n\rangle E_n\langle\varphi_n|,$$

$$\hat{H}^\dagger = \sum_n |\varphi_n\rangle E_n^*\langle\psi_n|. \tag{5}$$

The classical one-dimensional problem of a particle falling on a rectangular potential barrier of finite width is considered as an example. We introduce the linear size of the bounded area D. The corresponding potential is defined as follows:

$$U_b(x) = U_{b0}f_b(x), \quad f_b(x) = \begin{cases} 1, & |x| \le d/2, \\ 0, & |x| > d/2 \end{cases},$$

where $f_b(x)$ — the characteristic function that determines the width of the barrier, U_{b0} — the amplitude of the barrier, d — the width of the barrier.

We introduce into the system a second, purely imaginary dissipative potential $U_d(x)$, equal to zero in the region near the initial potential $U_b(x)$, and gradually increasing as we approach the boundaries of the considered region on the left and right

$$U_d(x) = iU_{d0}f_d(x),$$

$$f_d(x) = \left[1 - \frac{1}{\exp[-\sigma(x+\mu)] + \exp[\sigma(x-\mu)] + 1}\right].$$

Here $f_d(x)$ — the characteristic function defining the dissipative potential, U_{d0} — the amplitude of this potential, μ — the parameter specifying the position of the two dissipation regions, the parameter σ determines the growth rate of the imaginary potential. Figure 1 shows the

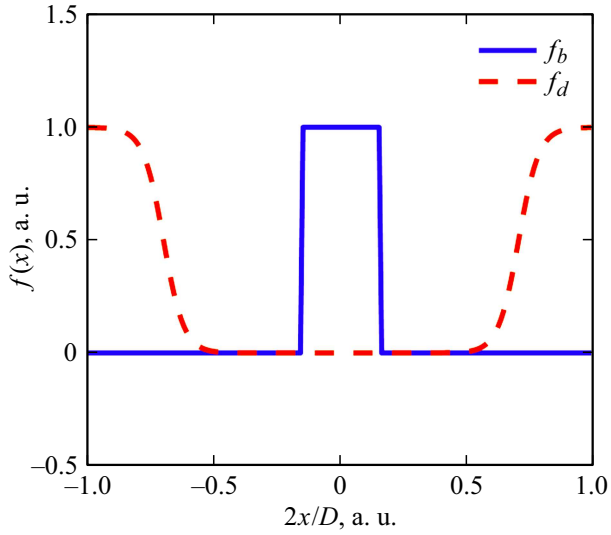

Figure 1. Characteristic functions $f_b(x)$ and $f_d(x)$ defining the real and imaginary parts of the potential, respectively.

functions $f_b(x)$ and $f_d(x)$, which are used to determine the distribution of real and imaginary potentials in the system.

The basis with a certain value of the wave vector $|k\rangle$ is used to represent the operator equation (1) in matrix form. The orthonormality and completeness relations for vectors $|k\rangle$ have the form

$$\langle k|k'\rangle = \delta_{kk'},$$

$$\sum_k |k\rangle\langle k| = 1.$$

Equation (1) in the selected basis, we represent as

$$\sum_{k'}\langle k|\hat{H} - E|k'\rangle\langle k'|\Psi(E)\rangle = \langle k|g\rangle. \qquad (6)$$

The states $|k\rangle$ are the eigenstates of the operator $\hat{p}$, so in this basis it is diagonal

$$\langle k|\hat{p}|k'\rangle = \hbar k\delta_{kk'}.$$

The potential energy operator is represented as the sum of two operators

$$U(\hat{x}) = U_b(\hat{x}) + U_d(\hat{x}).$$

Its matrix elements in the basis $|k\rangle$ are defined as follows:

$$U_{kk'} = \int dx\, dx'\langle k|x\rangle\langle x|U(\hat{x})|x'\rangle\langle x'|k'\rangle$$

$$= \frac{1}{D}\int dx\, U(x)\exp[-i(k-k')x],$$

where we took into account that

$$\langle x|U(\hat{x})|x'\rangle = U(x)\delta(x-x'),$$

$$\langle x|k\rangle = \frac{1}{\sqrt{D}}\exp(ikx).$$

As a result, the matrix Hamiltonian takes the following final form:

$$H_{kk'} = \frac{\hbar^2k^2}{2m_0}\delta_{kk'} + U_{kk'}.$$

By placing the local particle source at the point x_0, we will have

$$g(x) = \langle x|g\rangle = A\delta(x-x_0),$$

where A — some dimensional constant. In this case, the point x_0 is selected based on the condition $U_d(x_0) \cong 0$. Going to k-representation, we get

$$g_k = \langle k|g\rangle\int dx\langle k|x\rangle\langle x|g\rangle = \frac{A}{\sqrt{D}}\exp(-ikx_0).$$

Substitution of the eigenvectors of the Hamiltonian into (6) in accordance with the completeness condition (4) and expansion of (5) will result in

$$\sum_{k',n,n'}\langle k|\psi_n\rangle\langle\varphi_n|\hat{H} - E|\psi_{n'}\rangle\langle\varphi_{n'}|k'\rangle\langle k'|\Psi(E)\rangle = \langle k|g\rangle,$$

$$\sum_{k',n}\langle k|\psi_n\rangle(E_n - E)\langle\varphi_n|k'\rangle\langle k'|\Psi(E)\rangle = \langle k|g\rangle. \qquad (7)$$

The solution of equation (7), parametrically dependent on E, is written in the form

$$\Psi_k(E) = \langle k|\Psi(E)\rangle = \sum_{n,k'}\langle k|\psi_n\rangle\frac{1}{(E_n - E)}\langle\varphi_n|k'\rangle\langle k'|g\rangle$$

or

$$\Psi_k(E) = \sum_{k'}\langle k|\hat{G}(E)|k'\rangle\langle k'|g\rangle = \sum_{k'}G_{kk'}(E)g_{k'}, \qquad (8)$$

where the matrix elements $G_{kk'}(E)$ represent the Green function of the equation (7) in k-representation. The corresponding Green operator can be expressed as a biorthogonal expansion

$$\hat{G}(E) = \sum_n |\psi_n\rangle\frac{1}{E_n - E}\langle\varphi_n|.$$

Here E_n — is a complex quantity, and $\hat{G}(E)$ — is the inverse operator of the original equation (1):

$$\hat{G}(E) = (\hat{H} - E)^{-1}.$$

After calculation of the components of the wave function at a given energy value according to the formula (8) it remains to use its coordinate representation

$$\Psi(x;E) = \sum_k\langle x|k\rangle\langle k|\Psi(E)\rangle = \frac{1}{\sqrt{D}}\sum_k\exp(ikx)\Psi_k(E).$$

The obtained functions $\Psi(x;E)$ allow determining the flux density of the probability $j(x;E)$ corresponding to the

passing particle, and thus calculate the dependence of the transmission coefficient T on its energy. It is assumed that the particle moves from left to right. In the case of the considered one-dimensional problem, the ratio of the flow densities is reduced to the ratio of the squares of the wave amplitudes, which is written as follows

$$T(E) = \frac{j_1(E)}{j_0(E)} = \frac{|\Psi_1(E)|^2}{|\Psi_0(E)|^2}.$$

Here $|\Psi_1(E)|^2 = |\Psi(x_1;E)|^2$, and the coordinate $x_1 > d/2$ is located in the area where $U_d(x) \cong 0$. Note that the square of the amplitude $|\Psi(x;E)|^2$, calculated at $x < -d/2$, corresponds to the superposition of incident and reflected waves. If the amplitude of the incident wave is unknown, then it is easiest to determine it by solving an auxiliary problem in which there is no real potential barrier $U_b(x) = 0$. The solution $\Psi(x;E)$ in this case will have the form of a wave whose amplitude is almost constant near the center of the region under consideration and gradually fades as it approaches its boundaries. Thus, it is possible to approximate $|\Psi_0(E)| \cong |\Psi_0(0;E)| = \text{const}$.

2. Numerical calculation results

The rectangular potential barrier transmission coefficient, calculated numerically using the above method is compared as an illustration, with the known result of the analytical solution of this problem [12]:

$$T_a(E) = \frac{4k_0^2k_1^2}{(k_0^2 - k_1^2)\sin^2(dk_1) + 4k_0^2k_1^2},$$

where $k_0 = \sqrt{2m_0E}/\hbar$, $k_1 = \sqrt{2m_0(E - U_{b0})}/\hbar$.

It is assumed for implementation of the numerical calculation that the coordinate x changes discretely as $x_n = -D/2 + n\Delta x$, where $\Delta x = D/N$ — step, N — number of points, $n = 0, 1 \cdots, N-1$. The corresponding values of the wave vector are also discrete and are defined as $k_n = -\pi/\Delta x + n\Delta k$ with a step of $\Delta k = 2\pi/D$. The coordinate x changes continuously in the limit $N \to \infty$, and the values k are in the range $-\infty \cdots \infty$. N is selected as the finite for the numerical calculation and determines the accuracy of calculations. Next, the number of points was assumed to be $N = 200$, and the dimension of the matrices of the Hamiltonian and the Green operator was $N \times N = 200 \times 200$. This approach of discretization of x- and k-spaces arises naturally when calculating the energy spectrum and wave functions of charge carriers in semiconductor superlattices by the effective mass method [13,14]. The role of discrete variables x_n in this case is played by the Bravais lattice sites of the crystal, and k_n represent the vectors of the reciprocal superlattice.

Figure 2 shows the energy dependences of the rectangular barrier transmission coefficient calculated analytically $T_a(E)$ and numerically $T(E)$. As can be seen from the graph, the developed approach ensures high accuracy of compliance.

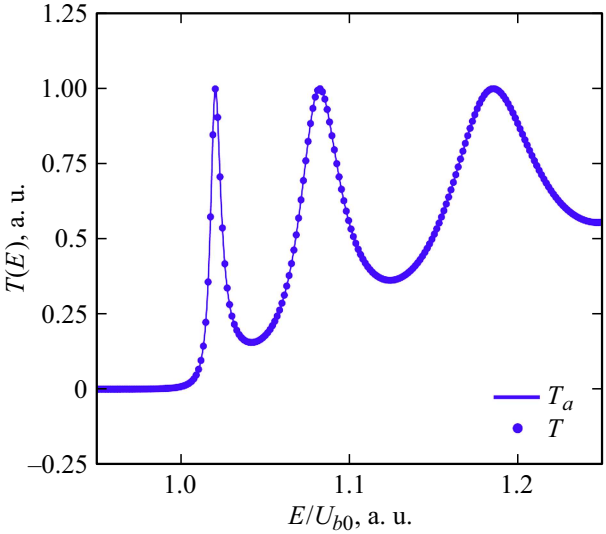

Figure 2. Dependence of the transmission coefficient of the rectangular barrier on energy.

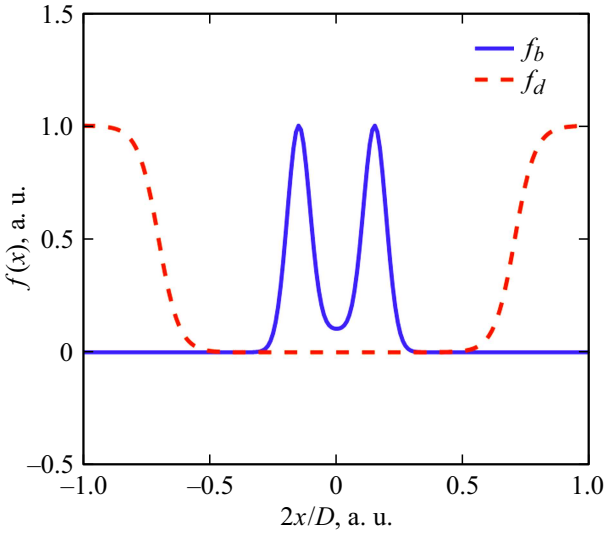

Figure 3. Characteristic functions defining the potential in a system with two Gaussian barriers.

As a second example, consider the dependence of the transmission coefficient $T(E)$ on the energy for a system with two barriers. Figure 3 shows the characteristic functions defining the real and imaginary parts of the potential. The real part of the potential is chosen in the form of two overlapping Gaussian functions. The amplitude of the barrier U_{b0} in this case will determine the value of the real potential at the points of maxima. Figure 4 shows the corresponding graph of the dependence $T(E)$. As follows from the figure, in this case, narrow peaks are present in the transmission spectrum at energies $E/U_{b0} < 1$, which correspond to the quasi-resonant states of the particle in a potential well formed by two Gaussian barriers.

Thus, the mathematical apparatus developed in this work makes it possible to obtain information about all quasi-

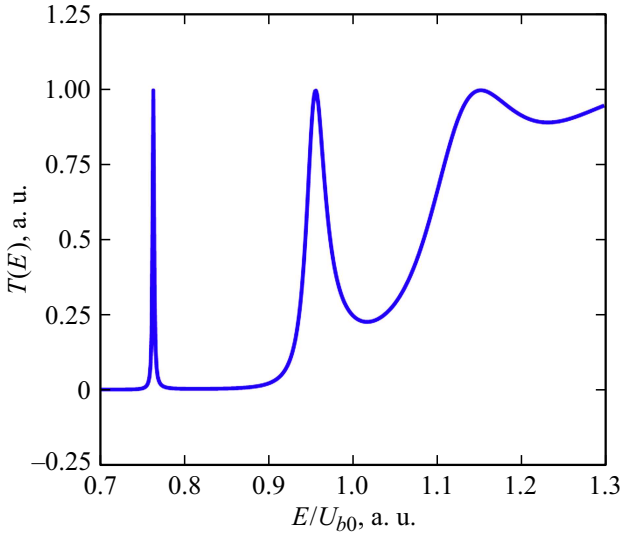

Figure 4. Dependence of the transmission coefficient on energy for a system with two Gaussian barriers.

resonant levels in the system, including those that are characterized by a long lifetime, i.e. a small broadening (the first maximum in Fig. 4). This theory makes it possible to investigate the effects of particle tunneling in the most general case, regardless of the specifics of a particular system and its parameters. It can be successfully used in the calculation of resonant tunneling effects in semiconductor heterostructures within the framework of the effective mass method.

Conclusion

A general approach to solving problems of resonant tunneling and scattering of particles using the method of Green's functions is proposed in the paper. The developed theoretical apparatus is based on the biorthogonal formalism of quantum theory, within which systems with non-Hermitian Hamiltonians are described. In particular, such operators naturally arise in the problems of tunneling and scattering of particles. An essential aspect of the described method is the spatial limitation and periodic continuation of the quantum system under consideration. This makes it possible to make the transition from continuous variables to discrete ones. The stationary Schrodinger equation with a particle source is reduced to a system of linear inhomogeneous algebraic equations as a result. The developed approach makes it possible to numerically and with high accuracy analyze the processes of tunneling and scattering of particles in structures with any number of potential barriers having an arbitrary shape.

Conflict of interest

The authors declare that they have no conflict of interest.

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