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Microscopic theory of resonant tunneling of charge carriers in semiconductor heterostructures

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A general approach to the study of resonant tunneling of charge carriers in semiconductor heterostructures has been developed. The tunneling problem is solved by introducing the Green's operator for the corresponding Schrodinger equation within the framework of the biorthogonal formalism of quantum theory. As an example, model heterostructures based on one-dimensional crystals are considered, for which it is possible to construct an accurate microscopic theory of tunneling. The exact results following from the proposed theory are compared with approximate data obtained by the method of smooth envelope functions, as well as the effective mass method. It is shown that the main contribution to the difference between microscopic theory and existing approximate methods is due to the nonparabolicity of the law of dispersion of charge carriers, whereas short-range interface fields play a secondary role in the tunneling process.

Keywords: effective mass method, Greenś function, biorthogonal quantum mechanics, resonant tunneling effects.

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1. Introduction

With the development of nanoelectronics it is becoming more pressing to design various devices where the effects of resonant tunneling of charge carriers are used, i. e., when the carriers are transferred through an alternating sequence of quantum barriers and quantum wells with an energy equivalent to the resonance in the considered system. This phenomenon, as well as the negative differential conductivity resulting from the potential tunneling, can be used, e.g., to implement infrared radiators of medium [1] and terahertz range [2] at intraband junctions in semiconductor superlattices — in „Wannier-Stark ladders“ [3]. There are other implementation options for nanoelectronics devices, the principle of which is based on resonant tunneling, for example, resonant-tunneling transistors [4] and logic gates formed on their basis [5]. Of practical interest here are the volt-ampere characteristics (VAC) of tunneling resonant devices, which can be obtained by calculating the dependence of the tunneling coefficient on the charge carriers energy.

To determine the tunneling coefficient energy dependence, various analytical approximations are usually applied in the literature, in particular, such as Breit-Wigner formulas [6,7]. Numerical methods using similar formulas for analyzing the particles scattering on barriers [8], as well as the method of transfer matrices should be mentioned [9,10]. In addition, there are various ways to calculate VAC of tunnel-resonance structures using equivalent electrical circuits that do not require finding the tunneling coefficient [11]. However, they are not highly accurate and cannot be used for a wide class of heterostructures.

All of the above approaches have their limitations and cannot be applied to describe tunneling in systems with potential barriers of arbitrary shape, or they allow us to study the energy spectrum of the tunneling coefficient only near the systems' resonant energies. However, as shown in [12,13], the analysis in a wide range of energies is possible within the Green's functions theory methods. Because of this approach it is possible to study the tunneling properties of the structure for arbitrary energy values away from the resonances of the structure.

The analysis of resonance tunneling, as a rule, is carried out within the effective mass approximation by approximating the differential equations solutions using the finite element method in the basis with a certain coordinate $|\mathbf{x}\rangle$ or by solving a system of linear algebraic equations within a single-band model in the basis with a certain value of the wave vector $|\mathbf{k}\rangle$. However, in this case, all the features of the band structure of the material are not taken into account, since the law of dispersion of charge carriers is approximated by a parabolic dependence.

In this study, a general approach to the analysis of resonant tunneling in multi-barrier structures is developed, allowing for the microscopic structure of potential barriers and all singularities of the band structure of the analyzed materials. The dependences of the tunneling coefficient on the energy of charge carriers are analyzed. The problem is formulated in a momentum representation, which makes it possible to reduce the solution of Schrodinger differential equation to the solution of a system of linear algebraic equations. The developed approach makes it possible to automatically provide for the boundary conditions on the heterointerfaces of the studied structures, which makes its at universal tool and gives an option for studying the systems with any number of arbitrary shape barriers.

2. Green's functions method in the framework of biorthogonal formalism

In general, Schrödinger equation for the intrinsic stationary states of a particle in the operator form his expressed as

$$\hat{H}|\psi\rangle = E|\psi\rangle, \tag{1}$$

where $\hat{H}$ — Hamiltonian of the considered problem, E and $|\psi\rangle$ — intrinsic energy and the corresponding eigen vector. To analyze the particle passing through the system a source of particles characterized by $|\rho\rangle$ vector is introduced. Then instead of the equation (1) It is necessary to consider the inhomogeneous Schrödinger equation

$$(\hat{H} - E)|\psi(E)\rangle = |\rho\rangle. \tag{2}$$

The solution of the inhomogeneous Schrödinger equation (2) is generally expressed in terms of the Green operator, which depends parametrically on the energy of the particle:

$$|\psi(E)\rangle = \hat{G}(E)|\rho\rangle, \tag{3}$$

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

Let us consider the problem of passing a particle through a certain structure formed by potential barriers of arbitrary shape. Such a system is open, which implies that the particle goes to infinity as a result of the scattering process. In such problems, the wave function in the coordinate representation turns out to be nonzero at infinity, and the Hamiltonian of the system is non-Hermitian [14]. In this regard, the formalism of quantum mechanics, corresponding to closed systems described by Hermitian operators, cannot be used to correctly represent the state of a particle.

In the developed approach, for subsequent numerical analysis, we will consider a system in a limited region of space, near the boundaries of which a phantom dissipative potential is introduced along with the potential of the structure. In this case, the wave function of the charge carrier smoothly decays in these regions. In the vicinity of the examined low-dimensional system, the solution of Schrödinger equation practically does not differ from the solution of a similar problem for an unlimited space, which makes it possible to replace the case of a particle fleeing to infinity [15,16].

A general approach to the analysis of quantum mechanical systems with non-Hermitian Hamiltonians is formulated within the quantum theory biorthogonal formalism in studies [17,18]. In this case, it is customary to consider two eigen problems:

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

$$\hat{H}^{\dagger}|\psi_n^{\mathrm{l}}\rangle = E_n^{*}|\psi_n^{\mathrm{l}}\rangle,$$

where $|\psi_n^{\mathrm{r}}\rangle$ and $|\psi_n^{\mathrm{l}}\rangle$ — are the so-called „right" and „left" eigen vectors corresponding to the complex eigen numbers E_n and E_n^{*} confined with biorthonormalization and completeness conditions:

$$\left.\begin{aligned} \langle\psi_n^{\mathrm{l}}|\psi_{n'}^{\mathrm{r}}\rangle &= \delta_{nn'} \\ \sum_n |\psi_n^{\mathrm{r}}\rangle\langle\psi_n^{\mathrm{l}}| &= 1 \end{aligned}\right\}.$$

Two biorthonormal sets of the eigenvectors of a non-Hermitian Hamiltonian allow to define the Green's operator in the form of the following expansion:

$$\hat{G}(E) = \sum_n \frac{|\psi_n^{\mathrm{r}}\rangle\langle\psi_n^{\mathrm{l}}|}{E_n - E}. \tag{4}$$

3. Microscopic theory of resonant tunneling of charge carriers

From a physical standpoint, a system of potential barriers is formed due to changes in the crystal potential in semiconductor heterostructures. In general, they can be considered as systems in which atoms of one material are replaced by atoms of another material. In this case, we will assume that the crystals forming the heteropair have the same symmetry, and the difference in parameters of the lattice can be ignored. When selecting one of the materials of the heterojunction, e.g., material B, as a reference, it is possible to create a microscopic Hamiltonian of such a system, taking into account the dissipative potential [19]:

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m_0} + U^{\mathrm{B}}(\hat{\mathbf{x}}) + \sum_{\mathbf{a}} f_{\mathrm{b}}(\mathbf{a})\Delta V(\hat{\mathbf{x}} - a) + iU_{0\mathrm{d}} f_{\mathrm{d}}(\hat{\mathbf{x}}), \tag{5}$$

where $\hat{\mathbf{p}}$ — momentum operator, m_0 — electron mass, $U^{\mathrm{B}}(\mathbf{x})$ — periodic potential created by atoms of material B, $f_{\mathrm{b}}(\mathbf{a})$ — the characteristic function that determines the position of atoms of crystal A in the lattice of crystal B, $\Delta V(\mathbf{x} - \mathbf{a})$ — difference of local potentials created by the atoms of materials in the cell numbered $\mathbf{a}$, $iU_{0\mathrm{d}} f_{\mathrm{d}}(\mathbf{x})$ — dissipative potential near the boundaries of a system with an amplitude of $U_{0\mathrm{d}}$.

When solving the Schrödinger equation (2) with the Hamiltonian (5), it is convenient to choose a basis of states with a certain value of the wave vector $|\mathbf{q}\rangle$, which in a solid can be represented as $|\mathbf{b} + \mathbf{k}\rangle$ states with certain values of the inverse lattice vector $\mathbf{b}$ and the wave vector $\mathbf{k}$. With this approach, the variables used are discrete, and the solution to the problem automatically satisfies the periodic Born-Karman conditions. In this case, there is no need to use difference schemes to solve Schrödinger equation, as is usually done when using a coordinate basis. The selected representation $|\mathbf{b}+\mathbf{k}\rangle$ is related to coordinate $|\mathbf{x}\rangle$ by means of the Fourier transform

$$\langle\mathbf{x}|\mathbf{b}+\mathbf{k}\rangle=\frac{1}{\sqrt{V}}\exp[i(\mathbf{b}+\mathbf{k})\mathbf{x}],$$

where V — the volume of the examined region.

In the selected basis, the abstract equation (2) takes the form of a system of linear algebraic equations. The elements of the Hamiltonian matrix of the microscopic theory (5) in it have the following form:

$$H_{\mathbf{bk},\mathbf{b}'\mathbf{k}'}=\hat{H}^{\mathrm{B}}_{\mathbf{bb}'}(\mathbf{k})\delta_{\mathbf{kk}'}+f_{\mathrm{b}}(\mathbf{k}-\mathbf{k}')\Delta V\left[(\mathbf{b}-\mathbf{b}')+(\mathbf{k}-\mathbf{k}')\right]$$
$$+iU_{0\mathrm{d}}f_{\mathrm{d}}\left[(\mathbf{b}-\mathbf{b}')+(\mathbf{k}-\mathbf{k}')\right],\qquad(6)$$

where $H^{\mathrm{B}}_{\mathbf{bb}'}(\mathbf{k})=\hbar^2(\mathbf{b}+\mathbf{k})^2\delta_{\mathbf{bb}'}/(2m_0)+U^{\mathrm{B}}(\mathbf{b}-\mathbf{b}')$ — Hamiltonian of the reference material, $U^{\mathrm{B}}(\mathbf{b}-\mathbf{b}')$ — Fourier transform of the periodic potential of the reference crystal, $f_{\mathrm{b}}(\mathbf{k}-\mathbf{k}')$ — Fourier transform of the characteristic function $f_{\mathrm{b}}(\mathbf{a})$, found by the formula

$$f_{\mathrm{b}}(\mathbf{k}-\mathbf{k}')=\frac{1}{N}\sum_{\mathbf{a}}f_{\mathrm{b}}(\mathbf{a})e^{-i(\mathbf{k}-\mathbf{k}')\mathbf{a}},$$

where N — number of unit cells having a volume of Ω $(V_{\mathrm{r}}=N\Omega)$, and a two-point „Furiier transform" of the difference of potentials $\Delta V(\mathbf{x})$ is found as

$$\Delta V[(\mathbf{b}-\mathbf{b}')+(\mathbf{k}-\mathbf{k}')]=\frac{1}{\Omega}\int\limits_V d\mathbf{x}\Delta V(\mathbf{x})e^{-i[(\mathbf{b}-\mathbf{b}')+(\mathbf{k}-\mathbf{k}')]\mathbf{x}}.$$

The corresponding Fourier transform of the characteristic functions of the phantom imaginary potential is written as

$$f_{\mathrm{d}}[(\mathbf{b}-\mathbf{b}')+(\mathbf{k}-\mathbf{k}')]=\frac{1}{V}\int\limits_V d\mathbf{x}f_{\mathrm{d}}(\mathbf{x})e^{-i[(\mathbf{b}-\mathbf{b}')+(\mathbf{k}-\mathbf{k}')]\mathbf{x}}.\qquad(7)$$

Finally, we obtain the following inhomogeneous Schrödinger equation with a microscopic Hamiltonian (6) in matrix form, as well as its solution $\psi_{\mathbf{bk}}(E)$:

$$\sum_{\mathbf{b}'\mathbf{k}'}(H_{\mathbf{bk},\mathbf{b}'\mathbf{k}'}-\delta_{\mathbf{bb}'}\delta_{\mathbf{kk}'}E)\psi_{\mathbf{b}'\mathbf{k}'}(E)=\rho_{\mathbf{bk}},$$

$$\psi_{\mathbf{bk}}(E)=\sum_{\mathbf{b}'\mathbf{k}'}G_{\mathbf{bk},\mathbf{b}'\mathbf{k}'}(E)\rho_{\mathbf{b}'\mathbf{k}'},$$

where Green's function $G_{\mathbf{bk},\mathbf{b}'\mathbf{k}'}(E)$ in the basis $|\mathbf{b}+\mathbf{k}\rangle$ is found by the formula

$$G_{\mathbf{bk},\mathbf{b}'\mathbf{k}'}(E)=\langle\mathbf{b}+\mathbf{k}|\hat{G}(E)|\mathbf{b}'+\mathbf{k}'\rangle$$
$$=\langle\mathbf{b}+\mathbf{k}|(\hat{H}-\hat{I}E)^{-1}|\mathbf{b}'+\mathbf{k}'\rangle,$$

and Fourier transform $\rho_{\mathbf{bk}}$ — by the formula

$$\rho_{\mathbf{bk}}=\langle\mathbf{b}+\mathbf{k}|\rho\rangle=\frac{1}{\sqrt{V}}\int\limits_V d\mathbf{x}\rho(\mathbf{x})e^{-i(\mathbf{b}+\mathbf{k})\mathbf{x}}.$$

The wave function in the coordinate representation for a given energy $\psi(\mathbf{x},E)$ is found using the inverse Fourier transform

$$\psi(\mathbf{x},E)=\frac{1}{\sqrt{V}}\sum_{\mathbf{b},\mathbf{k}}\exp[i(\mathbf{b}+\mathbf{k})\mathbf{x}]\psi_{\mathbf{bk}}(E).$$

4. Approximations of smooth envelopes of wave functions

The analysis within the smooth envelope function method is carried out by passing from the microscopic Hamiltonian (6) to an effective one-band Hamiltonian. In this case, the exact law of dispersion of charge carriers is taken into account for the considered band. The definition of the operator (5) in the basis of the eigen Bloch states of the reference crystal Hamiltonian in the one-band model allows obtaining an approximate expression for the elements of the effective Hamiltonian:

$$\langle n\mathbf{k}|\hat{H}|n\mathbf{k}'\rangle=E^{\mathrm{B}}_n(\mathbf{k})\delta_{\mathbf{kk}'}+f_{\mathrm{b}}(\mathbf{k}-\mathbf{k}')\Delta E_n+iU_{0\mathrm{d}}f_{\mathrm{d}}(\mathbf{k}-\mathbf{k}'),\qquad(8)$$

where $E^{\mathrm{B}}_n(\mathbf{k})$ — is the full dispersion branch of the reference material band structure, and the matrix element $\Delta V[(\mathbf{b}-\mathbf{b}')+(\mathbf{k}+\mathbf{k}')]$ in the Bloch basis determines, to a first approximation, the band discontinuity at the interface $\Delta E_n=E^{\mathrm{A}}_n(\mathbf{k}=0)-E^{\mathrm{B}}_n(\mathbf{k}=0)$ [19]. Moreover, if we take into account the smoothness of the change in the dissipative potential, we obtain the following simplification for the Fourier transform (7):

$$f_{\mathrm{d}}[(\mathbf{b}-\mathbf{b}')+(\mathbf{k}-\mathbf{k}')]\cong\frac{1}{N}\sum_{\mathbf{a}}f_{\mathrm{d}}(\mathbf{a})e^{-i(\mathbf{k}-\mathbf{k}')\mathbf{a}}$$
$$\times\frac{1}{\Omega}\int\limits_{\Omega}d\mathbf{y}e^{-i(\mathbf{b}-\mathbf{b}')\mathbf{y}}=\frac{1}{N}\sum_{\mathbf{a}}f_{\mathrm{d}}(\mathbf{a})e^{-i(\mathbf{k}-\mathbf{k}')\mathbf{a}}\delta_{\mathbf{bb}'}$$
$$=f_{\mathrm{d}}(\mathbf{k}-\mathbf{k}')\delta_{\mathbf{bb}'},$$

where the Fourier transform of the characteristic function of the smooth dissipative potential is introduced in the approximation of the envelope functions

$$f_{\mathrm{d}}(\mathbf{k}-\mathbf{k}')=\frac{1}{N}\sum_{\mathbf{a}}f_{\mathrm{d}}(\mathbf{a})e^{-i(\mathbf{k}-\mathbf{k}')\mathbf{a}}.$$

In the framework of the effective mass method, the one-band Hamiltonian (8) is further simplified by approximating the dispersion of charge carriers by a parabolic dependence near the extremum $E^{\mathrm{B}}_n(\mathbf{k}=0)$ [19]:

$$\langle n\mathbf{k}|\hat{H}|n\mathbf{k}'\rangle=\left[E^{\mathrm{B}}_n(0)+\frac{\hbar^2k^2}{2m^*_{\mathrm{B}}}\right]\delta_{\mathbf{kk}'}$$
$$+\Delta E_nf_{\mathrm{b}}(\mathbf{k}-\mathbf{k}')+iU_{0\mathrm{d}}f_{\mathrm{d}}(\mathbf{k}-\mathbf{k}').\qquad(9)$$

The solution of the following inhomogeneous Schrödinger equation with Hamiltonians (7)–(8) allows us to calculate the envelope of the wave function $F_{\mathbf{k}}^{(n)}(E)$ of the charge carrier at a given energy E:

$$\sum_{\mathbf{k}'}(H_{\mathbf{kk}'}^{(n)} - \delta_{\mathbf{kk}'}E)F_{\mathbf{k}'}^{(n)}(E) = \rho_{\mathbf{k}}^{(n)},$$

$$F_{\mathbf{k}}^{(n)}(E) = \sum_{\mathbf{k}'} G_{\mathbf{kk}'}^{(n)}(E)\rho_{\mathbf{k}'}^{(n)},$$

where the Green's function $G_{\mathbf{kk}'}^{(n)}(E)$ and the components $\rho_{\mathbf{k}}^{(n)}$ in the basis $|n\mathbf{k}\rangle$ are determined by the formulas

$$G_{\mathbf{kk}'}^{(n)}(E) = \langle n\mathbf{k}|\hat{G}(E)|n\mathbf{k}'\rangle = \langle n\mathbf{k}|(\hat{H} - \hat{I}E)^{-1}|n\mathbf{k}'\rangle,$$

$$\rho_{\mathbf{k}}^{(n)} = \sum_{\mathbf{b}}\langle n\mathbf{k}|\mathbf{b}+\mathbf{k}\rangle\langle\mathbf{b}+\mathbf{k}|\rho\rangle.$$

In this case, the smooth envelope wave function in **a**-representation is calculated using the inverse Fourier transform.

$$F_{\mathbf{a}}^{(n)}(E) = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}}\exp(i\mathbf{ka})F_{\mathbf{k}}^{(n)}(E).$$

Note that the Bloch wave functions of the reference bulk crystal used by us as a basis, which in the coordinate representation satisfy the periodic Born-Von Karman boundary conditions, form a complete orthonormal set of functions. This makes it possible, even in the presence of dissipative regions, to use them to represent the desired functions with zero boundary conditions.

5. Numerical calculation results

As an example, let us consider one-dimensional model heterostructures with two and three potential barriers for electrons in the lower band. x axis, along which the charge carriers are tunneled, is oriented perpendicular to the materials' layers. All geometric parameters are measured in units of a constant lattice a_0. At that, the energy is calculated in $E_0 = \hbar^2/(2m_0a_0^2)$. The thickness of barrier layers d_b is selected equal $3a_0$ and is equal to the distance between the layers d_w.

To perform numerical analysis within a one-dimensional problem, we will consider a limited area of space, the linear size of which is denoted as D. In this case, the values of the wave vector K in the Brillouin zone of crystals change discretely as $k_n = 2\pi/D[n-(N-1)/2]$, where $n = 0, 1, \ldots, N-1$, N is the total number of values of the vector $\mathbf{k}$. Further it was suggested that $N = 33$.

The characteristic function of the dissipative component of the potential for both tasks is selected as [15]

$$f_{\text{d}}(x) = 1 - \left[\exp\left(\frac{x-\mu}{\sigma}\right) + \exp\left(-\frac{x+\mu}{\sigma}\right) + 1\right]^{-1},$$

where μ is a parameter that determines the position of the dissipation regions in space, σ — is a parameter that describes the smoothness of the change in the imaginary potential.

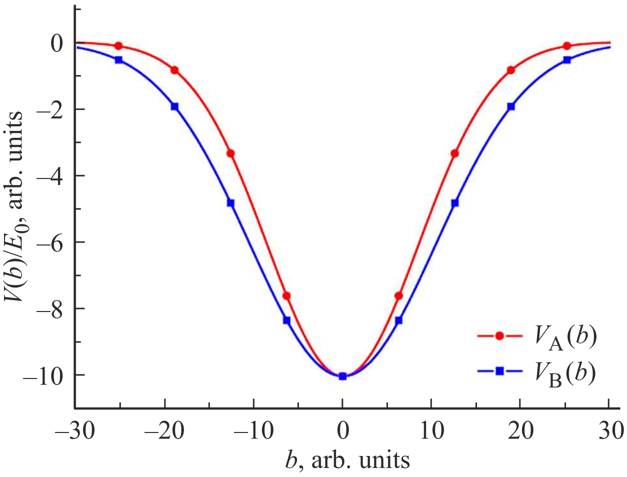

Figure 1. Model Fourier transforms of crystal potentials in material A (red line) and material B (blue line).

The band structures of materials are calculated using a model „Fourier transform" of the local atomic potential

$$V_{\text{A,B}}(q) = V_0^{\text{A,B}}\exp\left(-\frac{q^2}{d_{\text{A,B}}^2}\right),$$

where $V_0^{\text{A,B}}$, $d_{\text{A,B}}$ — parameters where the following values are selected: $V_0^{\text{A}}/E_0 = V_0^{\text{B}}/E_0 = -10$ arb. units, $d_{\text{A}}a_0 = 12$ arb. units, $d_{\text{B}}a_0 = 14.71$ arb. units. The order of the values of energies and distances, taking into account normalization, corresponds to the actual values of these parameters in real heterostructures. In this case, „Fourier transforms" $V_{\text{A,B}}(b)$ at points $q = b$, i. e., form factors, coincide with the Fourier transforms of the periodic crystal potential of materials $U_{\text{A,B}}(b)$.

To calculate band structures within the microscopic approach, it is necessary to select a finite number of points of S Fourier transforms of the crystal potential. Their number determines the number of inverse lattice vectors b. For further numerical analysis, $S = 9$ is selected — these points and the values of Fourier transforms in them are marked in Figure 1. At $N = 33$ and $S = 9$ the general dimensions of Hamiltonian — 297 × 297.

According to the band structures from the microscopic theory (Figure 2), the pattern of band discontinuities is determined (Figure 3 — two-barrier structure and Figure 4 — three-barrier structure), where the shaded areas correspond to the permitted energy bands.

The resulting diagrams (Figures 3 and 4) are determined by the energy difference in the center and at the boundary of the Brillouin zone. For the electrons of the lower energy band near its bottom, the selected materials form a system of potential barriers. At the same time, near the ceiling of the same band the barrier system turns into a system of tunnel-connected quantum wells for holes.

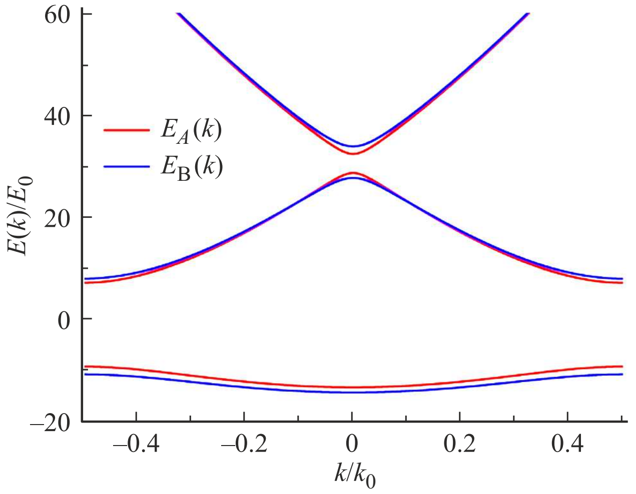

Figure 2. Band structures of materials A (red line) and B (blue line), $k_0 = 2\pi/a_0$.

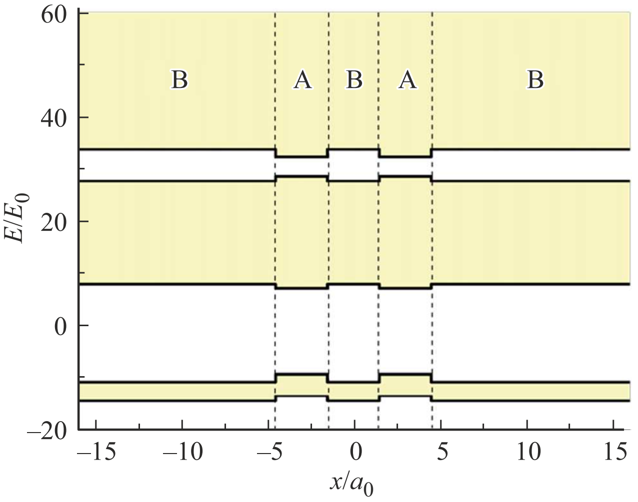

Figure 3. Energy band diagram of materials for a structure with two potential barriers for charge carriers of the low-lying energy band.

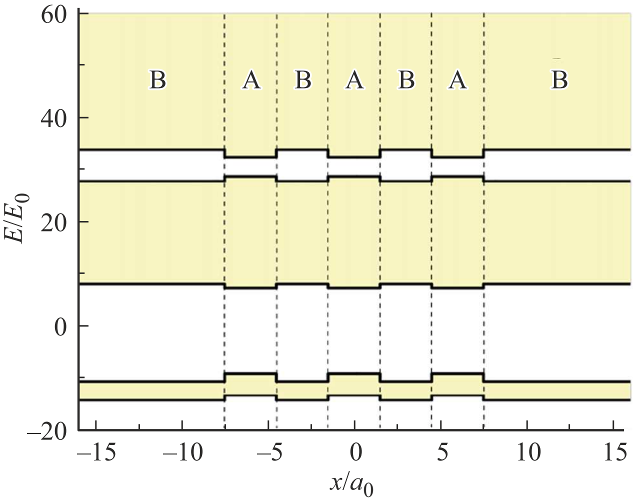

Figure 4. Energy band diagram of materials for a structure with three potential barriers for charge carriers of the low-lying energy band.

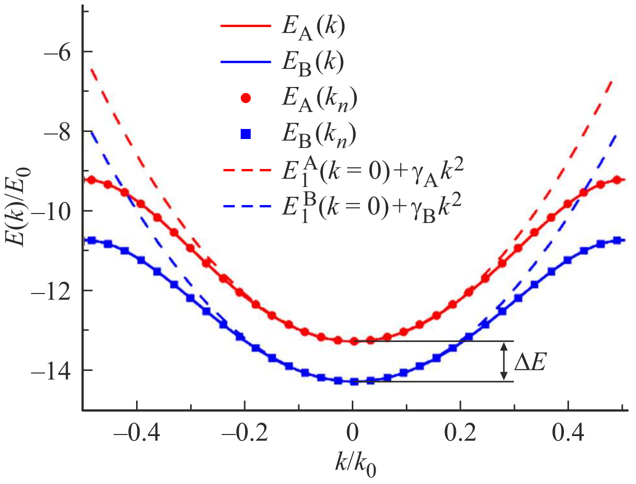

Figure 5. Lower dispersion branches of the band structures of materials A (red line) and B (blue line).

For subsequent analysis using the effective mass method, the obtained lower dispersion branches are approximated by parabolic dependencies (Figure 5) of the form $E_{A,B}(k) = E^{(1)}_{A,B}(0) + \gamma_{A,B}k^2$, where $\gamma_{A,B} = 1/m^*_{A,B}$. The obtained effective mass when calculated using a second derivative in the point $k = 0$: $m^*_A/m_0 = 0.73$ and $m^*_B/m_0 = 0.67$.

We calculate the dependences of the tunneling coefficient on the energy of the charge carriers for both structures using Hamiltonian of microscopic theory (6), as well as the Hamiltonians of smooth envelope function methods (8) and effective mass (9) — Figures 6 and 7. The energy of the particle is further calculated from the minimum of the lower dispersion branch of the reference crystal B. For convenience, potential barriers are shown here, determined by band discontinuities at the interfaces ΔE (Figures 3 and 4).

As follows from the presented data, resonances in the low-energy region (Figures 6 and 7) correspond to tunneling of charge carriers with energies corresponding to the first quasi-resonant levels in quantum wells formed by potential barriers. The number of resonant peaks in each series corresponds to the number of quantum wells formed by the barriers of the structure. In addition, the spectra of the tunneling coefficient show features in the energy range above the barrier (over-barrier reflection). Despite the qualitative coincidence of these dependences for the three methods used, there is some difference in the position of the resonant peaks, especially in the over-barrier reflection region. The dependences of tunneling coefficient on energy within the method of smooth envelope functions are in much better agreement with the solution following from microscopic theory, since this approximation takes into account the total dispersion of charge carriers in the entire Brillouin zone. However, unlike precise microscopic calculations, this approach does not take into account the contribution of short-range interface corrections. Thus, their effect should be considered small compared to the effects

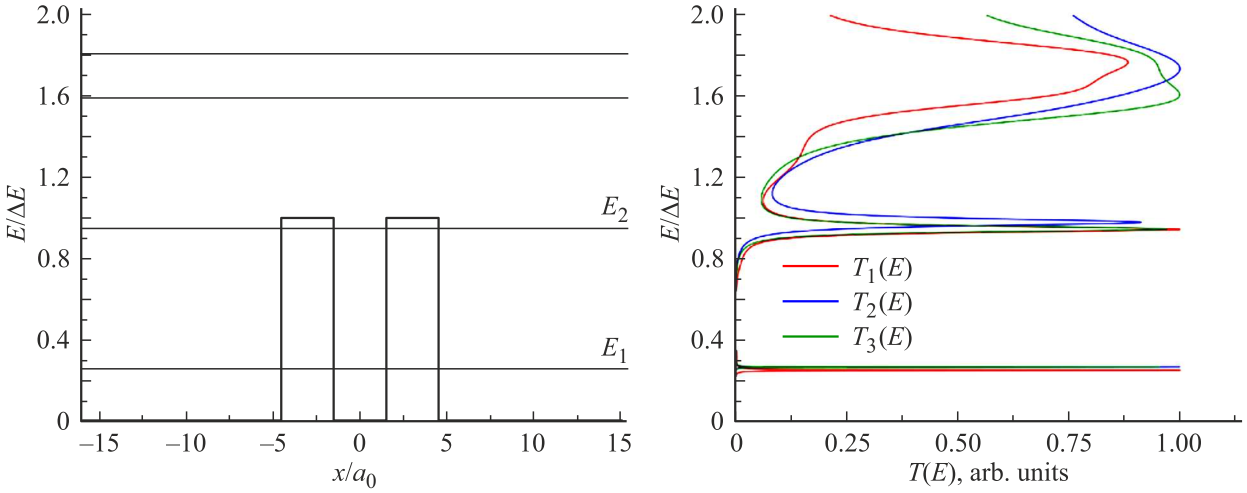

Figure 6. Dependences of the tunneling coefficient on the electron energy for a two-barrier structure: $T_1(E)$ — microscopic theory, $T_2(E)$ — smooth function envelopes method, $T_3(E)$ — effective mass approximation.

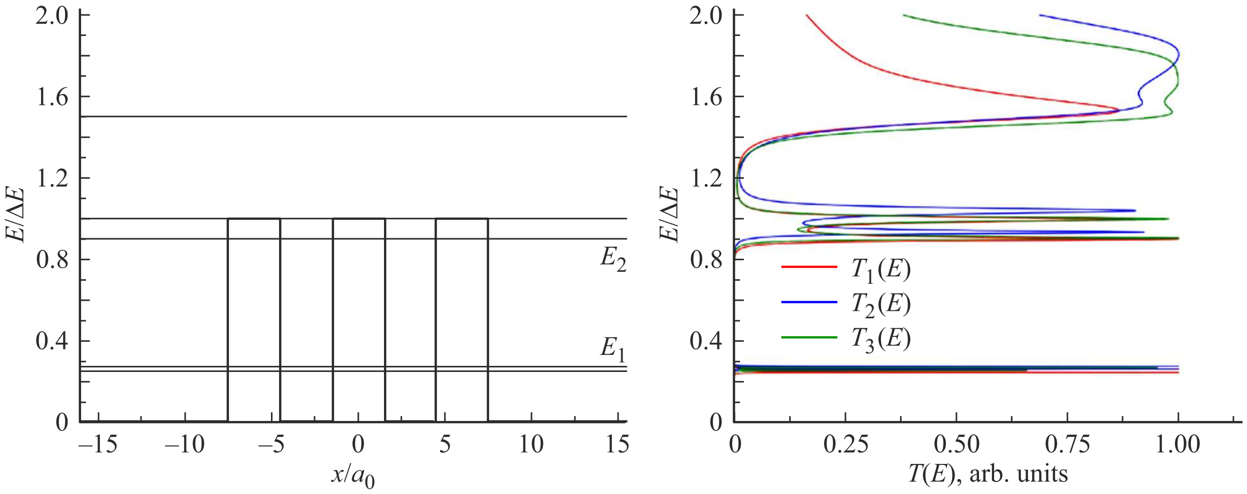

Figure 7. Tunneling coefficient versus electron energy for a three-barrier structure: $T_1(E)$ — microscopic theory, $T_2(E)$ — smooth function envelopes method, $T_3(E)$ — effective mass approximation.

of nonparabolicity in the dispersion law. The difference in the energy dependence calculated within the microscopic theory at energies above the height of the potential barrier is explained by nonparabolicity in the electron dispersion law, up to a change in the sign of the effective mass, as well as by contribution of the short-range component of the heterostructure potential. For this reason, the tunneling coefficient may not decrease to one in the quasi-resonance region (Figures 6 and 7).

Figures 8 and 9 show the exact $\psi(x)$ and envelope $F(x)$ wave functions of charge carriers for the two quasi-resonant levels in the system. In this case, the upper energy level E_2, in contrast to E_1, corresponds to a less localized wave function in space, which is due to the tunneling effect. This corresponds to a wider resonance in the transmission spectrum in this energy range and a shorter electron lifetime in this quasi-resonant state.

Thus, the width of the resonance lines, as expected, is directly related to the lifetime of the charge carrier at these levels. In our method, it is determined by the imaginary part of the pole of the Green's function in the lower half-plane-$\tau \propto 1/\mathrm{Im}\{E\}$. Consequently, the lifetime of the charge carrier, calculated within a precise microscopic theory, turns out to be long compared to the lifetimes calculated using the smooth envelope functions and effective mass methods.

6. Conclusion

A microscopic theory of resonant tunneling in the semiconductor heterostructures is organized. Resonant tunneling in systems with multiple potential barriers is studied using the example of two-barrier and three-barrier structures. The result of the exact problem numerical

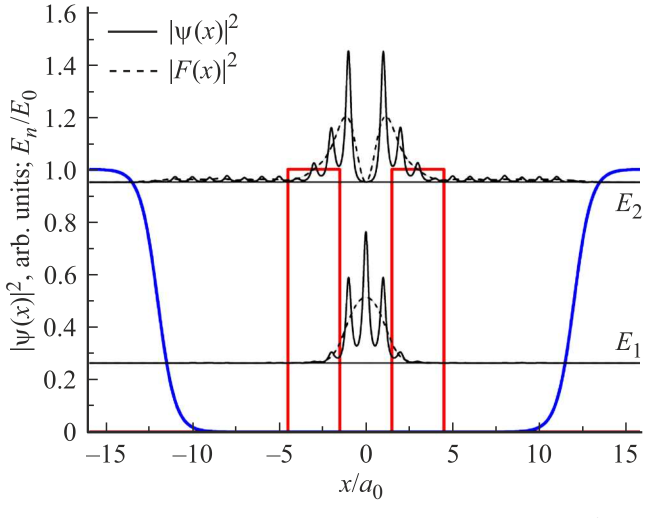

Figure 8. Squares of the modules of the exact $|\psi(x)|^2$ and envelope wave functions $|F(x)|^2$ of the charge carriers in a two-barrier structure (red and blue show the distribution of real and imaginary potentials, respectively, in the examined system).

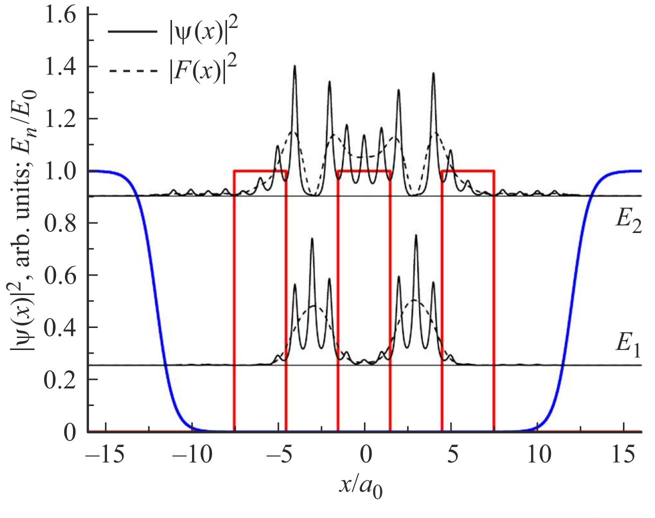

Figure 9. Squares of the modules of the exact $|\psi(x)|^2$ and envelope wave functions $|F(x)|^2$ of the charge carriers in a three-barrier structure (red and blue show the distribution of real and imaginary potentials, respectively, in the examined system).

solution is compared with calculations using the smooth envelope wave functions and the effective mass methods. It is shown that the data obtained using the method of smooth envelope wave functions, which takes into account the exact law of electron dispersion in the entire Brillouin zone, are in good consistency with the microscopic calculation data. Thus, it can be assumed that the interface effects caused by the short-acting part of the interface potential of the heterostructure are negligible compared to the effects of nonparabolicity in the dispersion law. The developed approach makes it possible to analyze the phenomenon of resonant tunneling in semiconductor heterostructures, taking into account all singularities in the band structure of the considered materials.

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Conflict of interest

The authors declare that they have no conflict of interest.

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