Properties of spectral characteristics of electron quasistationary states in an open multi-cascade nanostructure

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Motivation

With the appearance and development of nanodevices, the functioning of which is ensured by electronic transport through resonant tunneling nanostructures, the relevance of the theory of physical properties of quasi-particles in open nanostructures has significantly increased. Despite the significant progress of experimental research, the theory of physical processes in such devices is still not complete. The main problems in its development are related to mathematical complexities caused by non-localized wave functions and the quasistationary spectra of quasiparticles. Therefore, in the majority of theoretical papers, the research is performed in simplified models.

In this paper, we propose the developed theory of spectral characteristics of quasistationary states of an electron in a multi-cascade open nanostructure, being a typical element of a quantum cascade detector. For this, in the approximation of effective mass and rectangular potentials, using the transfer matrix method based on the solutions of the Schrödinger equation, an exact expression for the S-matrix is obtained. Its poles determine the resonance energies and resonance widths (lifetimes) of electron states.

Theory of S-matrix in open multi-cascade nanostructure

We consider an N-cascade nanostructure (Fig. 1), placed into an external bulk semiconductor medium-well. Taking into account that the magnitudes of the lattice constants of wells and barriers of semiconductor materials in isotropic nanostructures of typical quantum cascade detectors (QCD) [1] are close to each other, we will develop the theory of quasistationary states (QSS) of the electron in the model of position-dependent effective mass and rectangular potentials. In the Cartesian coordinate system with z-axis perpendicular to the nano layers of the structure, the effective mass and potential energy of the electron is written in the following form:

$$m(E,z)=\begin{cases} m_b(E)=m_b\left(1-\dfrac{(U-E)}{E_{gb}}\right), & j=1,3,5,\dots,P-2, i=1,2,\dots,N;\; j=P, i=N; \\ & z_{i,j-1}<z<z_{i,j}, \\ m_w(E)=m_w\left(1+\dfrac{E}{E_{gw}}\right), & j=2,4,\dots,P-1,\; i=1,2,\dots N;\; j=0, i=1;\; j=P+1, i=N; \end{cases} \tag{1}$$

$$U(z)=\begin{cases} U, & j=1,3,5,\dots,P-2, i=1,2,\dots,N;\; j=P, i=N; \\ & z_{i,j-1}<z<z_{i,j}, \\ 0, & j=2,4,\dots,P-1,\; i=1,2,\dots N;\; j=0, i=1;\; j=P+1, i=N; \end{cases} \tag{2}$$

where $z_{i,j}=z_{1,j}+(i-1)d$ are the coordinates of the hetero interfaces in the i-th cascade; $z_{i,P-1}=z_{i+1,0}$; $z_{1,-1}=-\infty$; $z_{N,P+1}=+\infty$; *d* is the linear size of the cascade; *P* is the total number of wells and barriers in in a separate cascade; *U* – heights of potential barriers; m_w, m_b are the effective masses of the electron in bulk analogues of well and barrier materials.

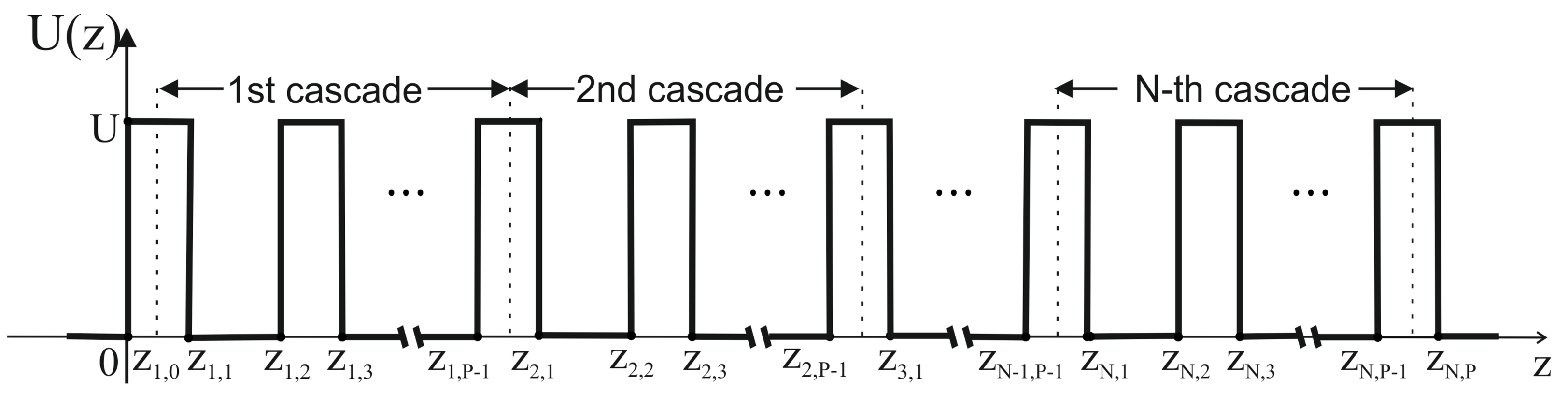

Fig. 1. Potential profile of an open multi-cascade nanostructure

The one-dimensional Schrödinger equation for an electron is written as

$$\left[-\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m(E,z)}\frac{d}{dz}+U(z)\right]\Psi(z)=E\Psi(z) \tag{3}$$

its solutions must satisfy the fitting conditions at the interfaces between all hetero layers of the studied nanostructure

$$\begin{cases} \Psi(z_{i,j}-\varepsilon)=\Psi(z_{i,j}+\varepsilon), \qquad (\varepsilon\to 0) \\ \left.\dfrac{1}{m(E,z)}\dfrac{d\Psi(z)}{dz}\right|_{z=z_{i,j}-\varepsilon}=\left.\dfrac{1}{m(E,z)}\dfrac{d\Psi(z)}{dz}\right|_{z=z_{i,j}+\varepsilon} \end{cases}, \tag{4}$$

and the normality condition

$$\int_{-\infty}^{+\infty}\Psi^*_{k'}(z)\Psi_k(z)dz=\delta(k-k'). \tag{5}$$

The wave function from equation (3) is found exactly

$$\Psi(z)=\begin{cases} A_{1,0}(e^{ikz}-Se^{-ikz}), & j=0, i=1; \\ A_{i,j}e^{\chi z}+B_{i,j}e^{-\chi z}, & j=1,3,5,\dots,P-2, i=1,\dots,N;\; j=P, i=N; \\ A_{i,j}e^{ikz}+B_{i,j}e^{-ikz}, & j=2,4,\dots,P-2, i=1,\dots,N; \\ A_{N,P+1}(e^{-ikz}-Se^{ikz}), & j=P+1, i=N; \end{cases} \tag{6}$$

where

$$k=\sqrt{\frac{2m_w(E)E}{\hbar^2}};\qquad \chi=\sqrt{\frac{2m_b(E)(U-E)}{\hbar^2}}. \tag{7}$$

S=*S*(*E*) is the scattering matrix.

All unknown coefficients $A_{i,j}$, $B_{i,j}$ and the S-matrix are uniquely defined from the fitting conditions (4) and the normality condition (5). Applying the method of the transfer matrix (T) [2, 3], the relationship between the coefficients of the wave functions in external semi-infinite media is obtained as

$$\begin{pmatrix} A_{1,0} \\ -A_{1,0}S \end{pmatrix}=\begin{pmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{pmatrix}\begin{pmatrix} -A_{N,P+1}S \\ A_{N,P+1} \end{pmatrix}. \tag{8}$$

A square equation is obtained for the S-matrix from (8).

$$S^2+\frac{t_{21}-t_{12}}{t_{11}}S-\frac{t_{22}}{t_{11}}=0, \tag{9}$$

which has two solutions

$$S_{1,2}=\frac{t_{12}-t_{21}}{2t_{11}}\left(1\pm\sqrt{1+\frac{4t_{11}t_{22}}{(t_{12}-t_{21})^2}}\right), \tag{10}$$

which are determined by all elements of the T-matrix and define two orthonormal wave functions.

In general, wave functions in the external semi-infinite media are written as linear combinations of both independent solutions.

$$\begin{cases} \Psi_{1,0}(z)=C_1(e^{ikz}-Se^{-ikz}), \\ \Psi_{N,P+1}(z)=C_N(e^{-ikz}-Se^{ikz}), \end{cases} \tag{11}$$

with known coefficients and S-matrix

$$S=\frac{S_1A^{(1)}_{i,j}+S_2A^{(2)}_{i,j}}{A^{(1)}_{i,j}+A^{(2)}_{i,j}};\; i=1, j=0;\; i=N, j=P+1. \tag{12}$$

It is known from the theory of scattering that in the complex energy plane ($E=E'-iE''$) the poles of the S-matrix, which are found as solutions of the equation

$$\frac{1}{S(E'-iE'')}=0, \tag{13}$$

determine the resonance energies ($E^S_n=E'_n$) and resonance widths ($\Gamma^S_n=2E''_n$) of electron states.

Properties of spectral parameters of electron QSSs in open multi-cascade nanostructure

The evolution of spectral parameters of electron QSS in multi-layer open nanostructure, depending on the number of cascades in it, is studied in a model of three-well cascade with GaAs wells of widths a_1=6.8 nm, a_2=2.4 nm, a_3=3.7 nm and with $\mathrm{Al_{0.33}Ga_{0.67}As}$-barriers of the same thickness (3 nm). Geometric sizes of potential wells and barriers in such a cascade simulate the general energy scheme of a single-well (a_1) active region with two operating states (*n*=1 and *n*=4), transitions between which occur with the absorption of electromagnetic radiation, and a double-well (a_2, a_3) extractor with two states (*n*=2 and *n*=3) of the phonon ladder. The physical parameters of the structure are known: $m_w=0.067\,m_e$, $m_b=0.095\,m_e$, *U* = 276 meV.

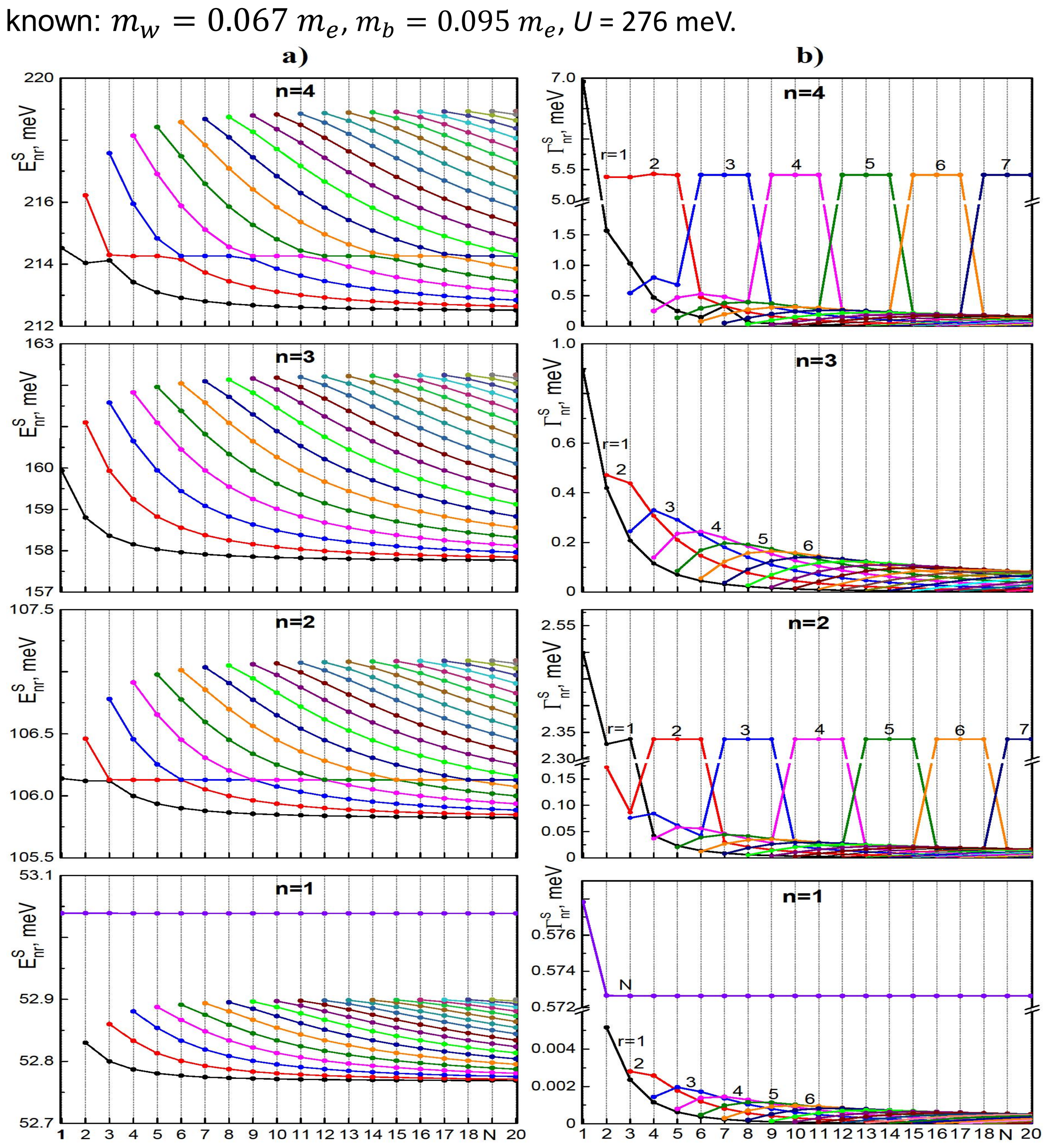

Fig. 2. Resonance energies E^S_{nr} (a) and resonance widths Γ^S_{nr} (b) of electron QSS as functions of the number of cascades (N) in the nanostructure

Dependences of resonance energies and widths of electron states on the number of cascades (*N*) in the nanostructure, numerically calculations by the solution of equation (13), are shown in Fig. 2. Figure proves that if the number of cascades *N* increases, the resonance energies of the QSS form the bands (numbered by n in the figure), the widths of which almost do not change when *N*>10. We should note that when *n*=2 and *n*=4, the anti-crossings are observed at E^S_{nr} functions of *N*. States with energies on horizontal sections located between anti-crossings are characterized by significant values of resonance widths (short lifetimes), Fig. 2b. In these states, the electron is either weakly localized in the second well (a_2) of the extractor (at *n*=2) of the last stage of the multi-cascade structure, or in the active well (a_1) of the first stage (at *n*=4). From the latter it can easily tunnel into the outer semi-infinite well. In the state with energy $E^S_{n=1r=N}$, the electron is characterized by a significant resonance width, Fig. 2b. It is caused by its weak localization in the active well (a_1) of the first cascade due to the high probability of tunneling into the left semi-infinite well.

The widths of all other states (Fig. 2b) have a qualitatively similar dependence on *N*. It shows the decreasing of Γ^S_{nr} with an increasing number of cascades. Their behavior is associated with an increasing lifetime of an electron in the layers of internal cascades, due to a decrease in the probability of an electron exiting a multi-cascade nanostructure to the outside with the gradual "addition" of new external cascades.

We should also note an interesting feature characteristic of the resonance widths determined by the poles of the S-matrix, which lays in the fact that for arbitrary *N* the sum of the widths of all QSSs in the *n*-th complex is equal, with high accuracy, to the width of the *n*-th state in a single-cascade (*N*=1) structure $\sum_{r=1}^{N}\Gamma^S_{nr}(N)=\Gamma^S_n(N=1)$.

Conclusions

1. The theory of spectral characteristics (resonance energies and resonance widths) of the electron QSSs in an open multi-cascade nanostructure is developed in the approximation of effective mass and rectangular potentials, using the transfer matrix method based on accurately obtained analytical expressions for the scattering matrix.

2. For the example of a $\mathrm{GaAs/Al_{0.33}Ga_{0.67}As}$ multi-cascade resonant-tunnel structure with three-well cascades, the peculiarities of resonance energies and resonance widths are investigated depending on the number of cascades. It is established that in the N-cascade nanostructure, in the energy regions that do not exceed the height of the potential barriers, four resonance complexes are formed. In each of which the poles of the S-matrix uniquely determine the resonance energies and resonance widths of the *N* electron QSS.

3. It is shown that with an increasing number of cascades, the resonance energies of the QSSs in the complexes form corresponding bands, the widths of which almost do not change at *N*>10. At the same time, anti-crossings appear at the dependences of energies on *N*. States with the energies on the horizontal sections between anti-crossings are characterized by significant values of resonance widths due to the localization of the electron in the extreme left or right cascades, and their values weakly depend on *N*. The widths of all other states localized in the internal cascades of the multi-cascade resonance-tunnel structure decrease rapidly with increasing number of cascades.

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