THE METHOD OF S-MATRIX IN THE THEORY OF RESONANCE ENERGIES AND WIDTHS FOR QUASISTATIONARY STATES OF AN ELECTRON IN ASYMMETRIC TWO-BARRIER RESONANCE-TUNNEL STRUCTURES

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By the methods of transfer- and S-matrices, we executed the analytic and numerical calculations of resonance energies and widths of quasistationary states of an electron in a plane two-barrier resonance-tunnel nanostructure with asymmetric rectangular (with different effective masses in barriers and wells) and δ-like potential barriers. By the example of the nanosystems GaAs/AlAs and $In_xAl_{1-x}As/In_xGa_{1-x}As$, we show that, as distinct from the exact values of resonance energies and widths in the model of rectangular potential barriers, the model of δ-like barriers which is often used in theoretical studies gives the errors of resonance energies overestimated by tens of percents, whereas the resonance widths are overestimated by tens of times.

1. Introduction

A great attention is given to the study of resonance-tunnel structures (RTS), because they are a base for the creation and operation of cascaded lasers in the THz range and resonance-tunnel diodes which possess unique perspectives for applications in nanodevices [1–3].

In the theory of RTS, the objects under study are the dynamical conduction $\sigma(\omega)$ or the response current $j(\omega)$, whose calculation is performed by solving the full Schrödinger equation for a system of electrons interacting with an electromagnetic field in a nanostructure. The theories of dynamical conduction $\sigma(\omega)$ and response current $j(\omega)$ were constructed in various models with the use of various mathematical procedures of calculations [4–10]. However, it was always necessary to know the resonance energy spectrum and the lifetimes (or resonance widths) of quasistationary states (QSS) of an electron in an open nanosystem.

In calculations of spectral parameters of an electron in RTS, the dominant majority of works use the method of effective mass and the model of rectangular potential barriers. In this case, with the purpose to simplify awkward analytic calculations, rectangular potential barriers are approximated very often by δ-like ones [4–9]. From the physical reasoning, it is clear that such an approximation leads to the loss of exactness in the determination of both spectral parameters, in particular of resonance widths, to which the dynamical conduction is very sensitive [4–6]. The second source of the inaccuracy of the δ-barrier approximation is also evident: this is the loss of the information about a difference of the effective masses of an electron in wells and barriers of RTS.

In the dominant majority of theoretical works, the calculations of the resonance energies (REs) and widths (RWs) in QSS of electrons in RTS were carried out with the use of the transparency coefficient. However, according to the general theory of scattering [11–13], these both spectral parameters are determined by complex-valued poles of the S-matrix. Therefore, it is important to clarify how values of the spectral parameters calculated by different methods correlate with one another.

The purpose of the present work consists in the development and application of a S-matrix-based method for the exact calculation of the spectral parameters of an electron in an open plane two-barrier nanostructure. By the example of two typical RTS

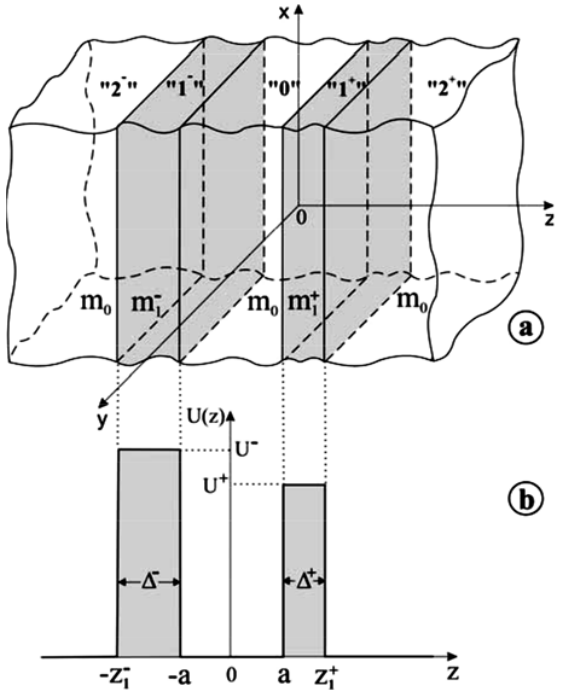

Fig. 1. Geometric (a) and energy (b) schemes of TBRTS

(GaAs/AlAs and $In_xAl_{1-x}As$/ $In_xGa_{1-x}As$) which are intensively studied theoretically and experimentally [14], we will find the dependences of REs and RWs on the geometric sizes of RTS and compare our results with those obtained by different methods in the approximation of the δ-barrier model [4–6]. We will analyze the reasons for the difference in values of the spectral parameters calculated in the approximate approaches and the exact S-matrix theory constructed in the models of rectangular barriers with different effective masses in barriers and wells.

2. Hamiltonian, S- and T-matrices and Spectral Parameters of an Electron in a Plane Open Two-barrier Nanosystem

We consider a plane open two-barrier resonance-tunnel structure (TBRTS) with geometric sizes indicated in Fig. 1. By assuming that the lattice constants $(a_0, a_1^{\pm})$ and the dielectric permeabilities of components of the nanosystem differ slightly (e.g., for the structures on the basis of InAS, GaAs, and AlAs), we use the model of effective masses $(m_0, m_1^{\pm})$ and rectangular potentials for electrons.

Hence, in the Cartesian coordinate system with the origin at the middle of a film-well with the $0Z$ axis which is normal to the planes of all films, we have

$$m(z) = \begin{cases} m_0, & 0 \le |\pm z| \le a,\ z_1^{\pm} \le |\pm z| \le \infty, \\ m_1^{\pm}, & a \le |\pm z| \le z_1^{\pm}, \end{cases} \tag{1}$$

$$U(z) = \begin{cases} 0, & 0 \le |\pm z| \le a,\ z_1^{\pm} \le |\pm z| \le \infty, \\ U^{\pm}, & a \le |\pm z| \le z_1^{\pm}. \end{cases} \tag{2}$$

The Hamiltonian of an electron in TBRTS takes the form

$$H = -\frac{\hbar^2}{2}\left(\frac{\partial}{\partial z}\frac{1}{m(z)}\frac{\partial}{\partial z} + \frac{1}{m(z)}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\right) + U(z). \tag{3}$$

Therefore, it is expedient to seek for a solution of the Schrödinger stationary equation

$$H\Psi(x,y,z) = E\Psi(x,y,z) \tag{4}$$

in the form

$$\Psi(x,y,z) = \Psi(z)\Psi_{\vec{k}_{\parallel}}(x,y), \tag{5}$$

where

$$\Psi_{\vec{k}_{\parallel}}(x,y) = \frac{1}{L}\, e^{i\vec{k}_{\parallel}(x\vec{n}_x + y\vec{n}_y)}. \tag{6}$$

Here, $\vec{k}_{\parallel}$ – quasimomentum of an electron in the $X0Z$ plane, and L – length of the basic domain in this plane.

We now obtain the following equation for the function $\Psi(z)$:

$$\left(-\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m(z)}\frac{d}{dz} + U_{k_{\parallel}}(z)\right)\Psi(z) = E\Psi(z). \tag{7}$$

Here, the quantity

$$U_{k_{\parallel}}(z) = U(z) + \frac{\hbar^2 k_{\parallel}^2}{2m(z)} = \begin{cases} \dfrac{\hbar^2 k_{\parallel}^2}{2m_0}, & 0 \le |\pm z| \le a, |z_1^{\pm}| \le |\pm z| \le \infty, \\ \dfrac{\hbar^2 k_{\parallel}^2}{2m_1^{\pm}} + U^{\pm}, & a \le |\pm z| \le |z_1^{\pm}|, \end{cases} \tag{8}$$

plays the role of the effective potential energy depending on $k_{\parallel}$. It is worth noting that, due to the difference of effective masses in barriers $(m_1^{\pm})$ and in wells (m_0), the potentials in wells and barriers are renormalized

differently at a fixed value of $k_\parallel$ (8). Since, as a rule, $m_1^\pm > m_0$, the effective potential barriers

$$\widetilde{U}^\pm = U^\pm - \frac{\hbar^2 k_\parallel^2}{2}\left(\frac{m_1^\pm - m_0}{m_1^\pm + m_0}\right)$$

decrease with increase in $k_\parallel$, which must cause a decrease of the lifetime (increase of RW) of QSS of an electron.

Taking into account that the system is open for the motion of an electron along the $0Z$ axis, we seek for a solution of Eq. (7) by the method of S-matrix [11]. That is, we write the wave functions in the form

$$\Psi(k_\perp z) = \\ = \begin{cases} \Psi_0(z) = A_0\ e^{ik_\perp z} + B_0\ e^{-ik_\perp z},\ -a \le z \le a, \\ \Psi_1^\pm(z) = A_1^\pm e^{z\chi_\pm} + B_1^\pm e^{-z\chi_\pm},\ a \le |\pm z| \le z_1^\pm, \\ \Psi_2^\pm(z) = B_2^\pm(e^{-ik_\perp z} + S_r e^{ik_\perp z}),\ z_1^\pm \le |\pm z| \le \infty, \end{cases} \tag{9}$$

where

$$k_\perp = \sqrt{\frac{2m_0E}{\hbar^2} - k_\parallel^2}, \quad \chi_\pm = \sqrt{\frac{2m_1^\pm}{\hbar^2}(U^\pm - E) - k_\parallel^2}. \tag{10}$$

The boundary conditions

$$\left.\begin{array}{l} \Psi_i(\pm z_i) = \Psi_{i+1}(\pm z_i) \\ \dfrac{1}{m_i}\dfrac{d\Psi_i(z)}{dz}|_{z=\pm z_i} = \dfrac{1}{m_{i\pm1}}\dfrac{d\Psi_{i\pm1}(z)}{dz}|_{z=\pm z_i} \end{array}\right\}\ (i = 0, \pm1) \tag{11}$$

and the normalization condition

$$\int\limits_{-\infty}^{\infty} \Psi^*_{k'_\perp}(z)\Psi_{k_\perp}(z)dz = \delta(k_\perp - k'_\perp) \tag{12}$$

determine uniquely all unknown coefficients $A_i^\pm$, $B_i^\pm$ and the scattering matrix S_r. In doing so, we use the method of transfer-matrix [15] which is, in our case, a second-rank matrix

$$T = \begin{pmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{pmatrix} \tag{13}$$

determined by the product of four matrices

$$T = (T_-^{01}T_-^{12})^{-1}\ T_+^{01}T_+^{12} \tag{14}$$

which are also of the second rank:

$$T_\pm^{01} = \begin{pmatrix} t_{\pm11}^{01} & t_{\pm12}^{01} \\ t_{\pm21}^{01} & t_{\pm22}^{01} \end{pmatrix};\ T_\pm^{12} = \begin{pmatrix} t_{\pm11}^{12} & t_{\pm12}^{12} \\ t_{\pm21}^{12} & t_{\pm22}^{12} \end{pmatrix}. \tag{15}$$

The analytic calculation of matrix elements gives the following result:

$$t_{\pm11}^{01} = \left(t_{\pm12}^{01}\right)^* = \\ = t_{\pm22}^{01} = \left(t_{\pm21}^{01}\right)^* = \frac{1}{2}\left(1 \mp i\frac{m_0\chi_\pm}{m_1^\pm k_\perp}\right)e^{\pm ik_\perp a}, \tag{16}$$

$$t_{\pm11}^{12}(\chi_\pm) = t_{\pm21}^{12}(-\chi_\pm) = \left(t_{\pm12}^{12}(\chi_\pm)\right)^* = \\ = \left(t_{\pm22}^{12}(-\chi_\pm)\right)^* = \frac{1}{2}\left(1+i\frac{m_1^\pm k_\perp}{m_0\chi_\pm}\right)e^{-\chi_\pm(z_1^\pm - a)}. \tag{17}$$

This allows us to uniquely determine all matrix elements of T-matrix (13) and yields a simple quadratic equation for the S_r-matrix,

$$S_r^2 + \frac{t_{22}\ e^{-2ik_\perp z_1^+} - t_{11}\ e^{-2ik_\perp z_1^-}}{t_{21}}S_r - \\ -\frac{t_{12}}{t_{21}}\ e^{-2ik_\perp(z_1^+ + z_1^-)} = 0, \tag{18}$$

which has two obvious solutions

$$S_r^{(1,2)}(k_\perp) = \frac{t_{11}\ e^{-2ik_\perp z_1^-} - t_{22}\ e^{-2ik_\perp z_1^+}}{2\ t_{21}} \times \\ \times\left(1 \pm \sqrt{1 + 4\frac{t_{12}\ t_{21}\ e^{-2ik_\perp(z_1^+ + z_1^-)}}{(t_{11}\ e^{-2ik_\perp z_1^-} - t_{22}\ e^{-2ik_\perp z_1^+})^2}}\right). \tag{19}$$

The upper index "1" corresponds to the sign "+", and the index "2" – to the sign "–".

According to the general theory [11], we extend the $S_r^{(1,2)}$-matrix into the complex plane of quasimomenta ($\tilde{k}_\perp = k_\perp - ik'_\perp$) or energies ($\tilde{E} = E - iE'$) and obtain the equations

$$\mathrm{Re}\left(S_r^{(1,2)}(E)\right)^{-1} = 0, \quad \mathrm{Im}\left(S_r^{(1,2)}(E)\right)^{-1} = 0 \tag{20}$$

for the determination of the spectra of REs and RWs, respectively.

As a rule, Eq. (20) cannot be exactly solved analytically. But, for specific nanosystems, the calculation of the spectral parameters (PE and RW) can be performed rapidly and with any accuracy with the use of a computer, which will be shown in what follows.

3. Analytic Calculation of the Spectral Parameters of an Electron in TBRTS with δ-like Barriers

We note that the model of rectangular potentials gives exact, but rather complicated analytic expressions for $S_r^{\pm}$-matrix (19) or for other quantities (in particular, for the transparency coefficient [15]) for an electron in TBRTS. Therefore, the majority of theoretical works [4–9] used δ-like potential barriers with the purpose to simplify the analytic expressions. In the case of the nanosystem under consideration, the potential energy of an electron takes the form

$$U(z) = U^+ \triangle^+ \delta(z-a) + U^- \triangle^- \delta(z+a). \tag{21}$$

As a result, the Schrödinger equation for the wave function $\Psi_{k_\perp}(z)$ reads

$$\begin{aligned}&(\frac{d^2}{dz^2} + k_\perp^2 - \frac{2m_0}{\hbar^2}(U^+\triangle^+\delta(z-a)+\\ &+U^-\triangle^-\delta(z+a)))\Psi_{k_\perp}(z) = 0\ ,\end{aligned} \tag{22}$$

where

$$k_\perp = \sqrt{\frac{2m_0 E}{\hbar^2} - k_\parallel^2}\ . \tag{23}$$

It is seen from Eq. (22) that, in this approximation, we loss the information on a difference of the effective masses of an electron in wells and in barriers, because this equation contains only m_0, rather than m_1.

A solution of Eq. (22) has form

$$\Psi(z) = \begin{cases} \Psi_0(z) = A_0\ e^{ik_\perp z} + B_0\ e^{-ik_\perp z}, & -a \le z \le a, \\ \Psi_\pm(z) = \pm\ C_\pm \sin(k_\perp z \pm \varphi), & a \le |\pm z| \le \infty. \end{cases} \tag{24}$$

We obtain the equation for the scattering phase φ and, because $S_\delta = e^{2i\varphi}$, for the S_δ-matrix from the conditions of integration of the quantity $d^2\Psi/dz^2$ in the vicinities of both barriers. That is, the direct integration yields

$$\begin{aligned}&I(\pm a) = \lim_{\varepsilon\to 0}\int\limits_{\pm a-\varepsilon}^{\pm a+\varepsilon}\frac{d^2\Psi}{dz^2}\ dz = \pm\ k_\perp C_\pm \times\\ &\times\cos(\pm k_\perp a \pm \varphi) \mp ik_\perp(A_0\ e^{\pm ik_\perp a} - B_0\ e^{\mp ik_\perp a}),\end{aligned} \tag{25}$$

and the integration with the use of the Schrödinger equation (22) gives

$$I(\pm a) = \frac{2m_0\Delta^\pm U^\pm}{\hbar^2}\Psi(\pm a)\ . \tag{26}$$

By introducing the notation $K_\perp = k_\perp a$ and $\gamma = \frac{A_0}{B_0}$ and by combining Eqs. (25) and (26), we get the system of two equations

$$\left.\begin{aligned}&\left(\frac{2m_0 a\Delta^+U^+}{\hbar^2K_\perp} - \mathrm{ctg}(K_\perp+\varphi)\right)\times\\ &\times(\gamma e^{iK_\perp} + e^{-iK_\perp}) = -i(\gamma e^{iK_\perp} - e^{-iK_\perp})\\ &\left(\frac{2m_0 a\Delta^-U^-}{\hbar^2K_\perp} - \mathrm{ctg}(K_\perp+\varphi)\right)\times\\ &\times(\gamma e^{-iK_\perp} + e^{iK_\perp}) = i(\gamma e^{-iK_\perp} - e^{iK_\perp}).\end{aligned}\right\} \tag{27}$$

Then we exclude the quantity γ from these equations, take the known relation

$$\mathrm{ctg}(\mathrm{K}_\perp+\varphi) = \frac{1+\mathrm{S}_\delta - \mathrm{i}(1-\mathrm{S}_\delta)\ \mathrm{tgK}_\perp}{(1+\mathrm{S}_\delta)\ \mathrm{tgK}_\perp + \mathrm{i}(1-\mathrm{S}_\delta)} \tag{28}$$

into account, and solve a resulting quadratic equation. This yields the exact analytic expressions for both $S_\delta^{(1,2)}$-matrices,

$$S_\delta^{(1,2)} = e^{-2iK}\frac{1+iZ_\delta^{(1,2)}}{1-iZ_\delta^{(1,2)}}, \tag{29}$$

where

$$\begin{aligned}&Z_\delta^{(1,2)} = \sin(2K_\perp)\ (\cos(2K_\perp)+\\ &+\frac{m_0 a(U^+\Delta^+ + U^-\Delta^-)}{\hbar^2K_\perp}\sin(2K_\perp)\pm\\ &\pm(1+(\tfrac{m_0 a}{\hbar^2K_\perp}\sin(2K_\perp))^2(U^+\Delta^+ - U^-\Delta^-)^2)^{\frac{1}{2}})^{-1}.\end{aligned} \tag{30}$$

It is seen from formulas (19) and (30) that the analytic formula for $S_r^{(1,2)}$ is exact but awkward, whereas that for $S_\delta^{(1,2)}$ is simple and convenient for the analysis. In particular, it is obvious that, in the case of symmetric barriers $U^+\Delta^+ = U^-\Delta^- = U\Delta$,

$$S_\delta^{(1,2)} = e^{-2iK_\perp}\ \frac{\pm\frac{m_0 aU\triangle}{\hbar^2K_\perp}\ (\mathrm{ctgK}_\perp)^{\pm 1} + i}{\pm\frac{m_0 aU\triangle}{\hbar^2K_\perp}\ (\mathrm{ctgK}_\perp)^{\pm 1} - i}. \tag{31}$$

By performing the analytic extension into the complex plane ($K = K_1 - iK_2$), we get, from the condition

$$(S_\delta^{(1,2)}(K_1 - iK_2))^{-1} = 0, \tag{32}$$

the system of two transcendental equations

$$\begin{cases} \dfrac{\Omega K_2}{K_1^2+K_2^2} + \dfrac{\mathrm{sh}K_2\ \mathrm{ch}K_2}{(\mathrm{sh}K_2)^2 + \begin{pmatrix} (\sin K_1)^2 \\ (\cos K_1)^2 \end{pmatrix}} = 1, \\ \dfrac{\Omega K_1}{K_1^2+K_2^2} \pm \dfrac{\sin K_1\ \cos K_1}{(\mathrm{sh}K_2)^2 + \begin{pmatrix} (\sin K_1)^2 \\ (\cos K_1)^2 \end{pmatrix}} = 0, \end{cases} \tag{33}$$

where

$$\Omega = \frac{2m_0 aU\Delta}{\hbar^2}.$$

The solutions of system (33) K_{1N} and K_{2N} determine the resonance energies E_N and widths Γ_N for a QSS of the electron,

$$E_N = \frac{\hbar^2(K_{1N}^2 - K_{2N}^2)}{2m_0a^2}, \quad \Gamma_N = \frac{2\hbar^2 K_{1N}K_{2N}}{m_0a^2}, \tag{34}$$

respectively.

4. Dependences of RE and RW of the Quasistationary Spectrum of an Electron on Geometric Sizes of TBRTS

Before the analysis of the spectral parameters of an electron within the accepted model of asymmetric TBRTS, we consider, for the sake of comparison (by using the introduced notation), the dispersion equation

$$\mathrm{tg}K + \frac{\hbar^2 K}{2m_0 a}\left(\frac{1}{U^+\Delta^+} + \frac{1}{U^-\Delta^-}\right) = 0, \tag{35}$$

Its solutions (K_N) determine the spectrum of resonance energies and the corresponding resonance widths

$$E_N^{\mathrm{asym}} = \frac{\hbar^2 K_N^2}{2m_0a^2}\ ,$$

$$\Gamma_N^{\mathrm{asym}} = \left(\frac{\pi N\hbar^2}{m_0a^2}\right)^3 \frac{K_N a^2}{2\pi N}\left(\frac{1}{(U^+\Delta^+)^2} + \frac{1}{(U^-\Delta^-)^2}\right) \tag{36}$$

which were obtained within the δ-barrier model and used in a number of works [4–6] for the calculation and analysis of the dynamical conduction of RTS. For simplicity, we set $K_\parallel = 0$ hereafter.

If both δ-barriers are identical ($U^+ = U^- = U$, $\Delta^+ = \Delta^- = \Delta$), then the spectrum of REs is determined by the equation [4]

$$\mathrm{tg}K + \frac{\hbar^2 K}{m_0 aU\Delta} = 0 \tag{37}$$

which is the exact limit of Eq. (35). For RWs, formula (36) yields

$$\Gamma_N^{\mathrm{asym}} = \frac{K_N}{\pi N}\ \Gamma_N, \tag{38}$$

where

$$\Gamma_N = \left(\frac{\pi N\hbar^2}{m_0a^2}\right)^3 \left(\frac{a}{U\Delta}\right)^2 \tag{39}$$

is a RW of the N-th quasistationary state of an electron in TBRTS with identical δ-barriers [4]. As seen, Γ_N^{asym} coincides well with Γ_N, if $K_N \approx \pi N$. According to Eq. (37), this is true under the condition $N \ll (m_0 aU\Delta)/(\pi\hbar^2)$.

We now pass to the analysis of the dependences of RE and RW of QSS of an electron on geometric sizes of TBRTS.

The numerical calculations were executed for two nanosystems: with symmetric barriers, GaAs/AlAs, and asymmetric barriers, $In_{0.52}Al_{0.48}As/In_{0.53}Ga_{0.47}As$. The choice of these nanosystems is caused by the fact that just they are intensively studied experimentally and theoretically and possess physical parameters (Table) which satisfy conditions of the theoretical model.

In Fig. 2, we present the results of calculations of resonance energies of an electron in the symmetric TBRTS GaAs/AlAs which are executed exactly by the method of S-matrix within the model of rectangular potentials at $m_0 \neq m_1$ (E_N^S), the model of rectangular potentials with the approximation $m_1 = m_0$ ($E_N^{S_0}$), and the model of δ-potentials ($E_N^{S_\delta}$), and by the method of dispersion equation (37) from work [4] (E_N). Here, we give the dependences of REs of QSS ($N = 1;\ 2;\ 8$) on typical thicknesses ($0.5\ \mathrm{nm} \leq \Delta \leq 1.5\ \mathrm{nm}$) and widths ($a = 10$ and 13.75 nm) characteristic of a similar TBRTS [4].

It is seen from Fig. 2 that, irrespective of the geometric parameters of the symmetric TBRTS, all three approximate methods of calculations give somewhat overestimated values of RE with the hierarchy

Parameters of components of the nanosystems

	m_e	a_0, nm	U, meV
GaAs	0.067	0.565	1040
AlAs	0.15	0.566	
$In_{0.53}Al_{0.47}As$	0.046	0.587	516
$In_{0.52}Al_{0.48}As$	0.089	0.587	

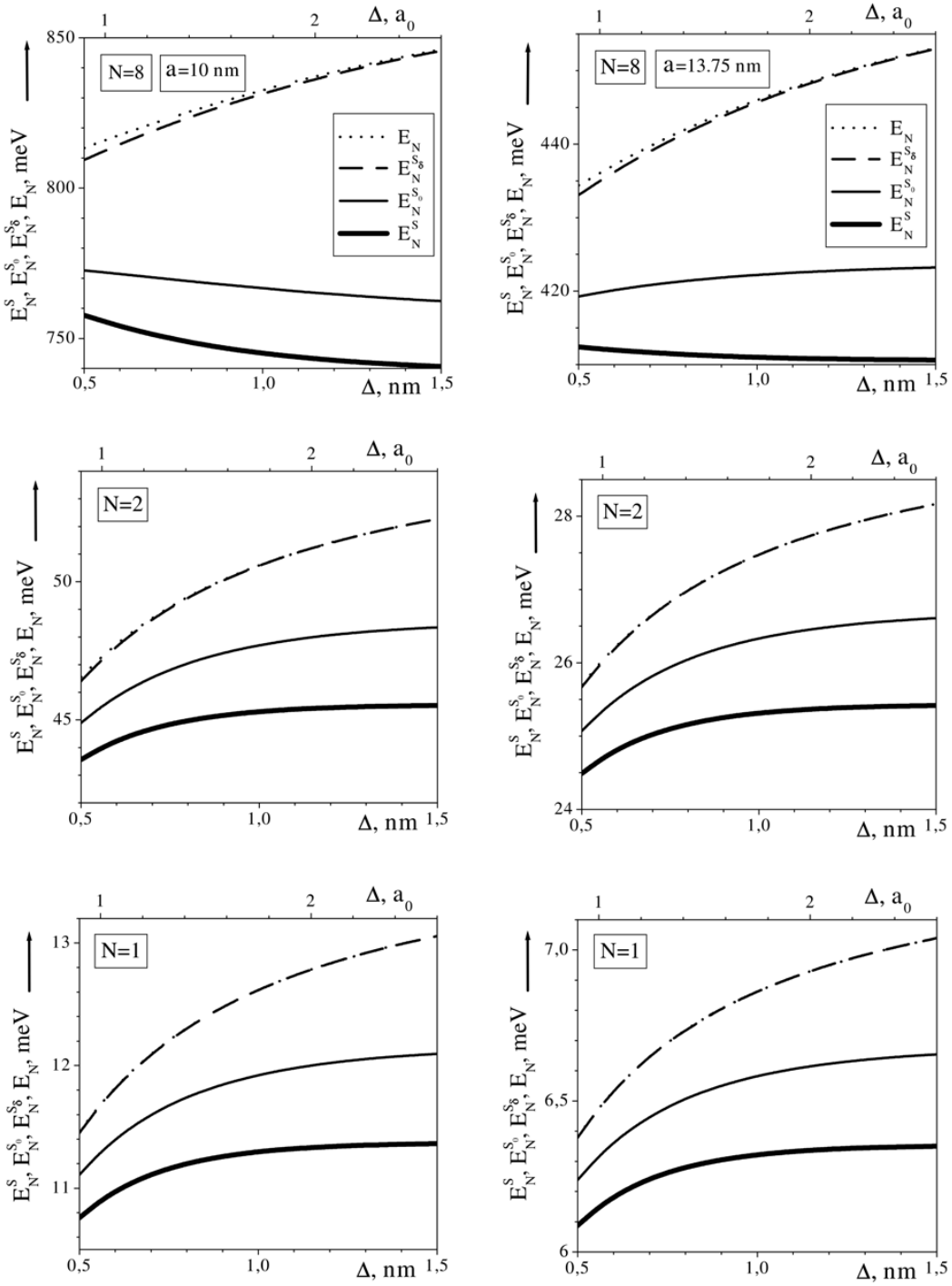

Fig. 2. Dependences of REs in QSS of an electron on the geometric parameters of TBRTS GaAs/AlAs calculated within different models

$E_N^S < E_N^{S_0} < E_N^{S_\delta} \approx E_N$. As for the exact values E_N^S, the relative errors of all RE within all approximate methods increase with the thicknesses of barriers Δ at fixed values of a and decrease with increase of N. In the studied interval of geometric parameters, the error of the quantity $E_N^{S_0}$ does not exceed 6%. In the δ-barrier

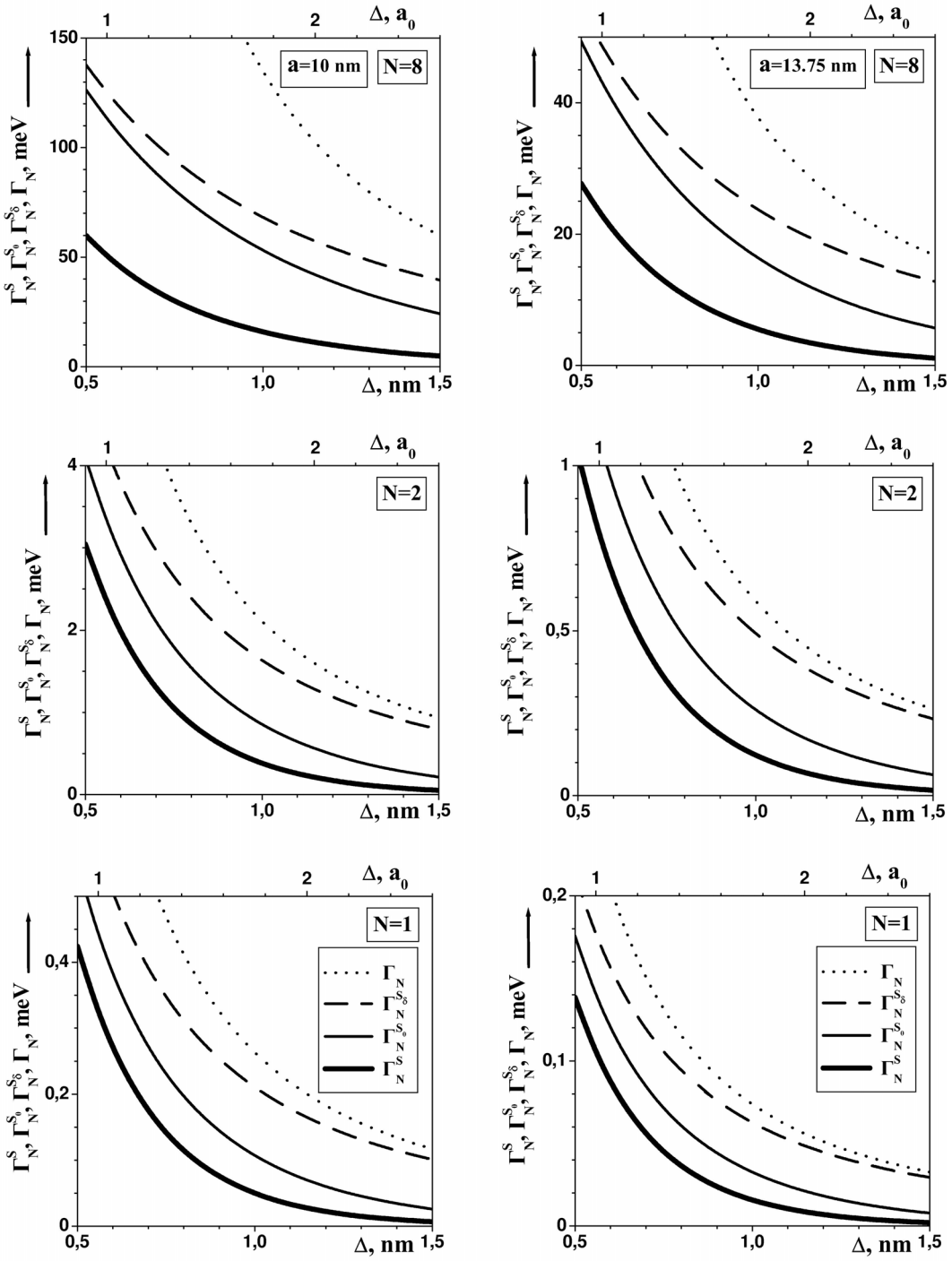

Fig. 3. Dependences of RWs in QSS of an electron on the geometric parameters of TBRTS GaAs/AlAs calculated within different models

model of TBRTS, both methods (the S-matrix method and the method of dispersion equation (37) [4]) give the close results with a maximal error of $\sim 25\%$.

In Fig. 3, we show the results of calculations of resonance widths in QSS of an electron in the symmetric TBRTS GaAs/AlAs. It is seen from this figure that,

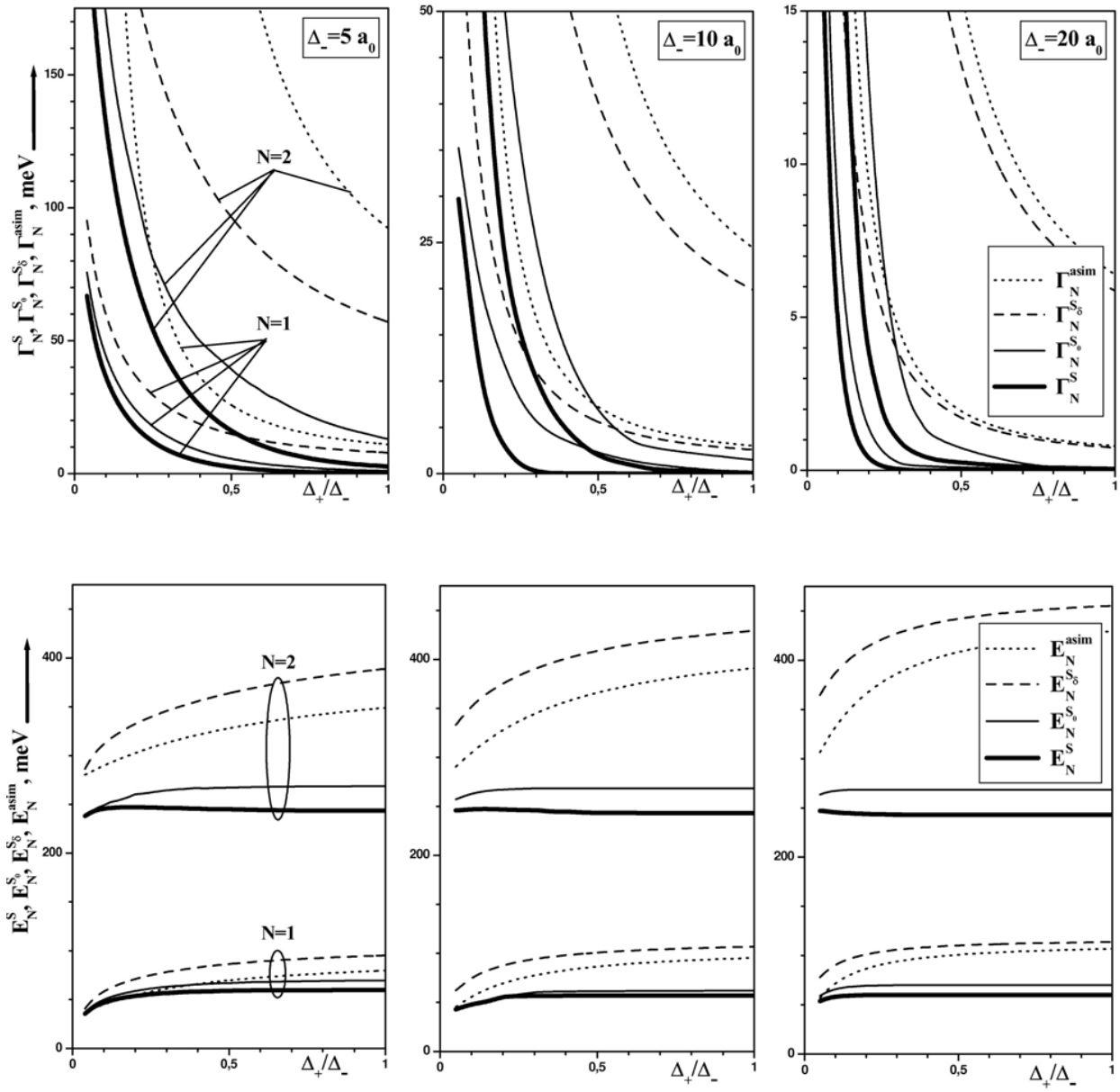

Fig. 4. Dependences of REs and RWs in QSS of an electron in the asymmetric TBRTS $In_{0,52}Al_{0,48}As/In_{0,53}Ga_{0,47}As$ on the geometric parameters calculated within different models; $a = 50a_0$

irrespective of geometric sizes of TBRTS, the resonance widths in QSS of an electron increase with the number N in all models. At fixed sizes of the well width a and values of N, an increase of the thicknesses of barriers Δ leads to a decrease of RW in all states in all models.

Figure 3 indicates that, irrespective of geometric sizes Δ of TBRTS, all three approximate methods give significantly overestimated values of RW with the hierarchy $\Gamma_N^S < \Gamma_N^{S_0} < \Gamma_N^{S_\delta} < \Gamma_N$. With increase in N, the errors of RW increase, as distinct from RE. An increase of the well width a decreases the errors, and an increase of the width of barriers Δ increases them for all three approximate methods of calculations. However, the errors of RW are quite large, as distinct from those of RE. For example, in the studied interval of the geometric parameters of TBRTS, the approximate methods give the following results: $1.3\Gamma_N^S \lesssim \Gamma_N^{S_0} \lesssim 5\Gamma_N^S$; $1.5\Gamma_N^S \lesssim \Gamma_N^{S_\delta} \lesssim 15\Gamma_N^S$; $2\Gamma_N^S \lesssim \Gamma_N \lesssim 18.3\Gamma_N^S$. Here, the

least and largest deviations correspond, respectively, to small ($\Delta = 0.5$ nm) and large ($\Delta = 1.5$ nm) thicknesses of barriers. It is obvious now that all approximations (at $m_1 = m_0$) give quite roughly overestimated values of all resonance widths in QSS of an electron in TBRTS GaAs/AlAs with thicknesses of barriers $\Delta \gtrsim 1$ nm.

The study of the spectral parameters of QSS of an electron in the asymmetric nanosystem $In_{0.52}Al_{0.48}As/In_{0.53}Ga_{0.47}As$ which is often investigated experimentally showed that the dependences of PE and RW in TBRTS with different barriers on the geometric parameters is qualitatively the same as in the system with symmetric barriers. Therefore, it remains to determine and analyze the evolution of the spectral parameters for the asymmetric TBRTS in various models depending on the ratio between the thicknesses of both potential barriers, Δ_+/Δ_-. The example of such dependences is shown in Fig. 4, which implies the following.

Resonance energies in the models of rectangular potentials with $m_1 \neq m_0$ and with $m_1 = m_0$ do not depend practically on the absolute and relative thicknesses of both barriers. The general hierarchy of values of RE in different models is as follows: $E_N^S < E_N^{S_0} < E_N^{\text{asym}} < E_N^{S_\delta}$. The error of $E_N^{S_0}$ does not exceed 10%, whereas the errors in both δ-barrier models are significant and vary in the limits $30\% \div 100\%$, as Δ_+/Δ_- changes from 0.1 to 1. The errors of RE in the symmetric δ-barrier model GaAs/AlAs are larger than those in the asymmetric $In_{0.52}Al_{0.48}As/In_{0.53}Ga_{0.47}As$ model, which is caused by the fact that the effective masses and the potential barriers are greater in the first system, than those in the second one.

As distinct from the resonance energies, the resonance widths in QSS of an electron in TBRTS with asymmetric barriers depend very strongly on the absolute and relative values of both barriers. Figure 4 yields the following hierarchy of RWs: $\Gamma_N^S < \Gamma_N^{S_0} < \Gamma_N^{S_\delta} < \Gamma_N^{\text{asym}}$. In this case, an increase of the absolute and relative values of both barriers decreases the values of RWs in all models.

Finally, it is important to note that the rate of relative increase of RW ($\Gamma_N^{\text{asym}}/\Gamma_N$) with decrease of the ratio Δ_+/Δ_- is 2–3 times less in the δ-barrier model than that in the exact model of rectangular potentials. In addition, the relative rate of variation of RW in the δ-barrier model does not practically depend on N, whereas it decreases with increase of N in the model of rectangular barriers.

5. Conclusions

We have developed an exact method of S-matrix-based calculations of RE and RW of electrons in a plane TBRTS with asymmetric rectangular potential barriers and different effective masses in wells and in barriers.

It is shown that the δ-barrier model TBRTS which is often used in the theory of QSS ignores, first, the difference of effective masses of an electron in wells and in barriers. Second, the form of a δ-like barrier introduces large errors to the spectral parameters of QSS. Thus, the δ-barrier model gives significantly overstated values of RE and RW of an electron in TBRTS and leads, as a result, to significant errors in values of the spectral parameters of QSS. For the asymmetric TBRTS $In_{0.52}Al_{0.48}As/In_{0.53}Ga_{0.47}As$ with typical geometric sizes from several to tens of nanometers, the errors of RE can reach 100 %, and the values of RWs turn out to be overestimated by twenty times.

Thus, it is obvious with regard for the results obtained that the δ-barrier model of TBRTS can be used only for rough qualitative evaluations in the theory of dynamical conduction or response current.

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МЕТОД S-МАТРИЦІ В ТЕОРІЇ РЕЗОНАНСНИХ ЕНЕРГІЙ І ШИРИН КВАЗІСТАЦІОНАРНИХ СТАНІВ ЕЛЕКТРОНА У НЕСИМЕТРИЧНІЙ ДВОБАР'ЄРНІЙ РЕЗОНАНСНО-ТУНЕЛЬНІЙ СТРУКТУРІ

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Р е з ю м е

Методом трансфер- і S-матриці виконано аналітичний і числовий розрахунки резонансних енергій та ширин квазістаціонарних станів електрона у плоскій двобар'єрній резонансно-тунельній наноструктурі з несиметричними прямокутними (з різними ефективними масами у бар'єрах і ямах) і δ-подібними потенціальними бар'єрами. На прикладі наносистем GaAs/AlAs і $In_xAl_{1-x}As/In_xGa_{1-x}As$ показано, що, на відміну від точних величин резонансних енергій і ширин, визначених у моделі прямокутних потенціальних бар'єрів, модель δ-подібних бар'єрів, яка часто використовується у теоретичних дослідженнях, дає завищені на десятки відсотків похибки резонансних енергій, а величини резонансних ширин завищені у десятки разів.