The over-barrier resonant states and multi-channel scattering by a quantum well

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ABSTRACT
We demonstrate an explicit numerical method for accurate calculation of the analytic continuation of the scattering matrix, describing the multi-channel scattering by a quantum well, to the unphysical region of complex values of the energy. Results of calculations show that one or several poles of the S-matrix exist, corresponding to the over-barrier resonant states that are critical for the effect of the absolute reflection at scattering of the heavy hole by a quantum well in the energy range where only the heavy hole may propagate over barriers in a quantum-well structure. Light- and heavy-hole states are described by the Luttinger Hamiltonian matrix. The qualitative behaviour of the over-barrier scattering and resonant states is the same at variation of the shape of the quantum-well potential, however lifetimes of resonant states depend drastically on the shape and depth of a quantum well.

1. INTRODUCTION

In [1] the multi-channel scattering by a quantum-well structure was studied for particle states obeying the system of ordinary differential equations

$$\left\{a\frac{d^2}{dz^2}+b\frac{d}{dz}+c+V(z)\right\}\Psi(z)=E\Psi(z) \tag{1}$$

where $V(z)$ is a bounded piecewise analytic potential function with a finite number of "pieces", and $V(z)\sim V_1^{\pm}/z+V_2^{\pm}/z^2+\dots$, $z\to\pm\infty$, $V^{\pm}$ are constants, ± superscript corresponds to the sign of ±∞; a, ib (i stands for imaginary unit), and c are piecewise constant hermitian $n\times n$ matrices; $\Psi(z)$ is the n-component wave function; E is the energy. At $z\to\pm\infty$ the solution
$\Psi_\alpha^{in}(z)$ of Eq. (1) has the form (in-state wave incident from the left)

$$\Psi_\alpha^{in}(z)\sim\frac{1}{\sqrt{|2\pi v_\alpha|}}\begin{cases} e^{ik_\alpha z}\cdot u_\alpha+\sum\limits_{\alpha'}X_{-\alpha',\alpha}\cdot e^{ik_{-\alpha'}z}\cdot u_{-\alpha'}, z\to-\infty \\ \sum\limits_{\alpha'}X_{\alpha',\alpha}\cdot e^{ik_{\alpha'}z}\cdot u_{\alpha'}, z\to+\infty \end{cases}, \tag{2}$$

where vectors u_α are determined from the equation $(-ak_\alpha^2 + ibk_\alpha + c - E)u_\alpha = 0$; v_α is the group velocity: $v_\alpha = iu_\alpha^*(2ik_\alpha a + b)u_\alpha$. Similarly for the in-state waves $\Psi_{-\alpha}^{in}(z)$ incident from the right (in the case $V_1^\pm \neq 0$, the quantities in exponents will contain logarithmic "Coulomb" phases (see [2]), omitted for brevity). The S-matrix component for the channel $\beta \to \alpha$ has the form: $S_{\alpha\beta} = X_{\alpha\beta}\left|v_\alpha / v_\beta\right|^{1/2}$. The S-matrix satisfies the unitary condition, namely, $S^* = S^{-1}$ (the symbol * stands for Hermitian conjugation) and the symmetry condition: $S_{\alpha\beta} = S_{-\beta,-\alpha}$. The quantities $\left|S_{\alpha\beta}\right|^2$ give transmission coefficients (when sgn(α) = sgn(β)) and reflection coefficients (sgn(α) = – sgn(β)).

Our study in the n = 2 case [1], when Eq. (1) describes the rectangular-quantum-well ($V(z)$ = const < 0 at $|z| < d/2$, $V(z) = 0$ elsewhere) two-channel system with two differing masses (i.e. heavy and light holes in a semiconductor quantum well), has revealed that within the range of E: $E_I < E < E_{II}$, where E_I, $E_{II} > 0$ are the eigenvalues of the matrix c, only the heavy particle may propagate over barriers, and scattering of the heavy particle is of the curious resonant nature: at various system parameters there are discrete E values of the absolute reflection, i.e. when $|S_{-H,H}|^2 = 1$. The nature of the states related to such pattern of scattering can be clarified by examining the analytic properties of the S-matrix [3]. So it is necessary to develop a method of calculation of analytic continuation of the S-matrix to the region of complex values of E in the case of the multi-channel scattering problem.

2. GENERAL FORMULATION OF THE METHOD

The light- and heavy-hole states in semiconductors are described by the 4 × 4 Luttinger Hamiltonian [4]. A unitary transformation [5, 6] block diagonalizes the Hamiltonian into two 2 × 2 blocks. We choose the z direction to be perpendicular to the interfaces in the quantum-well structure. Then, in the case of a symmetric quantum well, the Schrödinger equation is reduced to the Eq. (1) with n = 2, and, in the so-called axial approximation,

$$a = \begin{pmatrix} -1+\mu-\frac{6}{5}\delta & 0 \\ 0 & -1-\mu+\frac{6}{5}\delta \end{pmatrix}, \; b = k_1 \begin{pmatrix} 0 & -\sqrt{3}(\mu+\frac{4}{5}\delta) \\ \sqrt{3}(\mu+\frac{4}{5}\delta) & 0 \end{pmatrix},$$

$$c = k_l^2 \begin{pmatrix} (1+\frac{1}{2}\mu-\frac{3}{5}\delta) & \frac{\sqrt{3}}{2}(\mu-\frac{1}{5}\delta) \\ \frac{\sqrt{3}}{2}(\mu-\frac{1}{5}\delta) & (1+\frac{1}{2}\mu-\frac{3}{5}\delta) \end{pmatrix}. \quad (3)$$

Where k_l is the lateral quasi-momentum component (good quantum number):$k_l^2 = k_x^2 + k_y^2$; $\mu = (6\gamma_3 + 4\gamma_2)/5\gamma_1$, $\delta = (\gamma_3 - \gamma_2)/\gamma_1$, $\gamma_1, \gamma_2, \gamma_3$ are the dimensionless Luttinger parameters [4] ; energy and length are measured in units of $m_0 e^4 / 2\hbar^2\gamma_1$ and $\hbar^2\gamma_1 / m_0 e^2$, respectively. The realistic range of the parameters under consideration is: $0 \le \delta << \mu < 1$. In what follows, the case of a single symmetric quantum well with the potential $V(z)$ at $|z| < d/2$, $V(z) = 0$ elsewhere, is considered.

For further study it is convenient to represent Eq. (1) as a first-order equation for a 2n-component function $y(z) = \begin{pmatrix} \Psi(z) \\ d\Psi(z)/dz \end{pmatrix}$:

$$\frac{dy(z)}{dz} = A(z)y(z) \text{, where } A(z) = \begin{pmatrix} \hat{0} & \hat{1} \\ a^{-1}(E - c - V(z)) & -a^{-1}b \end{pmatrix}, \tag{4}$$

$\hat{0}$, and $\hat{1}$ are the null and identity $n \times n$ matrix, respectively. As it was shown in [1], at $k_l \neq 0$, within the energy range $E_I < E < E_{II}$, where $E_{I,II}$ are eigenvalues of the matrix c:

$$E_{I,II} = k_l^2 \left[1 \mp \left(\mu^2 - 0.9\mu\delta + 0.39\delta^2 \right)^{1/2} \right], \tag{5}$$

the eigenvalues of the matrix A_0, where $A_0 \equiv A(z)$at $|z| > d/2$, read as follows: $i\kappa$, q, $-q$,$-i\kappa$ (κ, $q > 0$), i.e. only the heavy hole can propagate over barriers, and the channel of conversion of the heavy hole into propagating light hole is closed (light-hole state is evanescent). Scattering within this energy range has a resonant nature, namely, at various system parameters characteristic feature is the occurrence of the well-defined peaks of the absolute reflection. In what follows we consider just this energy range where the multiplicity of the continuous spectrum equals two. It should be noted that in the case under consideration, to the continuous spectrum corresponds half-infinite interval $[E_{\min}, +\infty)$, where $E_{\min}$ equals either the positive solution of the equation 4det $a(E^2 - E \cdot tr(c) + \det c) = (E \cdot tr(a) - \det b - a_{11}c_{22} - a_{22}c_{11})$ or E_I - in the case of $\delta = 0$. Define a 4×4 matrix function Φ(z, E) in the following way:

a) The first and the third columns of Φ(z, E) are the solutions of the Eq. (4) which equal at $z > d/2$ to $\chi_1(E)e^{i\kappa z}$ and $\chi_3(E)e^{-qz}$ (κ, $q > 0$), respectively;
b) The second and the fourth columns of Φ(z, E) are the solutions of the Eq. (4) which equals at $z <$ - $d/2$ to $\chi_2(E)e^{+qz}$ and $\chi_4(E)e^{-i\kappa z}$, respectively;
c) At $|z| \leq$ d/2, i.e. in the interior of the quantum well, the matrix function Φ(z, E) is found by solving apparent Cauchy problems for the Eq. (4) (using e.g. the method of reccurent sequences, see [1], [2], [7], [8],).

Here χ_1, χ_2, χ_3, and χ_4 are the eigenvectors of the matrix A_0 corresponding to the eigenvalues $\lambda_1 = i\kappa, \lambda_2 = q, \lambda_3 = -q,$ and $\lambda_4 = -i\kappa$ ($\kappa, q > 0$), respectively. These eigenvectors have the form $\chi_j = \begin{pmatrix} u_j \\ \lambda_j u_j \end{pmatrix}$, where $u_j^* u_j = 1$.

Certain boundary conditions are imposed on the solutions at the points z = $\pm$ $d/2$. The conventional boundary conditions consistent with Hermitian character of the Hamiltonian, and implying the continuity of the solutions and of the probability current density (see, e.g., [6]) are used.

It follows from the results of [1] that, within the energy range under consideration, components of the S-matrix are inversely proportional to det Φ(z, E). Now we set at will a value of the coordinate z: $z = \hat{z}$, and obtain a function of the energy $f(E)$ = det$\Phi(\hat{z}$, E) that should be considered as defined at the upper edge of the interval (E_I , E_{II}) of the cut [E_{min}, $+\infty$), formed by the continuous spectrum. Then it is possible to make analytic continuation of the function $f(E)$ downward through this cut to the region of unphysical complex energies of the half-string $E_I <$ Re$E < E_{II}$, Im $E < 0$, and its zeroes there correspond to singular points of the scattering matrix. Since the function $f(E)$ is a product of a positive function, formed of modules of analytic functions, and of the analytic function $g(E)$, then zero E_0 of $g(E)$, lying immediately downward the continuous spectrum, is a resonance pole of the S-matrix, ReE_0 being the energy of the resonant state, -2ImE_0 - the resonant width, and $\hbar/(-2\mathrm{Im}E_0)$- resonant state lifetime [3]. Thus the problem is reduced to numerical solving the equation $f(E) = 0$.

3. RESULTS OF CALCULATIONS AND DISCUSSION

Complex values of S-matrix poles energies, and values of energies of the absolute reflection were calculated as functions of quantum-well width d, and lateral quasi-momentum component k_l for various realistic parameters μ and δ, the potential $V(z)$ shapes and depths. Qualitative results are the same and are in the following: at $k_l \neq 0$ there is one or several poles of the S-matrix, lying immediately downward the continuous spectrum, i.e. corresponding to resonant states, whose real parts of energies are within the interval $E_I <$Re$E< E_{II}$, and are close to energies of the absolute reflection, so it is these resonant states that are related to the effect of the absolute reflection.

For illustrative purpose some results of calculations of real and imaginary parts of energies of S-matrix poles and energies of the absolute reflection are demonstrated in Figures 1–4.

Parameters used correspond to a single quantum well with the rectangular or inverted bell-shaped (i.e., $V(z) = -a \exp(-bz^2)$) potential of the same width and depth and were taken from [6]: $\mu = 0.836$, $\delta = 0.057$, $\gamma_1 = 14.06$ (well material); $\mu = 0.832$, $\delta = 0.065$, $\gamma_1 = 11.72$ (barriers material); $V(0) = -134.9$ meV (InGaAsP/$Ga_xIn_{1-x}As$/InGaAsP, x=0.468 quantum-well structure [6]). Real parts of energies of S-matrix poles and energies of the absolute reflection as functions of quantum well width d and lateral quasi-momentum component are represented in Figures 1, 2 respectively. It can be seen from the Figure 1 that at small values of well width d there is one pole of the S-matrix (i.e. one resonant state) and one respective peak of the absolute reflection. Their energies steadily decrease with the increase of d. Then, at further increase of d, the second peak (resonant state) emerges and within some range of parameters there are two resonant states and two respective peaks of the absolute reflection (several, in general case). Then “the first” resonant state vanishes and the pattern is repeated (the second and the third set of lines in Figure 1). It is seen from the Figure 2 that there is only one pole of the S-matrix (i.e. one resonant state) and one respective peak of the absolute reflection at small values of k_l. The peak energies steadily increase with k_l. Then, at further increase of k_l, there are two resonant states and two respective peaks (several, in general case) of the absolute reflection.

Many-valuedness of the functions means that there are several peaks of the absolute reflection within the energy range $E_I < E < E_{II}$ and several respective S-matrix poles.

As evident from the Figures 1, 2 there is one or several poles of the S-matrix, whose real parts of energies are within the interval $E_I <$ Re $E < E_{II}$, and are close to energies of the absolute reflection, i.e. corresponding to resonant states. Qualitatively the behaviour of these values is the same for both considered shapes of the well, however the difference between energies of the absolute reflection and real parts of respective S-matrix poles energies obviously is larger in the rectangular-well case. This means (see [3]), that absolute values of imaginary parts of poles energies should be larger in the last case. Calculated imaginary parts of energies of S-matrix poles as functions of quantum well width d and lateral quasi-momentum component are shown in Figures 3, 4 respectively.

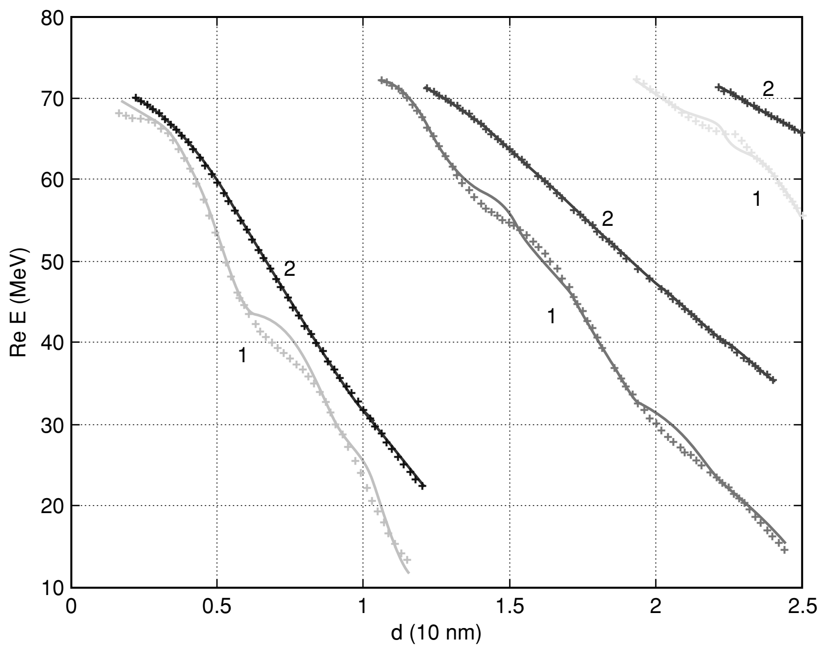

Figure 1 Real parts of energies of S-matrix poles (solid lines) and energies of the absolute reflection (crosses) as functions of *d*, k_l = 0.3 nm^{-1}. 1 – rectangular well, 2 – "bell-shaped" well. The different sets of lines correspond to individual peaks of absolute reflection.

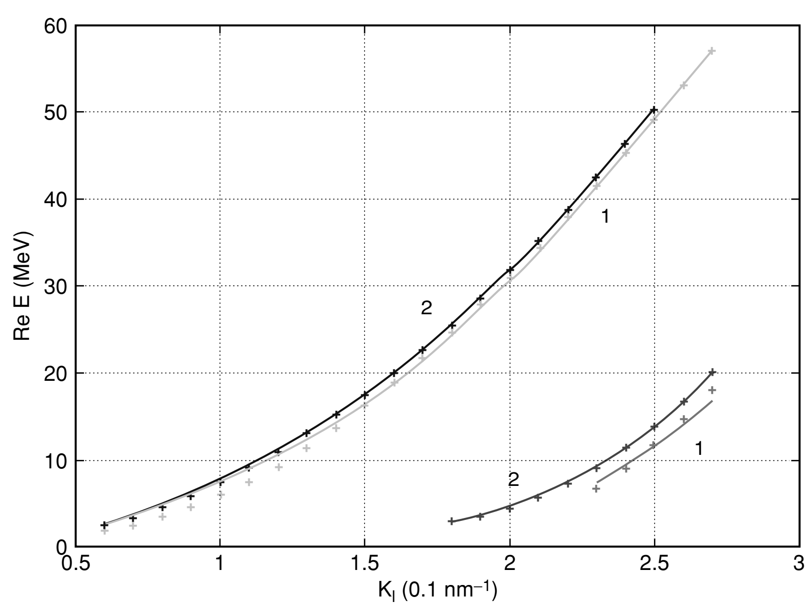

Figure 2 Real part of energies of S-matrix poles (solid lines) and energies of the absolute reflection (crosses) as functions of the lateral quasi-momentum component kl (d = 10 nm). 1 – rectangular well, 2 – "bell-shaped" well. The different sets of lines correspond to individual peaks of absolute reflection.

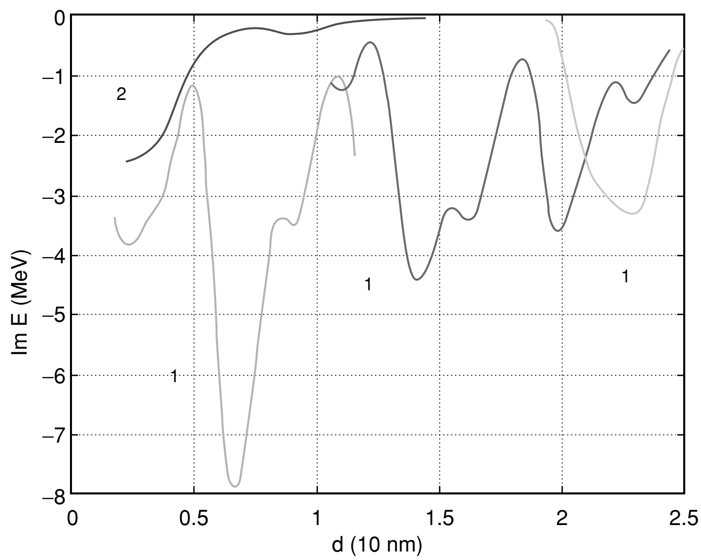

Figure 3 Imaginary parts of energies of S-matrix poles as functions of d, $k_l = 0.3\ nm^{-1}$. 1 – rectangular well, 2 – bell-shaped well.

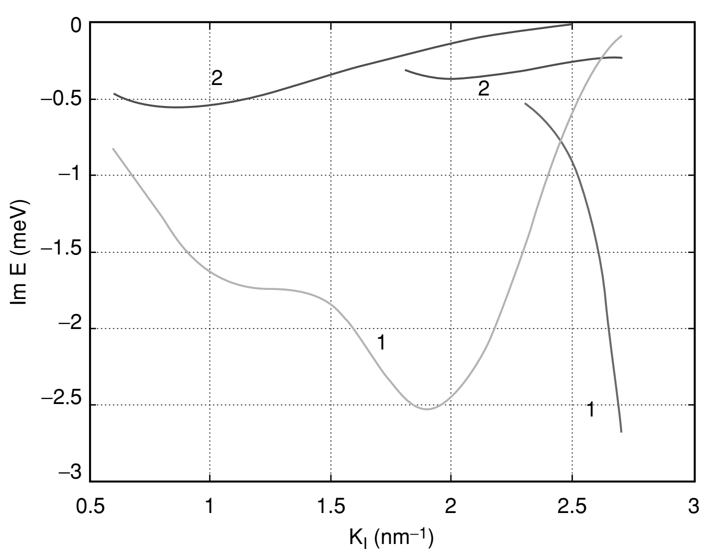

Figure 4 Imaginary parts of energies of S-matrix poles as functions of the lateral quasi-momentum component k_l (d = 10 nm). 1 – rectangular well, 2 – bell-shaped well.

In general, absolute values of imaginary parts of S-matrix poles in the case of smooth potentials of the well are substantially smaller than in the case of the conventional rectangular quantum well (curves 2 in Figure 3 is invisible at d >1.5 nm since magnitudes there are of the order of hundredths and thousandths of meV), i.e. lifetimes of resonant states in the former case considerably exceed ones in the latter.

It should be mentioned that in the case of a shallow quantum well there is in fact a long-living over-barrier resonant hole state. When one decreases the magnitude of the quantum-well depth, keeping the same values of other parameters, the resonance peak of absolute reflection becomes narrower, shifts towards the value E_{II} and then vanishes at sufficiently small values of $V(0)$. For example, in the case of the rectangular quantum well with $d = 7.1$ nm, $V(0) = -20$ meV (other parameters are identical to cited above), the energy of the absolute reflection equals 72.205975 meV that almost coincides with the value of real part of the energy of the S-matrix pole: $\mathrm{Re}E_p = 72.205974$ meV, resonance peak width at half-height equals $5.88 \cdot 10^{-4}$ meV, that is close to the value $-2\mathrm{Im}\, E_P = 5.89 \cdot 10^{-4}$ meV.

4. CONCLUSION

An explicit numerical method was developed for the accurate calculation of analytic continuation of the S-matrix, describing the multi-channel scattering by a quantum well, to the unphysical region of complex values of the energy. Numerical results demonstrated that one or several poles of the S-matrix, corresponding to the over-barrier resonant states that are critical for the effect of the absolute reflection at heavy-hole scattering by a quantum well, exist in the energy range where only the heavy hole may propagate over barriers in a quantum-well structure. Thus the effect of the absolute over-barrier reflection is explained by the existence of the over-barrier resonance states corresponding to the S-matrix poles. The qualitative behaviour of the over-barrier scattering and resonant states is the same at variation of the quantum-well potential shape however lifetimes of resonant states depend drastically on well shape and depth.

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