The Over-Barrier Resonant States and Multi-Channel Scattering in Multiple Quantum Wells

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ABSTRACT

We demonstrate an explicit numerical method for accurate calculation of the scattering matrix and its poles, and apply this method to describe the multi-channel scattering in the multiple quantum-wells structures. The S-matrix is continued analytically to the unphysical region of complex energy values. Results of calculations show that there exist one or more S-matrix poles, corresponding to the over-barrier resonant states critical for the effect of the absolute reflection of holes in the energy range where only the heavy ones may propagate over barriers in a structure. Light- and heavy-hole states are described by the Luttinger Hamiltonian matrix. In contrast to the single quantum-well case, at some parameters of a multiple quantum-wells structure the number of S-matrix poles may exceed that of the absolute reflection peaks, and at different values of parameters the absolute reflection peak corresponds to different resonant states. The imaginary parts of the S-matrix poles and hence the lifetimes of resonant states as well as the widths of resonant peaks of absolute reflection depend drastically on the quantum-well potential depth. In the case of shallow quantum wells there is in fact a long-living over-barrier resonant hole state.

1. INTRODUCTION

The multi-channel scattering by quantum-well structures was studied in [1] 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" (quantum wells), and $V(z)\sim V_1^{\pm}/z+V_2^{\pm}/z^2+\dots$, $z\to\pm\infty$; a, ib, 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: $S_{\alpha\beta} = X_{\alpha\beta}\left|v_\alpha / v_\beta\right|^{1/2}$. S-matrix satisfies the unitary condition, namely, $S^* = S^{-1}$ (the symbol * stands for Hermitian conjugation) and the symmetry condition (reciprocity theorem): $S_{\alpha\beta} = S_{-\beta,-\alpha}$. The quantities $|S_{\alpha\beta}|^2$ give transmission coefficients (when) and reflection 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 single 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]. The case of a single quantum well was discussed in [4]. In this work we generalize our study to the case of multiple quantum-wells structures.

2. FORMULATION OF THE METHOD

The light- and heavy-hole states in semiconductors are described by the 4×4 Luttinger Hamiltonian matrix [5]. A unitary transformation [6, 7] block diagonalizes the Hamiltonian into two 2×2 blocks. We choose the z direction to be perpendicular to the interfaces in the multiple quantum-wells structure. Then, in the case of symmetric quantum wells, the Schrödinger equation is reduced to the Eq. (1) with n = 2, and, in the so called axial approximation (see e.g. [6]),

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

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

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 [5]; 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: $0 \le \delta \ll \mu < 1$. In what follows, we consider the case of a structure of multiple identical symmetric quantum wells with the potential $V(z) < 0$, located at $|z| < D/2$ where $D = Nd_w + (N\text{-}1)\,d$, N - number of wells, d_w - wells width, d - barriers width, $V(z) = 0$ at $|z| > D/2$ (barriers).

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

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

$\hat{0}$, and $\hat{1}$ are the null and identity n×n matrix, respectively. As it was shown in [1], at $k_1 \neq 0$, within the energy range $E_I < E < E_{II}$, where $E_{I,II}$ are eigenvalues of the matrix c [4],

the eigenvalues of the matrix A_0, where $A_0 \equiv A(z)$ at $|z| > D/2$ at (in the barriers), read as follows: $i\kappa$, q, $-q$, $-i\kappa$ (κ, $q > 0$), i.e. only the heavy hole may propagate over barriers, and the channel of conversion of the heavy hole into propagating light hole is closed (light-hole state is evanescent). In what follows we consider just this energy range where the multiplicity of the continuous spectrum equals two. In the case under consideration, to the continuous spectrum corresponds half-infinite interval ($E_{\min}$,+∞), 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 - if $\delta = 0$. Define a 4×4 matrix function $\mathbf{\Phi}(z,E)$ in the following way:

1) The first and the third columns of $\mathbf{\Phi}(z,E)$ 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; **2)** The second and the fourth columns of $\mathbf{\Phi}(z,E)$ 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; **3)** At $|z| \leq D/2$, i.e. in the interior of the multiple quantum-wells structure, the matrix function $\mathbf{\Phi}(z,E)$ is found by solving apparent Cauchy problems for the Eq. (4) in each well region (using e.g. the method of reccurent sequences, see [1], [2], [8], [9]), and imposing the pertinent boundary conditions at each interface. 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. [7]) are used; **4)** The same boundary conditions are imposed on the solutions at the points $z = \pm D/2$.

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 $u_j^* u_j = 1$.

It follows from the results of [1] that, within the energy range under consideration, components of the S-matrix are inversely proportional to det $\mathbf{\Phi}(z,E)$. 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 ($E_{\min}$,+∞), 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 $E_I < \mathrm{Re}\, E < E_{II}$, $\mathrm{Im}\, E < 0$, 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, Re E_0 being the energy of the resonant state, –2 Im E_0 - the resonant width, and $\hbar/(-2\,\mathrm{Im}\,E_0)$ - resonant state lifetime [3]. The problem of S-matrix poles calculation is reduced to numerical solving the equation $f(E) = 0$

3. RESULTS AND DISCUSSION

The transmission and reflection coefficients were calculated as functions of the over-barrier energy of incident heavy hole for various parameters of multiple quantum-wells structures, including realistic material parameters, and lateral quasi-momentum component k_l. The complex values of S-matrix poles energies were calculated as functions of multiple quantum-wells parameters. Results of calculations show that at all realistic values of parameters there exist one or more S-matrix poles corresponding to the over-barrier resonant states critical for the effect of absolute reflection of the heavy hole in the energy range where only heavy holes may propagate over barriers in the structure. Real parts of pole energies are within the interval $E_{\mathrm{I}} < \mathrm{Re}\, E < E_{\mathrm{II}}$ ($\mathrm{Im}\, E < 0$) and are close to the energies of the absolute reflection peaks. The number of over-barrier resonant states and resonant peaks of absolute reflection, as well as their energies, depends on the widths of quantum wells and barriers, their number, and the value $k_l \neq 0$ of the lateral component of quasi-momentum. The values of material parameters used in calculations of Figures 1, 2 are as follows: $\gamma_1 = 14.06$, $\gamma_2 = 5.398$, $\gamma_3 = 6.198$ (wells material), $\gamma_1 = 11.72$, $\gamma_2 = 4.421$, $\gamma_3 = 5.180$ (barriers material). These parameters correspond to structures with InGaAsP/$Ga_xIn_{1-x}As$/InGaAsP quantum wells [7]. The value of the quantum wells depth used in calculations of Figures 1, 2 equals $V(0) = -134.9$ meV (x = 0.468 [7]).

Many-valuedness of the functions in Figures 1, 2 means that there are several S-matrix poles and respective peaks of the absolute reflection within the energy range $E_{\mathrm{I}} < \mathrm{Re}\, E < E_{\mathrm{II}}$, $\mathrm{Im}\, E < 0$.

In contrast to the single quantum-well case [4], at some parameters of multiple quantum-wells structures the number of S-matrix poles lying immediately downward the continuous spectrum may exceed that of the absolute reflection peaks. This case is illustrated in Figures 1, 2. As it can be seen from Figures 1, 2, the energy of the second peak (with higher energy) of the absolute reflection is close to the real part of the complex energy of pole 2 or 3 in different ranges of barriers width *d*, while the respective imaginary part is comparatively small, i.e. in these ranges the peak is related to different resonant states. Moreover, at some values of structure parameters a resonant state may exist whose complex energy has very small imaginary-part modulus, and real part that is closely set to the energy of the absolute reflection, i.e. a long-living one (see curve 3 in Figures 1, 2 at $d \approx 2.5$ nm).

Character of scattering, the imaginary parts of S-matrix poles, and hence the lifetimes of resonant states as well as the widths of resonant peaks of absolute reflection depend drastically on the quantum-wells potential depth. In the case of sufficiently shallow quantum wells there is in fact a single long-living over-barrier resonant hole state. When the magnitude of the quantum-well depth decreases, a residual resonance peak of the absolute reflection becomes extremely narrow (against the background of almost unity transmission at all energies except this narrow interval), shifts towards the energy value where the light-hole channel is opened, and then vanishes. The real part of S-matrix-pole energy almost coincides with the energy of the absolute reflection. Results of calculations of the transmission and reflection coefficients as functions of the over-barrier energy of the incident heavy hole for two strongly differing values of the depth of rectangular wells are demonstrated in Figures 3 and 4. Material parameters are identical to cited above. The energy range used in Figure 4 was selected in order to demonstrate the absolute reflection peak: transmission coefficient is close to unity (and the reflection one – to zero) at any energy value beyond this range. The energy of the absolute reflection peak in Figure 4 equals 72.4408 meV, that is close to the value 72.4407 meV of the real part of S-matrix pole energy, the resonance peak width at half-height equals 0.00247 meV, and the value $-2\, \mathrm{Im}\, E = 0.00246$ meV. It should be noted that in contrast to the single quantum-well case [1], at some parameters of multiple quantum-wells structures reflection coefficient may be close to unity almost in the whole range $E_{\mathrm{I}} < E < E_{\mathrm{II}}$ (see Figure 3).

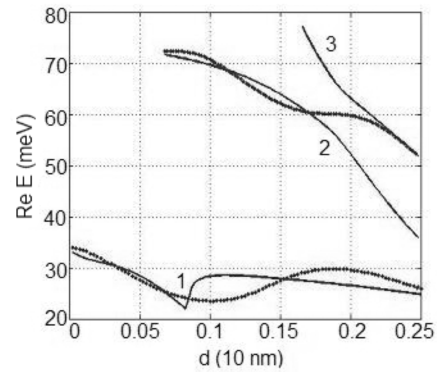

Figure 1. Real parts of S-matrix pole energies (solid lines) and energies of the absolute reflection peak (dots) as functions of barrier width d in a five-quantum-wells structure; d_w = 1.7 nm, k_l = 0.3 nm^{-1}; 1 ,2, 3 – pole number.

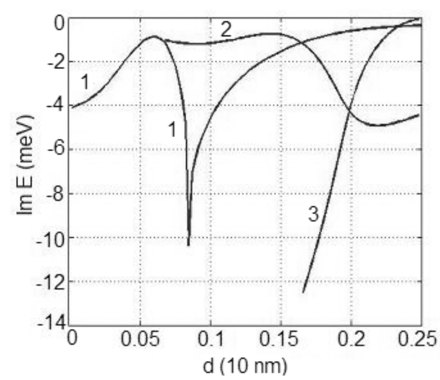

Figure 2. Imaginary parts of S-matrix pole energies as functions of barriers width d in a five-quantum-wells structure; d_w = 1.7 nm, k_l = 0.3 nm^{-1}; 1 ,2, 3 – pole number.

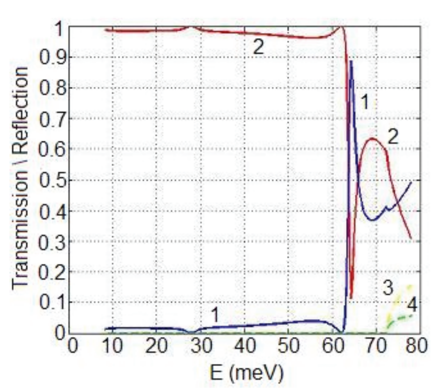

Figure 3. Transmission (1) and reflection (2) coefficients of heavy hole (without conversion into light hole) in a five-quantum-wells structure as functions of the over-barrier energy E; d_w = 1.7 nm, d = 1.5 nm, k_l = 0.3 nm^{-1}, wells depth V(0) = -134.9 meV; 3, 4 – reflection and transmission coefficients with conversion into light hole, respectively.

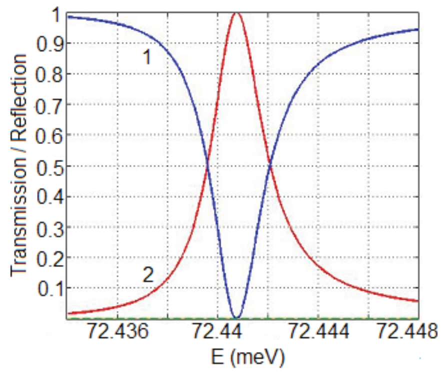

Figure 4. Transmission (1) and reflection (2) coefficients of a heavy hole (without conversion into a light hole) as functions of the over-barrier energy E in a five-quantum-wells structure; $d_w = 1.7$ nm, $d = 1.5$ nm, $k_l = 0.3$ nm^{-1}, wells depth V(0) = -15 meV.

4. CONCLUSION

An explicit numerical method was demonstrated for accurate calculations of the scattering matrix, and its poles in the unphysical region of complex energy values, describing the multi-channel holes scattering in the multiple quantum-wells structures. The results of calculations showed that at all realistic values of parameters there exists one or more S-matrix poles, corresponding to the over-barrier resonant states critical for the effect of the absolute reflection of holes in the energy range where only the heavy ones may propagate over barriers in the structure. In contrast to the single quantum-well case, at some values of parameters of multiple quantum-wells structures the number of S-matrix poles may exceed that of the absolute reflection peaks. In this case at different values of some parameter (e.g. barriers width) an absolute reflection peak is related to different resonant states. Moreover, at some values of parameters a resonant state may exist whose complex energy has very small imaginary-part modulus, and real part that is closely set to the energy of the absolute reflection, i.e. a long-living one. Character of scattering, the imaginary parts of S-matrix poles, and hence lifetimes of resonant states as well as widths of resonant peaks of absolute reflection depend drastically on the quantum-well potential depth. In the case of shallow quantum wells there is a single long-living over-barrier resonant hole state. The existence of over-barrier long-living hole resonant states may be one of the reasons for efficient holes capture by multiple quantum-wells structures.

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