Accurate solution of the eigenvalue problem for some systems of ODE for calculating holes states in polynomial quantum wells

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ABSTRACT
We demonstrate an explicit numerical method for accurate solving the eigenvalue problem for some systems of ordinary differential equations, in particular, those describing electron and hole bound states in semiconductor quantum wells with polynomial potential profiles. Holes states are described by the Luttinger Hamiltonian matrix. For solving the eigenvalue problem we use the recurrent sequences procedure that makes possible to derive exact analytical expression for the eigenfunctions,. Hole bound states energies and corresponding wave functions are calculated in a finite parabolic quantum well as functions of the lateral quasimomentum component and parameters of the potential.

Keywords: Ordinary differential equations, Eigenvalue problem, Quantum well polynomial potential, Bound states

1. INTRODUCTION

We consider eigenvalue problem for the equation

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

where $V(z)$ is polynomial function at $0 \le z \le d$

$$V(z)=\sum_{i=0}^{m}V_i z^i,\ (V(z)<0), \tag{2}$$

$V(z) = V = \text{const} \ge 0$ otherwise; $\hat{a}$, and $\hat{c}$ are Hermitian, and $\hat{b}$- anti-Hermitian piecewise constant $n \times n$ matrices; $\Psi(z)$ is n-component vector of solutions (wave function); E is the energy. A number of applied problems, in particular the problem of finding energies and wave functions of bound states of electrons and holes in semiconductor quantum wells (QW) is reduced to solving eigenvalue problem for Eq. (1). Various approximate

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numerical schemes are used for solving the problem even in the case of the conventional one-dimensional Schrödinger equation (i.e. when $n = 1$, $\hat{b} = 0$ in Eq. (1)), for example, multistep potential approximation [1], piecewise-linear potential approximation [2], finite-element methods, variational method [3], finite differences scheme [4, 5]. In the cases where a set of basis states is needed to describe a quantum system, for example in the problem of hole-bound states in a QW, the eigenvalue problem for the system of coupled differential equations ($n \geq 2$ in Eq. (1)) has to be solved. The problem then becomes much more complicated and usually finite-difference-scheme [4, 5] or numerical integration of the system of coupled ordinary differential equations (ODE) [6] based methods are used. In the present paper we demonstrate an explicit numerical method based on the recurrent sequences procedure [7, 8] for solving the eigenvalue problem for systems of ODE (1) that makes possible to derive exact analytical expression for the eigenfunctions and calculate accurately both eigenvalues and corresponding eigenfunctions. The method is used for calculation of hole bound-states energies and corresponding wave functions in a finite parabolic semiconductor quantum well as functions of the lateral quasimomentum component.

2. GENERAL FORMULATION OF THE METHOD

In this section the case of arbitrary but finite n and m in Eq. (1) is considered.

For further study it is convenient to represent Eq. (1) as a first-order equation for a 2n – component function

$$y(z) = \begin{pmatrix} \Psi(z) \\ d\Psi(z)/dz \end{pmatrix} \tag{3}$$

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

$\hat{0}$, and $\hat{1}$ are the null and identity $n \times n$ matrix respectively.

Since $V(z)$ is a polynomial function (2), matrix $A(z)$ in (4) assumes at $0 \leq z \leq d$ the form

$$A(z) = A_0 + A_1 z + A_2 z^2 + \cdots + A_m z^m, \tag{5}$$

where A_i, ($i = 0, 1,\ldots, m$) are constant $2n \times 2n$ matrices, and $A(z) = A = \text{const}$ at $z \leq 0$, $z \geq d$.

The following eigenvalue problem for Eq. (4) (corresponding to the one for Eq. (1)) is considered. It is necessary to find out such descrete values of the parameter E at which the following conditions for corresponding solutions are satisfied:

1) $y(z) \to 0$ as $z \to \pm\infty$
2) $y(z)$ is continuous at $z = 0$ and $z = d$.

It is necessary also to calculate corresponding eigenfunctions, i.e. normalized solutions $\Psi_E(z)$ of Eq. (1).

Note that more general conditions than 2) should be used in case when magnitudes of constant matrices $\hat{a}$, $\hat{b}$ and $\hat{c}$ are different at $0 \leq z \leq d$, $z < 0$ and $z > d$ (see e.g. [12]). For definiteness but without loss of generality let us next consider the case when they are constant at all values of z and conditions 2) are satisfied.

We consider the fundamental system of solutions of Eq. (4) seperately at $0 \le z \le d$, $z < 0$ and $z > d$.

Since $A(z)$ is polynomial matrix function (5) at $0 \le z \le d$ then the following formal power series for each particular solution satisfying the Eq. (4)

$$y(z) = \sum_{k=0}^{\infty} y_k z^k, \tag{6}$$

where y_k are constant (z-independant) 2n-components vectors obeying reccurent relations

$$(k+1) y_{k+1} = \sum_{l=0}^{m} A_l y_{k-l}, \; k = 0, 1, \; ... \tag{7}$$

converge at $|z| < \infty$ and give exact solutions of (4) (immediate corollary of [8, Theorem 4]). Here y_0 is some given 2n-vector that is one of 2n linear-independent 2n-vectors corresponding to particular solutions of the fundamental system of solutions of Eq. (4).

It is obvious that in actual calculations of the functions $y(z)$ one should truncate summation in Eq. (6) at sufficiently large value $k = k_{\max}$.

Since $A(z) = A =$ const at $z \le 0$, $z \ge d$ we have the following equation:

$$\frac{dy(z)}{dz} = Ay(z), \; A = \begin{pmatrix} \hat{0} & \hat{1} \\ \hat{a}^{-1}(E - V - \hat{c}) & -\hat{a}^{-1}\hat{b} \end{pmatrix}, \tag{8}$$

Solutions of Eq. (8) satisfying the definite conditions at $z \to \pm\infty$ are easy to find since they are superpositions of 2n-vectors (eigenvectors of the matrix A) multiplied by exponential functions with generally speaking complex arguments (eigenvalues of the matrix A). In the case of solving the eigenvalue problem one should consider those values of the parameter E that eigenvalues of the matrix A have nonzero real parts and one should retain only those exponentials in solutions which are decaying at $z \to \pm\infty$.

Let 2n by 2n matrix $A = A(E)$ has n eigenvalues with positive real parts and n eigenvalues with negative real parts at some values of E:

$$\lambda_1, \lambda_2, \ldots, \lambda_n \colon Re\lambda_i > 0, \; i = 1, \ldots, n; \; \lambda_{n+1}, \lambda_{n+2}, \ldots, \lambda_{2n} \colon Re\lambda_j < 0, \; j = n+1, \cdots, 2n, \tag{9}$$

At $z \le 0$ we have, as a matrix of n solutions of Eq. (8) tending to zero as $z \to -\infty$, the following $2n \times n$ matrix function

$$F(z) \equiv \left(u_1 \exp(\lambda_1 z), u_2 \exp(\lambda_2 z), \ldots, u_n \exp(\lambda_n z)\right). \tag{10}$$

Here n-elements vectors $u_1, \ldots, u_n$ are eigenvectors of the matrix $A(E)$ which correspond to its eigenvalues $\lambda_1, \ldots, \lambda_n$ with positive real parts. Using each of n columns of $2n \times n$ constant matrix $F(0)$ as a vector y_0 in (6), (7) we derive a $2n \times n$ matrix function $Y(z)$ which is built from n particular solutions $y_i(z)$ ($i = 1, \ldots, n$) of Eq. (4) at $0 \le z \le d$

$$Y(z) = \left(y_1(z), \dots, y_n(z)\right) = \sum_{k=1}^{\infty} Y_j z^j = \sum_{k=1}^{\infty} \left((y_1)_k, \dots, (y_n)_k\right) z^k,$$

$$(k+1)Y_{k+1} = \sum_{l=0}^{n} A_l Y_{k-l},\ k = 0,\ 1,\ \dots;\ Y_0 = F(0) = \left(u_1, \dots, u_n\right) \tag{11}$$

At $z \geq d$ we have, as a matrix of n solutions of Eq. (8) tending to zero as $z \to +\infty$, the following $2n \times n$ matrix function

$$\Gamma(z) = \left(u_{n+1}\exp(\lambda_{n+1}z), u_{n+2}\exp(\lambda_{n+2}z), \dots, u_{2n}\exp(\lambda_{2n}z)\right), \tag{12}$$

where $u_{n+1}, \dots, u_{2n}$ are eigenvectors of the matrix $A(E)$ which correspond to its eigenvalues $\lambda_{n+1}, \dots, \lambda_{2n}$ with negative real parts.

It is not difficult to compute $2n \times n$ matrix functions $Y(z)$ (11) and $\Gamma(z)$ (12) in the point $z = d$ at any value of the parameter E. It is obvious that for existence of the eigenfunction of Eq. (4) it is necessary and sufficient that such non-nil n-dimensional vectors of the matching $\Xi_1 = \Xi_1(E)$ and $\Xi_2 = \Xi_2(E)$ exist that the following condition is valid

$$Y(d)\,\Xi_1 = \Gamma(d)\,\Xi_2. \tag{13}$$

This implies that some value $E = E_0$ is the eigenvalue of Eq. (4) if the following equality is satisfied

$$\det M(E) = 0, \tag{14}$$

where $M = M(E)$ is a $2n \times 2n$ matrix

$$M \equiv (Y(d), -\Gamma(d)) \tag{15}$$

Thus the problem of finding eigenvalues of Eq. (4) is reduced to numerical solution of Eq. (14).

After computation of the eigenvalue $E = E_0$ and n-dimensional vectors Ξ_1 and Ξ_2 from Eq. (13), and normalization we derive the following expression for the corresponding eigenfunction

$$y_{E_0}(z) = \begin{cases} F(z)\Xi_1, z \leq 0, \\ Y(z)\Xi_1, 0 \leq z \leq d, \\ \Gamma(z)\Xi_2, z \geq d \end{cases} \tag{16}$$

Note that Eq. (16) gives exact analytical expression for the eigenfunctions of Eq. (4) and hence eigenfunctions and their first derivatives of Eq. (1). There are no restrictions on the properties of matrices $\hat{a}$, $\hat{b}$ and $\hat{c}$ in Eq. (1).

3. HOLE STATES IN A FINITE PARABOLIC QUANTUM WELL

The light- and heavy-hole states in semiconductors are described by the 4 × 4 Luttinger Hamiltonian matrix [9]. We choose z direction to be perpendicular to interfaces in a quantum-well structure (the direction of crystal growth). The potential $V(z)$ breaks the translational symmetry along z axis but components of quasi-momentum parallel to the interfaces (k_x, k_y) remain good quantum numbers. A unitary transformation [10] block diagonalizes the Hamiltonian 4 × 4 matrix into two 2 × 2 blocks. Then, in the case of symmetric quantum wells, after substitution $k_z \to -i\frac{d}{dz}$ in the Hamiltonian, the Schrödinger equation is reduced to the Eq. (1) with $n = 2$, and in the so called spherical approximation when one neglects the warping of the valence band matrices $\hat{a}$, $\hat{b}$ and $\hat{c}$ in Eq. (1) take on form

$$\hat{a} = \begin{pmatrix} -1+\mu & 0 \\ 0 & -1-\mu \end{pmatrix}, \hat{b} = k_l \begin{pmatrix} 0 & -\sqrt{3}\mu \\ \sqrt{3}\mu & 0 \end{pmatrix}, \hat{c} = k_l^2 \begin{pmatrix} 1+\frac{1}{2}\mu & \frac{\sqrt{3}}{2}\mu \\ \frac{\sqrt{3}}{2}\mu & 1+\frac{1}{2}\mu \end{pmatrix}. \tag{17}$$

Where k_l is the lateral quasi-momentum component (good quantum number): $k_l^2 = k_x^2 + k_y^2$; $\mu = (6\gamma_3 + 4\gamma_2)/5\gamma_1$, γ_1, γ_2, γ_3, are the dimensionless Luttinger parameters [9]; 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, m_0 is free electron mass. The realistic range of the parameter under consideration is: $0 \le \mu < 1$. Note that when $\mu = 0$ equations (1) become decoupled and each of them describes electron in a simple-conduction-band semiconductor QW [7, 5]. In what follows, we consider the case of a structure with a symmetric parabolic quantum well: $V(z) < 0$ at $0 \le z \le d$, and $V(z) = 0$ at $z \le 0$, $z \ge d$. Note that when $k_l = 0$ equations (1) become decoupled and are of the form of two one-dimensional Schrödinger equations describing heavy and light holes $\left(m_{h,l} = \frac{\gamma_1 m_0}{1 \mp \mu} \right)$. At $k_l \neq 0$ Eq. (1) become coupled and we designate hole states conventionally as a heavy- and light-hole states. After substitution (3) we obtain Eq. (4) with matrix function $A(z)$: $A(z) = A_0 + A_1 z + A_2 z^2$, where A_0, A_1, A_2 are constant 4 × 4 matrices. Eigenvalues of the matrix $A = A_0$ read as follows:

$$\lambda_{1,3} = \pm\sqrt{\frac{-E}{1-\mu} + k_l^2}, \quad \lambda_{2,4} = \pm\sqrt{\frac{-E}{1+\mu} + k_l^2} \tag{18}$$

We chose corresponding eigenvectors as:

$$\Phi_{1,3} = \begin{pmatrix} 1 \\ \phi_2^{1,3} \\ \lambda_{1,3} \\ \lambda_{1,3}\phi_2^{1,3} \end{pmatrix}, \phi_2^{1,3} = -\frac{\sqrt{3}k_l^2}{k_l^2 \mp 2k_l\lambda_1}; \Phi_{2,4} = \begin{pmatrix} \phi_1^{2,4} \\ 1 \\ \lambda_{2,4}\phi_1^{2,4} \\ \lambda_{2,4} \end{pmatrix}, \phi_1^{2,4} = -\frac{\sqrt{3}k_l^2}{k_l^2 \pm 2k_l\lambda_2}. \tag{19}$$

Thus matrix $F(z)$ from (10) equals

$$F(z) = \left(\Phi_1 \exp(\lambda_1 z), \Phi_2 \exp(\lambda_2 z)\right).$$

Using its value at $z = 0$ we find 4×2 matrix of solutions of Eq. (4) at $z = d$, namely

$$Y(d) = \sum_{k=0}^{\infty} Y_k d^k, (k+1)Y_{k+1} = \left(\sum_{l=0}^{n} A_l Y_{k-l}\right), \quad k = 0, 1, \ldots, Y_0 = F(0).$$

The 4×2-matrix function of solutions of Eq. (4) at $z \geq d$, tending to zero as $z \to +\infty$ is:

$$\Gamma(z) = \left(\Phi_3 \exp(\lambda_3 z), \Phi_4 \exp(\lambda_4 z)\right)$$

Eigenvalues are determined by numerical solution of the equation det $M(E) = 0$, where the 4×2 matrix M equals $M(E) = (Y(d), -\Gamma(d))$. Eq. (19) and (13) provide an eigenfunction for a particular value of $E = E_0$. Normalizing of wave functions is performed analytically.

3. RESULTS AND DISCUSSION.

Results of the calculations of the dispersions of *all* hole bound states in a GaAs symmetric parabolic quantum well, namely when the potential $V(z)$ is $V(z) = -U_0[1-(2z-1)^2]$, are represented in Fig. 1. Material parameters used in computations are: $\mu = 0.753$, $\gamma_1 = 6.85$. Calculated wave functions are shown in Figs. 2-4. Note, that no oscillatory theorem for the wave function is valid in the matrix case (i.e. if $n > 1$, in Eq. (1)) owing to admixture of

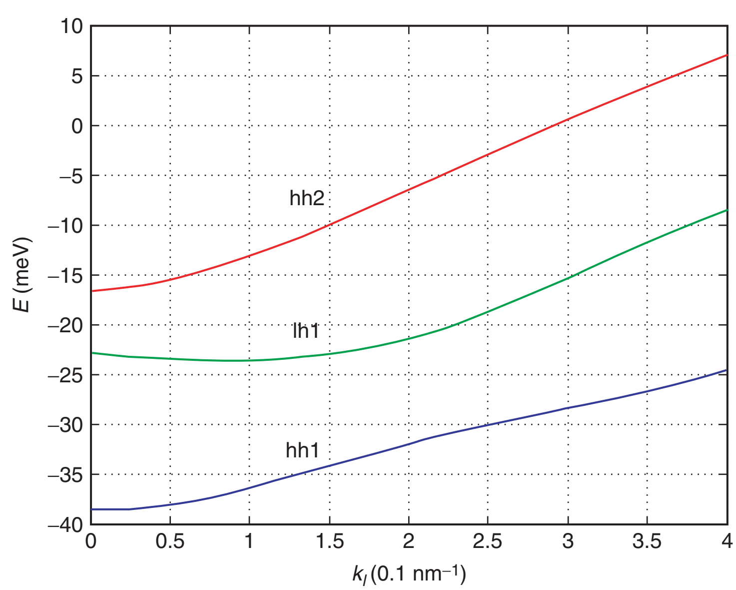

Figure 1 Dispersion of hole bound states in a single confined quantum well. d = 100 Å, U_0 =. 0,05 eV.

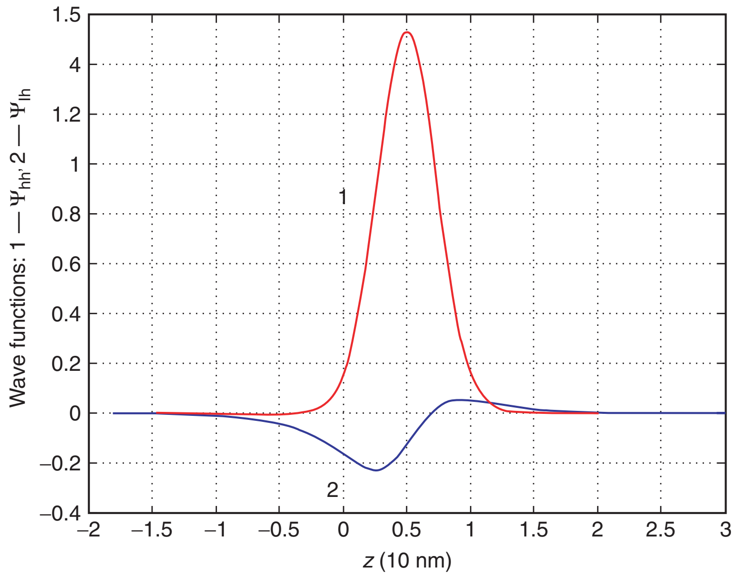

Figure 2 Wave function of the hole ground state (hh1) in a parabolic GaAs quantum well. U_0 = 0.05 *eV*, *d* = 10 *nm*, E_0 = –36.416 *meV*.

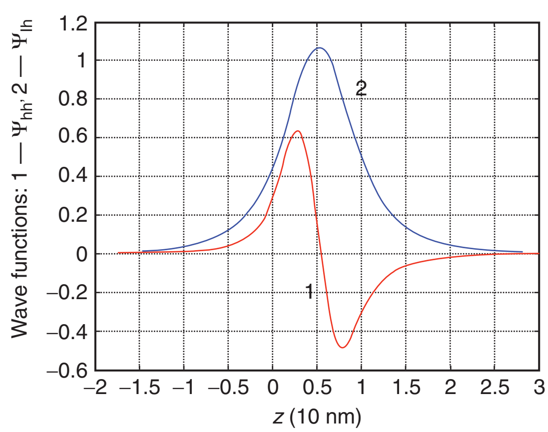

Figure 3 Wave functions of 1h1 state in GaAs single parabolic *QW*. Parameters are identical Parameters are those as in Fig. 1. *E* = -23.656 *meV*.

heavy- and light-hole states at $k_l \neq 0$ (one always obtains a light-hole exponential in asymptotic of solutions like in the 'Coulomb' case [11]). Moreover, it is possible to obtain a wave-function nil beyond the well (that is apparently seen in Fig. 4).

An explicit method was demonstrated for accurate solving the eigenvalue problem for some systems of ordinary differential equations. Exact analytical expressions for the eigenfunctions were derived. Energies and wavefunctions of hole bound states in a semiconductor finite parabolic quantum well were calculated as functions of a quasimomentum component parallel to interfaces in a structure.

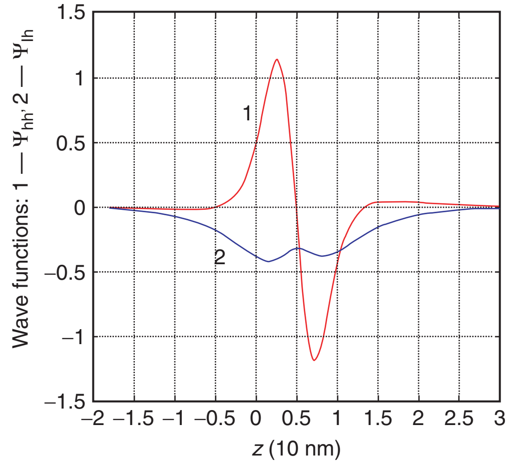

Figure 4 Wave functions of the hole second excited state (hh2) in a parabolic GaAs quantum well. Parameters are those as in Fig. 1, E_0 = –13.174 meV.

REFERENCES

[1] Ando Y., Itoh, T. Calculation of transmission tunneling current across the arbitrary potentials. J. Appl. Phys., 1987, Vol. 61, 1497–1501.

[2] Lui W.W., Fukuma M., J. Appl. Phys., 1986, Vol. 60, 1555–1559.

[3] Bastard G., Mendez E.E., Chang L., Esaki L. Variational calculation on aquantum well in an electric field. Phys. Rev., 1983, Vol. B28, 3241–3244.

[4] Ahn D., Chuang S.L., Chang Y.-C. Valence-band mixing effects on the gain and the refractive index change of quantum-well lasers, J. Appl. Phys., 1988, Vol. 64, 4056–4063.

[5] Harrison P. Quantum Wells, Wires and Dots. Theoretical and Computational Physics. 2011. J. Wiley & Sons.

[6] Ikoniĉ; Z., Milanoviĉ; V. Hole-bound-state calculation for semiconductor quantum wells, Phys. Rev., 1992, Vol. B45, 8760–8762.

[7] Polupanov A.F., Energy spectrum and wave functions of an electron in a surface energy well in a semiconductor, Sov. Phys. Semicond., 1985, Vol. 19, 1013–1015.

[8] Galiev V.I., Polupanov A.F., Shparlinski I.E., On the construction of solutions of systems of linear ordinary differential equations in the neighbourhood of a regular singularity, J. of Computational and Applied Mathematics, 1992, Vol. 39, 151–163.

[9] Luttinger J.M., Quantum theory of cyclotron resonance in semiconductors: General theory, Phys. Rev., 1956, Vol. 102, 1030–1041.

[10] Broido D.A., Sham L.J., Effective masses of holes at GaAs-AlGaAs heterojunctions, Phys. Rev. B, 1985, Vol. 31, 888–892.

[11] Galiev V.I., Polupanov A.F., Accurate solutions of coupled radial Schrödinger equations, J. Phys. A: Math. Gen., 1999, Vol. 32, 5477–5492.

[12] Polupanov A.F., Galiev V.I., Kruglov A.N. The over-barrier resonant states and multi-channel scattering by a quantum well. Int. J. of Multiphysics, 2008, Vol. 2 , 171–177.