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AN ANALYTICAL SOLUTION FOR CONICAL QUANTUM DOTS

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In the paper, an analytical method of the solution of a governing nonlinear eigenproblem is proposed. It can be directly applied into analysis of axisymmetric conical quantum dots embedded in a matrix. The method is based on the use of variational formulation combined with the method of the Rayleigh quotient and the series expansions. In order to explain the form of the series expansions (the Bessel and sine series), the analytical solutions for quantum dots are demonstrated and discussed. The solved example shows the efficiency of the method.

Key words: conical quantum dots, nonlinear eigenproblem, variational formulation, Rayleigh quotient

1. Introduction

Quantum effects begin to dominate as the size of semiconductor structures approaches the electron de Broglie wavelength. In low-dimensional semiconductor nanostructures (LDSN), the motion of electrons can be confined spatially, from one, two, and even three spatial directions. The operation of semiconductor quantum devices is based on the confinement of individual electrons and holes in one spatial dimension (quantum wells), two spatial dimensions (quantum wires) or three spatial dimensions (quantum dots – QDs). For instance the potential barriers, forming the well are provided primarily by either free surfaces, which impose essentially infinite confinement, or by sharply layered compositional differences. In the SiGe system, for example, the valence bands of uniform bulk Si and Ge are shifted in energy by 0.46 eV. Phonon induced relaxation of a charge to its ground state and other dynamics of excited charge carriers affects many important characteristics of nanoscale devices such as switching speed, luminescence efficiency and carrier mobility and concentration. Therefore, a better understanding of the processes that govern such dynamics has an important and fundamental technological implications. These phenomena are investigated experimentally through intraband transitions induced by carrier-phonon interactions in QDs and probed effectively by various time-resolved spectroscopy methods. Yet fundamental understanding of the underlying physics responsible for carrier dynamics and the specific role that phonons play in the relaxation mechanisms in QDs is still lacking. In such nanostructures, the free carriers are confined to a small region of space by potential barriers, and if the size of this region is less than the electron wavelength, the electronic states become quantized at discrete energy levels. The ultimate limit of low dimensional structures is the quantum dot, in which the carriers are confined in all three directions. Therefore, a quantum dot can be thought of as an artificial atom.

Many of the previous numerical modeling approaches for these quantum structures used spatial discretisation methods, such as the finite element or finite difference method (Grundmann *et al.*, 1995; Stier *et al.*, 1999; Johnson and Freund, 2001). As an alternative, the boundary element method was proposed by Geldbard and Malloy (2001). Voss (2006) employed the Rayleigh-Ritz method to solve the nonlinear eigenvalue problem where the eigenstates of the electron in QDs were derived with the use of the finite element method incorporated in the MATLAB package.

Lew Yan Voon and Willatzen (2004, 2005) found analytical solutions for paraboloidal and ellipsoidal QDs not embedded in the matrix. Various aspects of the evaluation of eigenenergies in closed periodic systems of quantum dots were also discussed in the literature – see e.g. Refs Li (2005) and Cattapan *et al.* (2009).

In the present paper, we intend to demonstrate the method of analytical solutions of the nonlinear eigenvalue problem for conical quantum dots embedded in the matrix. In the mathematical sense, the problem is described by the solution of the Helmholtz equation.

2. Governing relations

Let Ω_q be a 3D domain occupied by the quantum dot, which is embedded in a bounded matrix Ω_m of a different material – Fig. 1. A typical example is an InAs quantum dot embedded in a GaAs matrix. By adopting this continuum view of confinement in semiconductor quantum devices, the spectrum of confined states available to individual electrons or holes can be characterized by the steady state Schrdinger equation, given by

$$H_i(m_i)\Phi_i = E\Phi_i \tag{2.1}$$

where

$$H_i(m_i) = -\operatorname{div}\Big(\frac{\hbar^2}{2m_i}\operatorname{grad}\Phi_i\Big) + V_i(x)\Phi_i \qquad x \in \Omega_1 \cup \Omega_2$$

where H_i is the Hamiltonian function (operator), Φ_i means the wave function, E denotes the energy level (the identical value for the matrix and the quantum dot), $\hbar$ is the reduced Planck constant, and the index i corresponds to the quantum dot $(i = 1; q)$ and to the matrix $(i = 2; m)$, respectively. The electron effective mass m_i is assumed to be constant on the quantum dot and the matrix for every fixed energy level E and is taken as (Chuang, 1995)

$$\frac{1}{m_i(E)} = \frac{P_i^2}{\hbar^2}\Big(\frac{2}{E + E_{g,i} - V_i} + \frac{1}{E + E_{g,i} - V_i + \delta_i}\Big) \tag{2.2}$$

where the confinement potential V_i is piecewise constant, and P_i, $E_{g,i}$ and δ_i are the momentum matrix element, the band gap, and the spin–orbit splitting in the valence band for the quantum dot $(i = q)$ and the matrix $(2 = m)$, respectively. The values of the above constants are given in Table 1.

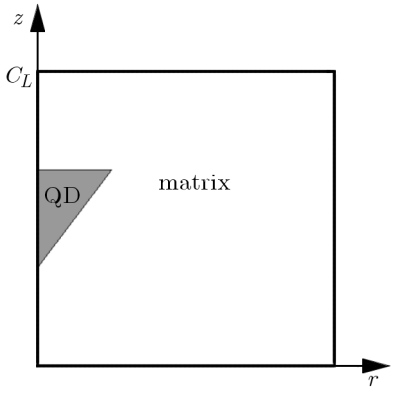

Fig. 1. Geometry of the quantum dot surrounded by the matrix

The aim of the study is to solve eigenvalue problem (2.1) and to determine the k-th eigenenergy. Since effective masses m_i (2.2) are, in fact, functions of the eigenergies, problem (2.1)

Table 1. Material properties of the quantum dot InAs and the matrix GaAs

	P_i	$E_{g,i}$	V_i	δ_i
$i = 1$ (q) InAs	0.8503	0.42	0	0.48
$i = 2$ (m) GaAs	0.8878	1.52	0.7	0.34

constitutes the nonlinear eigenvalue problem. Commonly, the wave function decays outside the quantum dot and the matrix very rapidly, it is then reasonable to assume homogeneous Dirichlet conditions, i.e.: $\Phi_i = 0$ on the outer boundaries. On the interface between the quantum dot and the matrix, the Ben Daniel-Duke condition (Chuang, 1995) holds

$$\frac{1}{m_1}\frac{\partial \Phi_1}{\partial n_1} = \frac{1}{m_2}\frac{\partial \Phi_2}{\partial n_2} \tag{2.3}$$

Here n_1 and n_2 denote the outward unit normal on the boundary of Ω_1 and Ω_2, respectively.

3. Solution to the boundary value problem

Steady state Schrödinger equation (2.1), which governs the behavior of individual charge carriers in strained devices, is in the form of the classical Helmholtz equation

$$\operatorname{div}\operatorname{grad}\Phi_i + k_i^2\Phi_i = 0 \qquad k_i^2 = \frac{2m_i(E - V_i)}{\hbar^2} \qquad i = 1, 2 \tag{3.1}$$

Let us assume rotational symmetry of the problem. Thus, in the cylindrical coordinateds the wave function can be written as $\Phi_i(r, z, \varphi) = R_i(r)Z_i(z)\sin(l\varphi)$, where $l = 0, \pm 1, \pm 2, \ldots$ is the electron orbital quantum number. Finally, after separation of the variables, Schrödinger equation (3.1) obtains the form:

$$\Big(\frac{1}{r}\frac{\partial}{\partial r}\Big(r\frac{\partial}{\partial r}\Big) + k_i^2 + s_i^2 - \frac{l^2}{r^2}\Big)R_i(r) = 0 \qquad \frac{\partial^2 Z_i(z)}{\partial z^2} + s_i^2 Z_i(z) = 0 \qquad i = 1, 2 \tag{3.2}$$

and s_i are the separation constants. If we rescale the spatial coordinate r in Eq. (3.2) and introduce a new variable $x = r\sqrt{k_i^2 + s_i^2}$, the first equation can be reduced to the classical form of the Bessel equation

$$\Big(\frac{1}{x}\frac{\partial}{\partial x}\Big(x\frac{\partial}{\partial x}\Big) + 1 - \frac{l^2}{x^2}\Big)X_i(x) = 0 \qquad X_i(x) = R_i(r) \tag{3.3}$$

Since the Bessel function $J_{-l}(x)$ tends to infinity at $x = 0$, the solutions of Schrödinger equation (3.1) can be expressed as follows

$$\Phi_i(r, z, \varphi) = [M_i \sin(s_i z) + N_i \cos(s_i z)]J_l\Big(r\sqrt{k_i^2 + s_i^2}\Big)\sin(l\varphi) \qquad i = 1, 2 \tag{3.4}$$

where M_i and N_i are the unknown constants. Using the Dirichlet boundary condition $\Phi_1(r, 0,) = 0$, one can find that $N_1 = 0$ and $\Phi_2(r, z = \overline{z}, \varphi) = 0$, $N_2 = -M_2 \tan(s_2\overline{z})$. The third boundary condition $\Phi_2(r = \overline{r}, z, \varphi) = 0$ leads to an infinite number of solutions being the zeroth of the Bessel functions of the l-th order, i.e.: $J_l\Big(\overline{r}\sqrt{k_2^2 + s_2^2}\Big) = 0$. Let us note that with the use of that relation, it is possible to determine the value of the separation constant s_2.

4. Variational formulation

The analytical form of solution (3.4) is not very convenient for direct numerical computations of eigenenergies due to the existence of boundary condition (2.3). Therefore, we adopt herein the variational formulation. Multiplying (2.1) by $\boldsymbol{\Psi}$ in the Sobolev space $H_1^0(\Omega)$, $\Omega = \Omega_1 \cup \Omega_2$ and integrating by parts, one gets the variational form of the Schrödinger equation

$$a(\boldsymbol{\Phi}, \boldsymbol{\Psi}; E) = \sum_{i=1}^{2} \int\limits_{\Omega} \Big(\frac{\hbar^2}{2m_i} \operatorname{grad} \boldsymbol{\Phi} \cdot \operatorname{grad} \boldsymbol{\Psi} + V_i(x) \boldsymbol{\Phi} \cdot \boldsymbol{\Psi} \Big)\, d\Omega = E \int\limits_{\Omega} \boldsymbol{\Phi} \cdot \boldsymbol{\Psi}\, d\Omega = E b(\boldsymbol{\Phi}, \boldsymbol{\Psi}) \quad (4.1)$$

If the quadratic form $a(\boldsymbol{\Phi}, \boldsymbol{\Phi}; E)$ is a positive, monotonically decreasing function then a unique positive solution exists

$$E(\Phi) = \frac{a(\boldsymbol{\Phi}, \boldsymbol{\Phi}; E)}{b(\boldsymbol{\Phi}, \boldsymbol{\Phi})} \quad (4.2)$$

and the corresponding eigenvectors $\boldsymbol{\Phi}_k$ are stationary elements of $E'(\boldsymbol{\Phi}_k)$. If the quadratic form a does not dependent on E, then the above Rayleigh functional is just the well known Rayleigh quotient. The evaluation of the Rayleigh functional is based on the discretization method of the eigenvectors $\boldsymbol{\Phi}_k$. Since the solution to equations (3.3) can be represented in form of the Bessel function, we propose to define the radial part of the eigenvectors in form of the orthogonal Bessel functions

$$R(r) = \sum_{m=1}^{\infty} A_m J_l\Big(\frac{\mu_m^{(l)}}{r_0} r \Big) \quad (4.3)$$

where the symbols $\mu_m^{(l)}$ denote the m-th zero of the Bessel function J_l at $r = r_0$. The expansion in form given by equation (4.3) is assumed to be valid in the whole space occupied by the quantum dot and the matrix. In the z direction the function $Z(z)$ can be expressed in form of the classical Fourier series, i.e

$$Z(z) = \sum_{n=0}^{\infty} C_n \sin\Big(\frac{n\pi(z - z_0)}{z_1 - z_0} \Big) \quad (4.4)$$

where z_1 and z_0 denote the upper and lower boundaries of the quantum dot, respectively (see Fig. 1). Similarly, as in Section 3, in the cylindrical system of coordinates, the representation of the eigenfunctions can be defined as the multiplication of series (4.3), (4.4) and function $sin(l\varphi)$. In equation (4.1), the integration over the variables r, φ and z is separated. Using the properties of the Bessel function, the numerator in equation (4.1) takes the form

$$a(\boldsymbol{\Phi}, \boldsymbol{\Phi}) = \sum_{i=1}^{2} \Big(\frac{\hbar^2}{2m_i} D_1 + V_i D_2 \Big) \quad (4.5)$$

and

$$D_2 = \frac{r_0^2 dz}{2} F(A_m) \sum_{n=0}^{\infty} \Big(\frac{n\pi}{z_1 - z_0} C_n \Big)^2$$

$$D_1 = -dz \sum_{n=0}^{\infty} (C_n)^2 \sum_{m,k=0}^{\infty} A_m A_k \frac{\mu_m^{(l)} \mu_k^{(l)}}{r_0^2} \int\limits_0^{r_0} dr\; J_{l-1}\Big(\frac{\mu_k^{(l)} r}{r_0} \Big) J_{l+1}\Big(\frac{\mu_m^{(l)} r}{r_0} \Big)$$

whereas the denominator

$$b(\mathbf{\Phi},\mathbf{\Phi}) = \frac{r_0^2 dz}{2} F(A_m) \sum_{n=0}^{\infty} (C_n)^2 \qquad F(A_m) = \sum_{m=0}^{\infty} \left[A_m J_l'(\mu_m^{(l)}) \right]^2$$
$$dz = \frac{z_1 - z_0}{2} \tag{4.6}$$

The computation is carried out in the iterative way in two steps:

1. For the assumed value of the eigenenergy E_0 the minimum of the functional $a(\mathbf{\Phi},\mathbf{\Phi}) - -E_0 b(\mathbf{\Phi},\mathbf{\Phi})$ is searched for, with respect to the unknown coefficients A_m and C_n
2. For the calculated values of A_m and C_n, rational matrix eigenvalue problem (4.2) is solved to determine a new eigenvalue E_1.

The procedure is repeated until the required accuracy is reached. The computations are conducted with the use of the symbolic package Mathematica.

5. Numerical example

Figure 1 demonstrates the axisymmetrical conical quantum dot embedded in the matrix. The radius and the height of the QT are equal to 10, whereas the radius and the height of the matrix are equal to 40 and 30, respectively. The physical properties of the materials are given in Table 1. The boundary conditions are assumed to be in the Dirichlet form, i.e. the wave functions are equal to zero on the boundaries.

Table 2 shows results of the computations. The results are presented for the first six eigenvalues and compared also with the results available in the open literature.

Table 2. Eigenvalues for the quantum dot embedded in the matrix

l	Eigenvalue	
	present analysis	Voss (2006)
0	0.254607	0.254585
1	0.387332	0.384162
0	0.466941	0.467239
2	0.502889	0.503847
0	0.560774	0.561319
1	0.599138	0.598963
3	0.622213	0.617759

l – the electron orbital quantum number

The computed eigenvalues show quite good agreement with the results obtained by Voss (2006). In the presented computations, the maximal number of terms in expansion (4.3) was equal to 50, and approximation (4.4) was cut off on 15 to 20 terms. It is worth to note that the lowest values of the eigenvalues do not correspond to the lowest values of the electron orbital quantum number.

6. Concluding remarks

The presented method shows the possibility of analytical computations of the nonlinear boundary value problem characterized by the Helmholtz equations. In this way, it is possible to find not only the energy spectrum and wave functions of an electron in a quantum dot but also the acoustic

eigenfrequencies and eigenmodes of the pressure field inside an acoustic cavity. Eigensolutions are presented in a convenient form of the series expansions. The analysis can be conducted for an arbitrary form of the potential function, however having the axisymmetry with respect to the axis of rotations.

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Rozwiązanie analityczne dla stożkowych kropek kwantowych

Streszczenie

W pracy zaproponowano analityczną metodę do rozwiązania nieliniowego problemu własnego. Może ona być bezpośrednio zastosowana do analizy osiowosymetrycznych stożkowych kropek kwantowych osadzonych w osnowie. Polega na wykorzystaniu wariacyjnego sformułowania w połączeniu z metodą Rayleigha i rozwinięciem w szereg. Przedstawiono i przeanalizowano analityczne rozwiązania dla kropek kwantowych z wykorzystaniem różnych form rozwinięć w szereg (Bessela i Fouriera). Rozwiązany przykład pokazuje skuteczność przedstawionej metody.

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