Eigenvalue problem of confined quantum dots

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Abstract: The analysis of optoelectromechanical properties of nanostructures in band structure engineering is discussed in the paper. It is demonstrated that the design of semiconductors is based on the solution of different forms of the Schrödinger (Helmholtz) equation, dependent on the form of the Hamiltonian characterizing quantum effects. The formulation can lead to the linear or nonlinear eigenvalue problems. Then, the methods of solutions are also presented.

1. Introduction

Today the advances in chemical synthesis and manufacture techniques have led to novel nano-sized materials demonstrating unique and often unexpected properties. These new nanosystems offer the ability to control their electronic and optical behavior through the sample’s size, shape and topology [1-4]. In recent decades semiconductor quantum dots (QD) have been the subject of many experimental, theoretical and technological investigations [5-9]. The design of nanoelectronic devices requires a clear understanding of the fundamental properties of nanomaterials. When nanomaterials absorb a light quantum, two charged particles are created simultaneously, an electron and a hole. Knowledge of photoinduced charge carrier dynamics in nanomaterials will help to achieve an effective functionality of prospective nanonelectronic devices. Here, the eigenproblems analysis is presented for selected QD having the conical shape embedded in a cylindrical matrix.

2. Materials and methods

2.1 Quantum dots

QDs are tiny dimensionally confined (typically semiconductor) objects where quantum effects become obvious, for example, energy spectra become discrete. Of particular interest is the class of devices that are composed of combinations of lattice mismatched materials. These material combinations, such as Si$_x$Ge$_{1-x}$/Si and In$_x$Ga$_{1-x}$As/GaAs, where x indicates the fractional content of alloying material, are selected primarily on the basis of their electronic properties and to some extent for convenience of processing [10]. 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) [2].

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. Usually, the QD is buried in the host matrix (figure 1) with differing elastic constants and lattice parameter. Because of the lattice mismatch, both the QD and host matrix strain and relax elastically to accommodate this mismatch and thus admit a state of stress. As is well known, the electronic structure and the consequent optoelectronic properties of QDs are severely impacted due to this lattice mismatch induced strain. The host matrix boundaries do not impact its strain state, if the distance of the QD from any free boundary is significantly larger than, e.g., the QD radius (typically \( \sim 3R \)).

**Figure 1.** Spherical quantum dot embedded in host matrix

**Figure 2.** Schematic view of the structure (QD - InAs separated by wide gap material layers e.g. GaAs)

The typical QD infrared light system is plotted in figure 2. A lot of QDs constitute a set of separated layers.

### 2.2 Computational model

Many of the previous numerical modeling approaches for quantum dots used spatial discretisation methods, such as the finite element or finite difference method [5–7]. As an alternative, the boundary element method was proposed by Geldbard and Malloy [11]. Voss [12] 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. Voon and Willatzen [13–14] found analytical solutions for paraboloidal and ellipsoidal QDs not embedded in the matrix. Various aspects of the evaluation of the eigenenergies in closed periodic systems of quantum dots were also discussed in the literature - see, e.g., [15–16].

Even in devices free of misfit dislocations, the strain induced by lattice mismatch can strongly affect electronic properties. However, this effect has not been thoroughly studied, particularly in submicron sized structures in which quantum mechanics governs the device properties and in which strains are highest and most nonuniform. In order to analyze strain effects in semiconductor quantum structures, it is necessary to adopt a model for electronic properties. Simple quantum mechanical models have long been available for describing the electronic properties of semiconductor devices based on the transport and confinement of single charge carriers. The study of quantum dots and quantum wires has renewed the interest in these models. The effects of uniform, coherent strain on electronic properties have also been well understood for many years and have been identified experimentally by Zaslavsky et al. [17]. There have been some attempts to model strain effects in quantum dots – see, e.g., [7]. Further, many quantum dot structures have a well-pronounced piezoelectric effect which does contribute to their overall properties in a non-trivial manner. These coupled electromechanical effects will become increasingly important for the current and future applications of such nanostructures [18–19]. 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 Schrödinger equation, given by:

\[
H_{\alpha\beta}(\vec{r})\psi_\beta(\vec{r})+V_{\alpha\beta}(\vec{r})\psi_\beta(\vec{r})=E\psi_\alpha(\vec{r})
\]
where $H_{\alpha\beta}$ is the Hamiltonian function coupling the energy of a charge carrier between energy bands $\alpha$ and $\beta$, $\psi_\beta$ is the quantum mechanical wave function associated with energy band $\beta$, $V_{\alpha\beta}$ is an effective potential field coupling energy bands $\alpha$ and $\beta$, and $E$ is the energy (the eigenvalue) of a particular quantum mechanical state.

The form of the Hamiltonian function is directly associated with the type of semiconductors, and especially with the form of the energy band. In view of that, we introduce the following division:

1. One band envelope-function formalism for electrons and holes in which the effective Hamiltonian is given by:

$$H_{\alpha\alpha} = -\text{div}\left(\frac{\hbar^2}{2m_0\lambda}\nabla\psi_\alpha\right)$$

where $\hbar$ is the reduced Planck constant, and the index $i$ corresponds to the quantum dot ($i=1$) and to the matrix ($i=2$), respectively. Such a description is valid for the direct band gap and for instance is valid for an InAs quantum dot embedded in a GaAs matrix. In the present analysis 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 [5]:

$$\frac{1}{m_i(E)} = \frac{P_i^2}{\hbar^2} \left(\frac{2}{E + E_{g,i}^\dagger - V_i} + \frac{1}{E + E_{g,i} - V_i + \delta_i}\right)$$

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

**Table 1.** The material properties of the quantum dot InAs and the matrix GaAs.

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

2. The highest energy valence subbands. This basis consists of the two degenerate heavy hole subbands and the two degenerate light hole subbands, in reference to the relative masses of the charge carriers when treated as classical particles. The form of the Hamiltonian is given by:

$$H_{\alpha\beta} = -\frac{\hbar^2}{2m_0} L_{\alpha\beta}(\vec{r}) \psi_{\beta\alpha}^2, \alpha, \beta, k, l = 1, 2$$

where:

$$L_{\alpha\beta}(\vec{r}) = \begin{bmatrix} g^{k_1}_{l_1} & g^{k_1}_{l_2} & g^{k_1}_{l_3} \\ g^{k_2}_{l_1} & g^{k_2}_{l_2} & g^{k_2}_{l_3} \\ g^{k_3}_{l_1} & g^{k_3}_{l_2} & g^{k_3}_{l_3} \end{bmatrix}$$
This Hamiltonian can be used to model the medium in a Si$_x$Ge$_{1-x}$ structure $g^H_1, g^H_2, g^H_3, g^H_4, g^H_5, g^H_6$ – see Singh and Muc et al. [20-21]. With the use of the relation (3) it is possible to use the identical approximations of the wavefunctions in the equations (4) and (5), since the different properties of the QD and the matrix are hidden in table 1. Using the properties of the Bessel function the numerator in the equation (3) takes the form:

$$a(\Phi, \Phi) = \sum_{m=1}^{\infty} \left( \frac{\hbar^2}{2m} D_m + V D_2 \right)$$  \hspace{1cm} (6)$$

whereas the denominator:

$$b(\Phi, \Phi) = \frac{\hbar^2}{2} F(A_m) \sum_{n=0}^{\infty} C_n \left( \frac{\hbar^2}{2} F(A_m) = \sum_{n=0}^{\infty} A_n A_l \frac{\mu^{k_1 l_1}_m}{r_0} \int \mathcal{J}_{l_1}^2 \left( \frac{\mu^{k_1 l_1}_m}{r_0} \right), \right.$$  \hspace{1cm} (7)$$

The computation is carried out in the iterative way in two steps. Firstly for the assumed value of the eigenenergy $E_0$ the minimum of the functional $a(\Phi, \Phi) - E_0 b(\Phi, \Phi)$ is searched for, with respect to the unknown coefficients $A_m$ and $C_m$. Next for the calculated values of $A_m$ and $C_m$ a rational matrix eigenvalue problem (4) 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.

3. Results and discussion

We have applied our method on two different problems in order to test its efficiency and effectiveness. Figure 3 demonstrates the axisymmetrical conical quantum dot embedded in the axisymmetric cylindrical matrix.

![Figure 3. Axisymmetric problem - conical QD surrounded by cylindrical matrix.](image)

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

| The electron orbital quantum number | Eigenvalue - present analysis | Eigenvalue - Voss [12] |
|------------------------------------|----------------------------|------------------------|
|                                    | Fourier expansion 15 to 20 terms | Finite element 30 (linear) | Wavelet L=12 | Finite element (planar) |
| 0                                  | 0.254607                        | 0.255243 | 0.258931 | 0.254585 |
| 1                                  | 0.387332                        | 0.386121 | 0.395571 | 0.384162 |
| 0                                  | 0.466941                        | 0.469542 | 0.471121 | 0.467239 |
| 2                                  | 0.502889                        | 0.503891 | 0.504005 | 0.503847 |
| 0                                  | 0.560774                        | 0.564551 | 0.564551 | 0.561319 |
| 1                                  | 0.599138                        | 0.604511 | 0.597138 | 0.598963 |
| 3                                  | 0.622213                        | 0.634115 | 0.623356 | 0.617759 |

The radius and the height of the QD 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 the results of the computations. The results are presented for the first six eigenvalues and compared also with the results available in the open literature. The computed eigenvalues shows quite good agreement with the results obtained by Voss [12]. In present the computations the maximal number of terms in the expansions of the function \( Z(z) \) is different, however, the use of the linear finite element or the wavelet approximations seems to be much more reasonable that the application of the finite element discretization with the use of the triangular elements. The approximation in the radial direction (10) was cut off on the maximal 50 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.

4. Summary

The present method shows the possibility of analytical computations of 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 the convenient form of the series expansions. The analysis can be conducted for the arbitrary form of the potential function, however having the axisymmetry with respect to the axis of rotations.

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