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Computation of intersubband transition energy in normal and inverted core–shell quantum dots using finite difference technique

Arpan Deyasi [a], S. Bhattacharyya [b], N.R. Das [c,*]

[a] RCC Institute of Information Technology, Canal South Road, Beliaghata, Kolkata, West Bengal 700 015, India
[b] Modern Institute of Engineering and Technology, Bandel, Hooghly, West Bengal 712123, India
[c] Institute of Radio Physics and Electronics, University of Calcutta, 92 APC Road, Kolkata 700 009, India

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ABSTRACT

In this paper, intersubband transition energy is computed for core–shell (normal and inverted) quantum dots (CSQD) of cubic and spherical geometries by solving time-independent Schrödinger equation using finite-difference technique. Sparse, structured Hamiltonian matrices of order $N^3 \times N^3$ for cubic and $N \times N$ for spherical dots are produced considering N discrete points in spatial direction. The matrices are diagonalized to obtain eigenstates for electrons. Computed results for the lowest three eigenstates and intersubband transitions are shown for different structural parameters taking GaAs/$Al_xGa_{1-x}As$ based CSQD as example. Transition energy decreases with increase in core thickness. When compared, spherical CSQDs show higher transition energy between two subbands than cubic CSQDs of similar size and same material composition. Also, in inverted configuration, transition energy decreases for a cubic dot while increases for a spherical dot as core size is increased. Wide tuning range for intersubband transition by tailoring dot dimensions indicates important applications for optical emitters/detectors.

1. Introduction

In recent years, there has been increasing interest in semiconductor nanostructures because of their key roles in novel electronic [1,2] and photonic [3,4] devices. Thanks to the advancement of

* Corresponding author. Tel.: +91 33 2350 9115x44; fax: +91 33 2351 5828.
E-mail addresses: deyasi_arpan@yahoo.co.in (A. Deyasi), swapanbhattacharyya@ieee.org (S. Bhattacharyya), nrd@ieee.org (N.R. Das).

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technology [5,6], it has become possible to fabricate new devices of various geometries and controllable dimensions. In a nanostructure, dimension is comparable to or less than the de-Broglie wavelength of electrons, and so the carriers are confined due to the restricted motion along the reduced dimensions, resulting in quantization of states. Energy quantization due to complete carrier confinement in a quantum dot (QD) introduces remarkable novelty in the performance of QD-based transistors, optical transmitters, modulators, receivers, etc. [7–10]. Recently, core–shell quantum dots (CSQDs) have emerged as potential candidates for electronic and photonic devices due to their tailorable intersubband transition energy [11,12]. In a normal CSQD, lower bandgap 'core' is surrounded by higher bandgap 'shell' material, while in an inverted CSQD, core layer is made of higher bandgap material and shell is made of lower bandgap material. Recently, it is reported that core–shell nanostructures exhibit much higher photoluminescence [13] than single-layered geometries. It also improves quantum yield due to the localization of carriers in the core area from all possible dimensions and, thus, reduces the interaction with interface trap states [14]. These core–shell structures have the potential of higher absorption cross-sections and lower Auger recombination coefficient [15]. This property along with tuning ability of eigenenergy provides a wider range of absorption and emission spectra [16]. Position-controlled doping in CSQD helps in biomedical diagnosis [17]. It is recently reported that inverted core–shell structure show better lasing performance [16,18] than other quantum dots. Properties of these electronic and optoelectronic devices are dependent on their confinement levels, which in turn, is dependent on geometry, dimension and material composition of the structure. Therefore, a systematic investigation of electron states of core–shell quantum dot is very essential.

Energy is obtained by solving time-independent Schrödinger equation, but, in many cases, because of complex geometry, it is very difficult to solve the equation using analytical method. Therefore, numerical procedure is an alternative choice for solving such problems. Several methods have already been considered by theoretical researchers e.g., variational method [19], finite-element method [20], shooting method [21] and finite-difference method [16,22]. Researchers computed ground state energy using FD technique which matches with earlier result for larger base width, but deviates for lower values [21]. Among these different methods, finite-difference technique is capable of simulating the arbitrary nanostructure profiles [22–24]. It is a very intuitive and versatile modeling technique, which allows the user to specify the material at all points within the computational domain by employing grid structures. This technique has a number of very good absorbing boundary conditions to choose from, which simulates the effect of free space beyond the boundary forever. By making sparse, structured Hamiltonian matrices, grid dimension can be made smaller than the size of the actual device. Accuracy and computational time depends heavily on the dimension of discretization. In the present paper, energy eigenvalues of core–shell (normal and inverted) quantum dots of cubic and spherical geometries are calculated using finite-difference technique. Hence, intersubband transition energies are computed for the lowest three energy sates by varying dot dimensions. In Section 2, the mathematical model for the computation is given. Results are plotted and discussed in Section 3. Finally, in Section 4, a conclusion is given.

2. Mathematical model

In this section, we present a theoretical background for the numerical solution of Schrödinger equation using finite-difference technique to obtain the energy eigenvalues in a CSQD. For this purpose, the structure is discretized into a large number of uniform grids in three dimensions. Geometry of the grid structure depends on the choice of possible coordinate system. The solution considers conduction band discontinuity and effective mass mismatch at core–shell junctions [25]. It is assumed that the wavefunction (ψ) vanishes outside the shell. Calculations for cubic and spherical geometries are shown below:

2.1. Cubic quantum dot

Let us consider the schematic structure of a cubic quantum dot as shown in Fig. 1a. The time-independent Schrödinger equation for electron wavefunction ψ in Cartesian coordinate system is given by,