Physica E 76 (2016) 203–208

Contents lists available at ScienceDirect

Physica E

journal homepage: www.elsevier.com/locate/physe

Optical properties of a semispherical quantum dot placed at the center of a cubic quantum box: Optical rectification, second and third-harmonic generations

S.A. Mohammadi [a], R. Khordad [b,*], G. Rezaei [b]

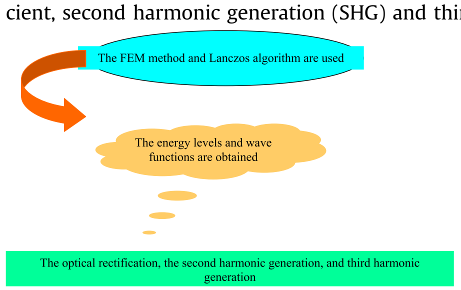
[a] Department of Mathematics, College of Sciences, Yasouj University, Yasouj, Iran
[b] Department of Physics, College of Sciences, Yasouj University, Yasouj, Iran

HIGHLIGHTS

- Optical properties of a quantum dot system are studied.
- The rectification coefficient, second and third harmonic generations is studied.
- The peak positions in optical properties change with quantum size.

GRAPHICAL ABSTRACT

We apply finite element method (FEM) and Arnoldi algorithm to obtain energy eigenvalues and eigenfuctions of a semispherical quantum dot located at the center of a cubic box. Then, the compact-density matrix approach and an iterative method are used to find the optical rectification (OR) coefficient, second harmonic generation (SHG) and third harmonic generation (THG).



ARTICLE INFO

Article history:
Received 3 August 2015
Received in revised form
11 October 2015
Accepted 13 October 2015
Available online 23 October 2015

Keywords:
Optical rectification
Second and third-harmonic generations
Quantum box

ABSTRACT

In the present paper, we first apply finite element method (FEM) and Arnoldi algorithm to obtain energy eigenvalues and eigenfuctions of a semispherical quantum dot located at the center of a cubic box. Then, the compact-density matrix approach and an iterative method are used to find the optical rectification (OR) coefficient, second harmonic generation (SHG) and third harmonic generation (THG). Numerical calculations are performed for the typical $GaAs/Ga_{1-x}Al_xAs$ system. It is found that OR coefficient has a red-shift when the semispherical radius R becomes larger. Raising R and potential height V_0, the magnitude of OR coefficient, SHG and THG are increased. Moreover, the position of resonant peaks of OR coefficient, SHG and THG are affected by the semispherical radius and potential height.

1. Introduction

In the past two decades, quantum dots (QDs) have been received considerable attention by researchers [1–3]. Quantum dots are semiconductor nanostructures with vast applications across many industries. Modern nanotechnology has allowed scientists to fabricate quantum dots with various geometrical shapes such as spherical, cubic, cylindrical, ellipsoidal, cone-like, lens-shape, and pyramidal shape [4–8]. Quantum dots confine charge carriers in three dimensions and their properties can be controlled in experiments. Almost, all parameters of QDs such as size, number of electrons, coupling between dots, as well as external parameters, like temperature, magnetic and electric field can be varied in a controlled way.

* Corresponding author.
E-mail address: khordad@mail.yu.ac.ir (R. Khordad).

http://dx.doi.org/10.1016/j.physe.2015.10.016
1386-9477/

During the past few years, the optical properties of quantum dots, in particular second and third harmonic generations or optical rectification, have attracted lots of attention in theoretical and applied physics [9–17]. The study of optical properties of QDs is important and interesting because the optical susceptibility of these structures is adjustable by changing their size and shape, the surrounding environment and the external applied fields. Also, investigation of optical properties of QDs has practical usage in novel optoelectronic devices such as QD lasers, quantum cryptography, and QD infrared photodetector.

So far, the optical properties of QDs have became subject of intensive experimental and theoretical studies in the last decade. For example, in 1999, Sauvage et al. [18] studied the third-harmonic generation in InAs/GaAs self-assembled quantum dots in both theoretical and experimental cases. Several groups have investigated QDs in a well infrared photodetectors both theoretically and experimentally [19–21]. Maikhuri et al. [22] have studied the linear and nonlinear optical properties of ZnO quantum dots embedded in SiO_2 matrix. Zeng et al. [23,24] have investigated the optical susceptibilities in singly charged ZnO colloidal QDs embedded in different dielectric matrices.

It is fully known that the key problem in the study of optical properties of QDs is to obtain the energy levels of the confined carriers. Theoretically, in order to obtain the QD energy levels, one can use the effective mass approximation. In this case, one should solve the Schrödinger equation by means of a numerical method. In some cases like simple geometrical shapes, the infinity barrier approximation is used. However, when the geometrical shape of QDs is not simple or when QDs embedded in dielectric matrices, the calculation of energy levels is a nontrivial task which requires considerable theoretical effort. So far, several theoretical approaches have been put forth for the calculation of the energy levels and wave functions of various QDs. For instance, Tablero [25] has applied a model to determine the electronic structure of self-assembled quantum arbitrarily shaped dots. Sa'ar et al. [26] proposed a local-envelope state expansion; Pescetelli et al. [27] used a tight-binding approach for T- and V-shaped quantum wires and Ammann et al. [28] used a quasi-factorization scheme. In most of these investigations the barrier encountered by the confined electrons at the surface of the dot has been assumed to be infinite.

In the present work, we intend to study the second and third harmonic generations and optical rectification of a semispherical quantum dot placed at the center of a cubic quantum box. Due to the complicated form of the structure, we have applied the finite element method (FEM) to obtain energy levels and wave functions numerically. Then, we have used analytical expressions to determine the second and third harmonic generations and optical rectification.

2. Energy levels and wave functions

In the effective mass approximation, the Hamiltonian of a charge carrier in a quantum dot is given by (see Fig. 1)

$$H_0 = -\frac{\hbar^2}{2m^*}\nabla^2 + V(x, y, z), \tag{1}$$

where m^* is the effective mass of electron and the confining potential $V(x, y, z)$ is given by

$$V(x, y, z) = \begin{cases} V_1 = 0 & Inside \\ V_2 = V_0 & Outside \end{cases}, \tag{2}$$

where V_0 is the potential height between GaAs and $Al_xGa_{1-x}As$. In the following, we briefly present our calculation procedure for finding the energy levels and wave functions of the Hamiltonian of Eq. (1).

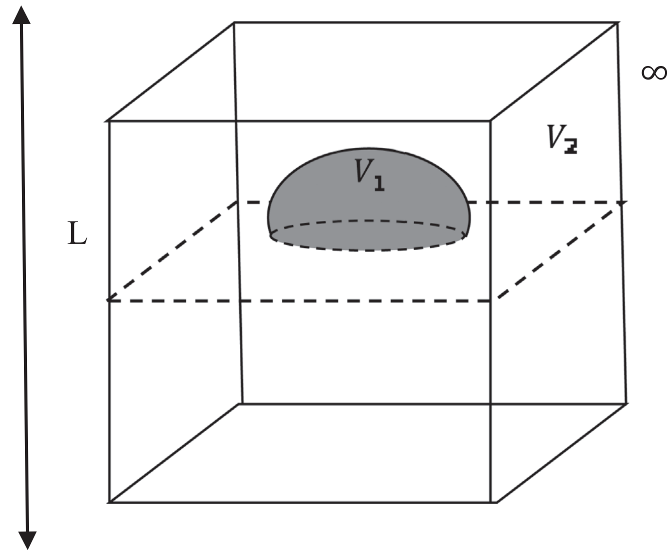


Fig. 1. Schematic diagram of a semispherical quantum dot embedded in a cubic quantum box.

Let Ω_1 be a domain occupied by the quantum dot, which is embedded in a bounded matrix Ω_2 of different material (see Fig. 1). A typical example is a GaAs semispherical quantum dot embedded in a cubic $Al_xGa_{1-x}As$ As matrix. One can write the Schrödinger equation for a charge carrier in the quantum dot as

$$\begin{cases} -\frac{\hbar^2}{2m_1}\nabla^2\psi + V_1\psi = E\psi, & (x, y, z) \in \Omega_1 \\ -\frac{\hbar^2}{2m_2}\nabla^2\psi + V_2\psi = E\psi, & (x, y, z) \in \Omega_2 \end{cases}, \tag{3}$$

where ψ is the wave function and E is the energy. It is clear that the wave function decays outside the quantum dot very rapidly, therefore, we can consider homogeneous Dirichlet conditions $\psi = 0$ on the outer boundary of Ω_2 and the Ben Daniel–Duke condition on the interface between Ω_1 and Ω_2 as

$$\frac{1}{m_1}\frac{\partial\psi}{\partial n_1}|_{\Omega_1} = \frac{1}{m_2}\frac{\partial\psi}{\partial n_2}|_{\Omega_2}, \tag{4}$$

where n_1 and n_2 are the outward unit normal on the boundary of Ω_1 and Ω_2, respectively. To solve the Schrödinger equation (3), we apply the finite element method (FEM) [29,30]. To construct an approximate solution of Eq. (3), we write the wave function ψ as

$$\psi = \sum_{j=1}^{m} c_j\varphi_j, \quad \psi(p_j) = c_j, \quad j = 1, 2, \ldots, m, \tag{5}$$

where $\{\varphi_1, \varphi_2, \ldots\}$ is the set of basis function with the following conditions:

$$\varphi_i(p_j) = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases} \quad i, j = 1, 2, \ldots, m. \tag{6}$$

Inserting Eq. (5) into Eq. (3), multiplying Eq. (3) by φ_i and integration by parts, we can obtain the generalized eigenvalue equation $KX = EMX$ where K is the stiffness matrix, M is the mass matrix and $X = [c_1, c_2, \ldots, c_m]^T$ is the eigenvector corresponding to the eigenvalue E. The elements of matrices K and M are given by