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Influence of impurity on binding energy and optical properties of lens shaped quantum dots: Finite element method and Arnoldi algorithm

R. Khordad [a,*], H. Bahramiyan [b], S.A. Mohammadi [c]

[a] *Department of Physics, College of Sciences, Yasouj University, Yasouj, 75914-353, Iran*
[b] *Department of Optics and Laser Engineering, Marvdasht Branch, Islamic Azad University, Marvdasht, Iran*
[c] *Department of Mathematics, College of Sciences, Yasouj University, Yasouj, Iran*

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A B S T R A C T

In the present work, we have studied the effects of the impurity position on the donor binding energy and optical properties of a lens shaped quantum dot with a finite confining potential. To this end, we have calculated the energy levels, wave functions and the binding energy using the finite element method and the Arnold algorithm for various impurity locations. Applying the compact density matrix and an iterative method, the refractive index changes and absorption coefficients have been determined in the presence of the impurity. Our results show that the binding energy decreases when the quantum dot height and radius increase. The absorption coefficients and refractive index changes decrease and shift toward the higher energies in the presence of the impurity. Generally, the impurity location plays an important and considerable role in the electronic and optical properties of a lens shaped quantum dot.

1. Introduction

Nanotechnology, which is one of the fastest growing research fields of the 21th century, constitutes a challenge for the modeling of physical phenomena in the range of nanometer scales. Nowadays, nanotechnology applications have entered our daily lives and its progresses have led to design and manufacturing of new types of low-dimensional semiconductor structures such as nanotubes, quantum dots (QDs), quantum wells and quantum wires [1,2].

Different kinds of low-dimensional semiconductor structures can be fabricated using chemical lithography, chemical vapor deposition, molecular beam epitaxy, and etching [3–5]. Quantum dots with various geometrical shapes are one of certain kinds of nanostructures which are manufactured using nanolithography [6–9]. In the past few years, many researchers have tried to study the electronic, optical and transport properties of QDs with particular geometrical shapes such as pyramid, lens-shape, and cone-like [10–13]. It is fully known that the properties are sensitive to external factors such as temperature, pressure, electric and magnetic fields, and impurity states. So far, many studies have been performed on electronic and optical properties of QDs under the external factors particularly in simple geometrical shapes like spherical and cylindrical QDs [14–16].

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

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We know that the impurity states have an important role in electronic and optical properties of QDs. For this reason the impurity states, which are included donors and acceptors, have been extensively investigated in theoretical and experimental procedures [17–19]. It is well-known that Bastard, for the first time, has studied the binding energy of a hydrogenic impurity in a quantum well [20]. After this study, many authors have investigated the binding energy and effect of the external factors on it for other nanostructures like quantum dots and quantum wires [21–27]. They have deduced that the nanostructure geometry and impurity position play important roles in the binding energy. For more information, the reader is referred to [14–27].

It is worth mentioning that the information about electronic and optical properties of nanostructures in the presence of impurity is of topmost importance in sciences and industries. It is fully known that investigation of optical properties of QDs has practical usage in novel optoelectronic devices such as QD lasers, quantum cryptography, and QD infrared photo detector [28–34].

In this work, we study the energy levels, binding energy and optical properties of a lens shaped quantum dot in the presence of impurity. The layout of the rest of this paper is as follows: the Hamiltonian, a brief description about the finite element method (FEM), the relevant wave functions and energy levels are described in Section 2. The analytical expressions of the optical absorption coefficients and refraction index changes are presented in Section 3. Numerical calculations and detailed discussions are given in Section 4. Finally, conclusion is presented in Section 5.

2. Theory and model

The Hamiltonian of a hydrogenic donor impurity located at the position r_0 in a lens shaped quantum dot is expressed by (see Fig. 1):

$$H = -\frac{\hbar^2}{2m^*}\nabla^2 + V(x,y,z) - \frac{e^2}{\varepsilon|r - r_0|} \tag{1}$$

Where m^2 and $V(x,y,z)$ are the electron effective mass and the confining potential, respectively. The confining potential is given by

$$V(x,y,z) = \begin{cases} 0 & \text{Inside} \quad (\Omega_1) \\ V_0 & \text{Outside} \quad (\Omega_2) \end{cases}, \tag{2}$$

where V_0 is the potential height between GaAs and $Ga_{0.5}\,In_{0.5}\,As$.

It is clear that the third term in Eq. (1) represents the coulomb interaction between electron and hydrogenic donor impurity. Up to our best knowledge, Hamiltonian (1) has not an analytical solution for the lens shaped quantum dot. Therefore, we find the energy levels and wave functions of the ground and first excited states of Hamiltonian (1) using numerical methods. We compute relevant energy states and corresponding wave functions employing the finite element method (FEM). In the following, we briefly present the used numerical method to solve the Schrödinger equation. FEM is a powerful numerical technique for finding approximate solutions of partial differential equations [35–38].

Let Ω_1 be the first domain occupied by a typical material (for example GaAs) and Ω_2 be the second domain of different material (for example $Ga_{0.5}\,In_{0.5}\,As$). The Hamiltonian of a charge carrier in the quantum dot is given by

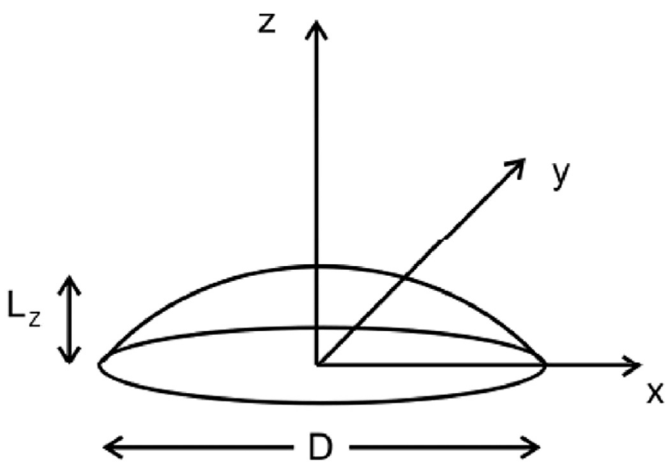

Fig. 1. Schematic diagram of lens shaped quantum dot.