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The intersubband optical properties of a two-electron quantum dot-quantum well heterostructure

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ABSTRACT

In this paper, both linear and third-order nonlinear optical properties of two-electron in a semiconductor core/shell/well/shell quantum dot (QD) heterostructure for cases with and without a hydrogenic donor impurity have been investigated in a detailed manner as depending on the structure parameters. For this purpose, first, the energy eigenvalues and corresponding wave functions of the structure have been computed as a function of the layer thicknesses by means of the self-consistent solution of the Poisson and Schrodinger equations in envelope function effective mass approximation. Second, using these energy eigenvalues and their wave functions obtained from the calculations, both linear and third-order nonlinear optical properties of the multi-shell QD (MSQD) with two-electron have been determined as a function of the photon energies and shell thicknesses. Also, all procedures mentioned above have been repeated for negatively charged donor impurity (D^-) located in the center of the same structure. Finally, obtained results have been presented comparatively for cases with and without the impurity.

1. Introduction

In the last two decades, the zero dimensional QD hetero nanostructures have attracted the most attention among the semiconductor nanostructures because of their interesting physical properties and device applications based on principles of quantum mechanics. Hence, the electronic and optical properties of QDs have been intensively examined by many authors [1–4]. Recently, some optical properties of low-dimensional semiconductors QD, such as dipol transitions [5–7], oscillator strengths [8–10], linear [11–13] and nonlinear [14–16] optical absorption coefficients, photoionization cross-sections [17], and refractive indices [18–21], have been investigated both theoretically and experimentally.

On the other hand, the application of some external perturbations on QDs, for example, electrical and/or magnetic field, hydrostatic pressure, and temperature etc. induces some important changes on their electronic and optical properties. Therefore, these effects have been studied by many researchers [22–29]. Xie [30–32] has investigated the optical properties of double electron QD with different confinement potential shapes, Gaussian and Wood-Saxon potentials, depending on confinement strength, impurity and magnetic field in the effective mass approximation by using matrix diagonalization method and compact-density matrix approach. Sahin [33] has reported the optical properties of one- and two-electron spherical QD as a function of radius, light intensity and photon energy for cases with and without a hydrogenic donor impurity. Lu et al. [34] have examined the optical absorption coefficients and refractive indices of a double electron QD using compact-density

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matrix approximation. Lu and Xie [35] have worked on an external electric field effects on optical properties of a QD with two-electron using perturbation method. In addition to these the same structure mentioned above has been investigated by Mengesha and Malnev [36], using both variation and perturbation methods to get its low energy levels and optical properties. All of these studies make serious contributions to intelligibility of the physical properties of these structures thoroughly.

In the literature, there is no reported study on the optical properties of the MSQD with double electron so far. In our previous study [37], we have reported a detailed investigation of the electronic properties of a MSQD with two-electron for cases with and without a donor impurity as a function of the core radius, shell thickness and well width. In this study, we have carried out the linear and third-order nonlinear optical properties of the same structure as a function of shell thickness and photon energy. The results have been analyzed depending on core radii and shell thicknesses, and probable reasons leading to these situations have been discussed in a detail. As a result of these analyses, in this contribution, we demonstrate that the optical properties of this structure are dependent strictly on its geometric parameters such as shell thicknesses.

2. Model and theory

In this study, we have considered a multi-shell spherical CdSe/ZnS/CdSe/ZnS quantum dot nanocrystal with two-electron. The CdSe core material with radius R_1 is coated with ZnS shell which has a wider band gap than that of the CdSe. The shell thickness is $T_s = R_2 - R_1$ and the well width is $T_w = R_3 - R_2$. The potential profile of the structure is shown in Fig. 1.

We have considered interacting two electrons in the structure. In the framework of effective mass approximation and BenDaniel–Duke boundary condition, the single particle Schrödinger equation with existing of the impurity is given as

$$\left[-\frac{\hbar^2}{2}\vec{\nabla}_r\left(\frac{1}{m_e^*(r)}\vec{\nabla}_r\right) - e\phi_{sc} - \frac{Ze^2}{\kappa(r)r} + V_e(r)\right]R_{n\ell}(r) = \varepsilon_{n\ell}R_{n\ell}(r). \tag{1}$$

Here, first term is kinetic energy term of the electron, $\hbar$ is reduced Planck constant, $m_e^*(r)$ is the position-dependent effective mass of the electron, e is the unit electronic charge, ϕ_{sc} is the self-consistent Hartree potential between the electrons, the third term is the Coulomb interaction between electron and donor impurity, Z is charge of the impurity, $V_e(r)$ is the position dependent confining potential of the electron, $\kappa(r)$ is the position dependent dielectric constant, $\varepsilon_{n\ell}$ is the single particle energy eigenvalue and $R_{n\ell}(r)$ is the radial wave function of the electron. It is noted that $Z = 1$ cases correspond to existing of the on-center impurity. In this case, the two-electron quantum structure is called as a negatively charged donor impurity (D^-). If $Z = 0$, the structure is called as a QD with two electrons.

The mathematical expression of the confining potential of the considered structure is given by

$$V_e(r) = \begin{cases} 0, & r \leqslant R_1 \quad \text{and} \quad R_2 \leqslant r \leqslant R_3 \\ V_b, & R_1 < r < R_2 \quad \text{and} \quad r > R_3 \end{cases}, \tag{2}$$

where V_b is the conduction band offset between CdSe and ZnS.

The electrostatic Coulomb potential originated from the interaction between electrons is calculated by solving of the Poisson equation. In the manner including interface polarization the Poisson equation can be expressed as

$$\vec{\nabla}\kappa(r)\vec{\nabla}\phi_{sc} = \frac{e}{\varepsilon_0}\rho_e(r), \tag{3}$$

where $\rho_e(r)$ is the electron density, and ε_0 is the dielectric permittivity of the vacuum. The electron density is determined by means of

$$\rho_e(r) = \frac{1}{4\pi}q\left|R^{elec}_{nq,\ell q}(r)\right|^2. \tag{4}$$

The details of the electronic structure calculation can be found elsewhere [37].

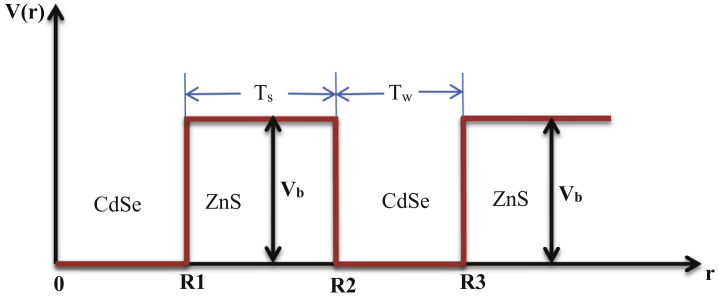

Fig. 1. The potential profile of multi-shell CdSe/ZnS quantum dot heterostructure.