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Linear and nonlinear optical absorption coefficients of two-electron spherical quantum dot with parabolic potential

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ABSTRACT

Linear and nonlinear absorption coefficients of two-electron spherical quantum dot (QD) with parabolic potential are investigated in this paper. Wave functions and energy eigenvalues of the $1s^2$, 1s1p, 1s1d and 1s1f electronic states have been computed by using an optimization approach, which is a combination of Quantum Genetic Algorithm (QGA) and Hartree–Fock Roothaan (HFR) method. It is found that the strength of S→P transition is stronger than P→D and D→F transitions. Also the peak positions and amplitudes of the absorption coefficients are sensitive to the electron spin. It should be noted that the peak positions and amplitudes of absorption coefficients are strongly dependent on the parabolic potential. Additionally, dot radius, impurity charge, incident optical intensity and relaxation time have a great influence on the linear and nonlinear absorption coefficients.

1. Introduction

In recent years, it has now become possible to fabricate low-dimensional semiconductor structures(confined quantum systems) like quantum wells, well-wires and dots due to the fast development of nanotechnology. Confined quantum systems have been one of the most important subjects of investigation. Therefore, due to their fundamental properties and their wide range of technological applications [1], a great deal of theoretical works on these structures has been reported extensively by using different methods like a finite element method [2,3], perturbation [4], density functional [5,6], configuration interaction [7,8], variational [9,10], exact solution [11], quantum genetic algorithm and Hartree–Fock Roothaan method [12] and other methods [13,14]. Understanding of the electronic and optical properties in such structures is important because these properties are strongly affected by the presence of impurity. Therefore, several researchers have investigated the various optical properties such as the linear and nonlinear absorption coefficients and the refractive index changes of one-electron QDs [15–35] and two-electron QDs [36–41] with finite and infinite confining potential surface. QDs are also called as artificial atoms because of having discrete energy levels and shell structures. The charge carriers(electrons and holes) of QDs are confined in all three-dimensions. Three-dimensional quantum confinement of these carriers leads to the formation of discrete energy levels and the change of electronic and optical properties. In a two-electron QD, Huang and Libin [36] investigated the optical absorption coefficients in a GaAs parabolic QD by using the exact diagonalization method and the compact density matrix approach. The linear and nonlinear absorption coefficients and refractive index changes in a two-electron QD with parabolic potential were calculated by using exact analytical method [37]. A detailed investigation of the linear and nonlinear optical properties in a spherical one- and two-electron QD was performed by Şahin [38]. Xie [39] calculated the linear and nonlinear absorption coefficient and the oscillator strength for two-electron QD subjected to the parabolic confinement. Very recently, Kumar et al. [40] carried out the absorption coefficients and the refractive index changes in a two-electron GaAs/$Ga_{1-x}Al_xAs$ QD with and without the inclusion of polaronic effect. Coden et al. [41] studied a detailed analysis of the electronic and optical properties of two-electron QDs and they investigated the impurity effects under a two-dimensional Gaussian confinement potential. In two-electron QD (2e-QD), all of the above mentioned theoretical studies have been performed only the optical absorption transition between the lowest energy states, which is the transition of the ground state S ($L=0$) to the first excited state P ($L=1$), L denotes the total angular momentum of electrons. Therefore, the theoretical studies related to the absorption coefficients of 2e-QD for higher states are still important, especially in transitions among higher excited electronic states ($L=2$ and 3). To our knowledge, there has been no report of the absorption coefficients including the optical transitions between higher states ($L=2$ and 3) in 2e-QD with

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parabolic potential.

In the present study we have calculated the linear and nonlinear absorption coefficients of 2e-QD with parabolic potential, assuming a spherical symmetric confining potential of infinite depth. The wave functions and energy eigenvalues of 2e-QD have been computed by using QGA and HFR methods over Slater type basis sets. The effects of parabolic potential, electron number, impurity charge, dot radius, incident photon energy and relaxation time will be investigated on the singlet and triplet linear and nonlinear absorption transitions.

2. Theory and formulations

Let us consider a 2e-QD confined by an infinite spherical potential well. Within the effective mass approximation, in atomic units (au), the nonrelativistic Hamiltonian of such a system in the presence of impurity and parabolic potential term is given by

$$H = \sum_{i=1}^{2}\left[-\frac{\nabla_i^2}{2m^*} - \frac{Z}{\varepsilon r_i} + \frac{1}{2}\gamma_p^2 r_i^2\right] + \frac{1}{\varepsilon r_{12}} + V_c(r_1, r_2), \tag{1}$$

where m^* is the effective mass of electron, ε is the electric constant of medium, Z is impurity charge, r_i is the distance to impurity of ith electron and r_{12} is the distance between electrons. $\gamma_p = \hbar\omega_0/2R_y^*$, ω_0 is the frequency of harmonic oscillator and R_y^* is the effective Rydberg constant. The term $V_c(r_1, r_2)$ is the confinement potential, and it has the form following

$$V_c(r_1, r_2) = \begin{cases} 0, & \text{if} \quad r_1 \text{ and } r_2 < R \\ \infty, & \text{if} \quad r_1 \text{ or } r_2 \geq R \end{cases}, \tag{2}$$

where R is dot radius.

According to the Pauli principle, a many-electron system's wave function must be antisymmetric according to interchange of any two electrons, and this wave function can be written as a single or linear combination of Slater determinants, which are contracted by the one electron spin orbitals, $u_\mu(q_i)$, μ denotes the quantum numbers n*l*mm$_s$. The one electron spin orbitals include the spatial function $\phi_{nlm}(\mathbf{r})$ and spin function $\sigma_{\mathbf{m_s}}(s)$, that is, $u_\mu(q_i) = \phi_{nlm}(\mathbf{r})\sigma_{\mathbf{m_s}}(s)$. Since the Hamiltonian given in Eq. (1) does not contain spin terms, the energy is unaffected by inclusion of the spin factor in the wave functions of the ground and excited states. The one-electron spatial wave function may be written as a linear combinations of the unnormalized Slater type orbitals (STOs),χ, as follows

$$\phi_j(\mathbf{r}) = \sum_{k=1}^{t} c_{jk}\chi_k(\mathbf{r}, \zeta_k), \tag{3}$$

where t is the number of basis sets.

Using the normalized wave function, the singlet energy E^S and the triplet energy E^T states of the 1s*nl* configuration of system are given by

$$E^S = I(1s) + I(nl) + J(1s, nl) + K(1s, nl) \tag{4}$$

$$E^T = I(1s) + I(nl) + J(1s, nl) - K(1s, nl) \tag{5}$$

in which nl are the arbitrary quantum numbers, $I(nl)$ is one-electron integral, $J(1s, nl)$ and $K(1s, nl)$ are the electron–electron Coulomb and Exchange energy integrals respectively. For the ground state(1s^2), these integrals are modified as $nl = 1s$ and K (1s,1s)=0. In order to compute the energies given in Eqs. (4) and (5), one should calculate one- and two-electron molecular integrals appearing in HFR approximation. For QDs, one- and two-electron integrals given in Eqs. (4) and (5) can be easily evaluated by modifying for appropriate consideration of the boundaries the expressions of atomic systems [42,43].

The nonlinear optical properties have been taken into account potentially useful for optical limiting and switching applications [44]. In QDs, intersubband optical transitions occurring by absorbing a photon between an initial state (i) and a final state (f) are called as the photoabsorption process. In order to calculate the linear, nonlinear and total absorption coefficients, we consider the interaction between the polarized electromagnetic wave (EMW) of angular frequency ω and the QD. If the wave length of the progressive EMW is larger than the dimension of QD (10^3 Å for UV light), the amplitude of EMW may be considered as a constant throughout the QD. Then the electric field of an incident wave can be expressed as

$$E(t) = 2\tilde{E}Cos(\omega t) = \tilde{E}e^{i\omega t} + \tilde{E}e^{-i\omega t}. \tag{6}$$

The electronic polarization $P(t)$ originated by the incident field $E(t)$ is expressed by

$$P(t) = \varepsilon_0\chi^{(1)}(\omega)\tilde{E}e^{i\omega t} + \varepsilon_0\chi^{(2)}(2\omega)\tilde{E}^2e^{2i\omega t} + \varepsilon_0\chi^{(3)}(3\omega)\tilde{E}^3e^{3i\omega t} + c.\,c.\,, \tag{7}$$

where terms up to the third-order in $\tilde{E}$ are retained. The linear, the second- and the third-order nonlinear optical susceptibilities are labeled by the terms $\chi^{(1)}(\omega)$, $\chi^{(2)}(2\omega)$ and $\chi^{(3)}(3\omega)$, respectively, and ε_0 is the electrical permittivity of the vacuum. Since our system is spherical symmetric, the term $\chi^{(2)}(2\omega)$ is not taken into account. The second-order susceptibility term occurs only in non centrosymmetric structures. Such structures can not produce second-order optical interactions. We considered the electric field along the z-axis.

The linear $\alpha^{(1)}(\omega)$ and nonlinear $\alpha^{(3)}(\omega, I)$ absorption coefficients in 2e-QDs are defined by [36,38,39]

$$\alpha^{(1)}(\omega) = \omega\sqrt{\frac{\mu}{\varepsilon_r}}\frac{\rho\hbar\Gamma_{fi}}{\left(E_{fi} - \hbar\omega\right)^2 + \left(\hbar\Gamma_{fi}\right)^2}\left\langle M_{fi}\right\rangle^2, \tag{9}$$

and

$$\alpha^{(3)}(\omega, I) = -\,\omega\sqrt{\frac{\mu}{\varepsilon_r}}\frac{2I\rho\hbar\Gamma_{fi}}{n_r\varepsilon_o c\left[\left(E_{fi} - \hbar\omega\right)^2 + \left(\hbar\Gamma_{fi}\right)^2\right]^2}\left\langle M_{fi}\right\rangle^4. \tag{10}$$

From here, the total absorption coefficient is given as follows

$$\alpha(\omega, I) = \alpha^1(\omega) + \alpha^3(\omega, I). \tag{11}$$

Here μ, n_r and c are the magnetic permeability, the refractive index and the speed of light in vacuum. $I = 2\varepsilon_0 n_r c\left|\tilde{E}\right|^2$ is the incident optical intensity and $\varepsilon_r = \varepsilon_0 n_r^2$ is the real part of the permittivity. $\Gamma_{fi}(f \neq i)$ is a relaxation rate of the final and initial state and $\tau_{fi} = 1/\Gamma_{fi}$, τ_{fi} is known as the relaxation time. $M_{fi} = \langle f|ez_1 + ez_2|i\rangle$ is the electric dipole moment matrix element of two electrons and $E_{fi} = E_f - E_i$ is the energy difference between i and f electronic levels. Electric dipole moment operator does not depend on the electron spin. The dipole transitions must be between energy states of different parity and these transitions are allowed only between the states with the same spin in systems with two-electron, that is, the dipole transitions are allowed between singlet-singlet and triplet-triplet energy states with different parity. In order to more realistic calculate the linear and nonlinear absorption coefficients of 2e-QD, it should be considered the electron density as $\rho = N/V_{QD}$, where N is the number of electron in QD and V_{QD} is the volume of QD.