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Influence of image charge effect on impurity-related optical absorption coefficients and refractive index changes in a spherical quantum dot

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A B S T R A C T

We have investigated the influence of an image charge effect (ICE) on the energies of the ground and first few excited states of a hydrogen-like impurity in a spherical quantum dot (QD) in the presence of an external electric field. The oscillator strengths of transitions from the 1*s*-like state to excited states of $2p_x$ and $2p_z$ symmetries are calculated as the functions of the strengths of the confinement potential and the electric field. Also, we have studied the effect of image charges on linear and third-order nonlinear optical absorption coefficients and refractive index changes (RICs). The results show that image charges lead to the decrease of energies for all the hydrogen-like states, to the significant enhancement of the oscillator strengths of transitions between the impurity states, and to comparatively large blue shifts in linear, nonlinear, and total absorption coefficients and refractive index changes. Our results indicate that the total optical characteristics can be controlled by the strength of the confinement and the electric field.

1. Introduction

In recent years, with the development of experimental techniques, theoretical and experimental studies of the electronic and optical properties of the impurities doped inside the semiconductor nanostructures have attracted much attention [1,2]. The optical properties of QDs are very important for hi-tech optoelectronic device applications in far-infrared photodetectors [3–5], lasers [6], and high-speed electro-optical modulators [7]. Impurity-doped semiconductor quantum dots (QDs) have potential in future THz applications due to the observed smaller energy separation between impurity states. Electronic and optical properties related to impurities can be changed effectively by engineering the size of the system, the position of the impurity in the structure and the strength and direction of applied fields [8,9].

Due to the dielectric contrast between a semiconductor nanostructure and its dielectric environment, the interaction between carriers and their dielectric images strongly renormalize bare single particle states. Thus, the dielectric mismatch often turns into a key factor in the understanding of the physical properties of various nanostructures [10–16]. Particularly, the effect of image charge potential on qubit dynamics in a double quantum dot system has been studied by means of a specific local-in-time non-Markovian master equation [10]. The ground-state binding energy of a hydrogenic impurity placed on the axis of a cylindrical quantum-well wire has been calculated including the effect of image charges [11]. The

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enhancement of oscillator strength of silicon QDs by image charge and excitonic electron-hole attraction has been examined theoretically using a simple effective-mass model [12]. Muljarov et al. have developed a theoretical model for the calculation of exciton binding energies in semiconductor/insulator superlattices by taking into account image potentials [13]. It has been shown that the huge value of exciton binding energies is governed by the strong increase of electron-hole interaction due to image-charge effects (ICEs) for ultrathin semiconductor layers placed in a small refractive index surrounding [14]. The effect of a Coulombic dot-lead coupling on the dynamics of a QD has been studied by taking into account the interaction between charge fluctuations on the dot and the dynamically generated image charge in the leads [15]. The ICEs are properly taken into account in the calculations of electronic states in strained cleaved-edge-overgrowth quantum wires and QDs [16]. The effect of the electron-phonon interaction on the exciton states [17,18] as well as impurity-bound states have been investigated in a spherical QD embedded in a nonpolar matrix by taking into account the image charge potential [19,20]. Recently, we have investigated impurity-related electronic states and oscillator strengths for the transitions between these states in quantum dots in the presence of an electric field by taking into account both polaron and image charge effects [21–23].

The study of the linear and nonlinear optical properties of QDs such as optical absorption and refractive index changes (RICs) have attracted considerable attention from many scientists both experimentally and theoretically [24–38]. In Ref. [38] a study of the off-center impurity energy spectrum as well as linear optical absorption coefficient of the spherical QD has been performed within a rectangular potential well model by taking into account the polarization charges at the boundary.

In this article, we present a study of the effect of image charges on impurity-related optical properties in a spherical QD with parabolic confinement in the presence of an electric field. The parabolic confinement is more appropriate when the QDs are fabricated by the etching process on a quantum well, by ion implantation or by the application of electrostatic gates [39]. To the best of our knowledge, this is the first study devoted to the effect of image charges on linear and nonlinear optical absorption coefficients and RICs in the presence of an external electric field.

2. Theory

The Hamiltonian of the system can be written as

$$H = -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega_0^2 r^2 + |e|Frcos\theta + V_c(r), \tag{1}$$

where m is the electron effective band mass, ω_0 is the parabolic confinement strength and can be chosen as $\omega_0 = \hbar/(2mR^2)$, R is the nominal value of the dot radius, F is the intensity of the electric field, and θ is the angle between $\mathbf{r}$ and $\mathbf{F}$. $V_c(r)$ is the electrostatic energy for the electron inside the quantum dot interacting with impurity and image charges arising due to the difference in dielectric constants inside and outside the dot [19,40]:

$$V_c(r) = -\frac{e^2}{\varepsilon_\infty|\mathbf{r}-\mathbf{r_i}|} + \sum_{j=0}^{\infty}\left(\frac{1}{\varepsilon_d}-\frac{1}{\varepsilon_\infty}\right)\frac{\varepsilon_d(j+1)}{\varepsilon_\infty j+\varepsilon_d(j+1)}\left(\frac{r}{R}\right)^{2j}\frac{e^2}{2R} - \sum_{j=0}^{\infty}\left(\frac{1}{\varepsilon_d}-\frac{1}{\varepsilon_\infty}\right)\frac{\varepsilon_d(j+1)}{\varepsilon_\infty j+\varepsilon_d(j+1)}\frac{e^2}{R}\left(\frac{rr_i}{R^2}\right)^j P_j(cos\vartheta), \tag{2}$$

where ε_∞ is the high-frequency dielectric constant, ε_d is the dielectric constant of the embedding medium, $\mathbf{r_i} = (r_i, \theta_i, \varphi_i)$ is the radius-vector of the impurity, $P_j(x)$ is a Legendre polynomial, ϑ is the angle between $\mathbf{r}$ and $\mathbf{r_i}$. The first term in Eq. (3) is conditioned by the electron interaction with the impurity; the second and the third terms describe the electron interaction with its image charges and with impurity image charges, respectively. In particular, the electron interaction energy with the image charges of the hydrogen-like impurity located in the center of the spherical quantum dot is given by $-(e^2/\varepsilon_d R)(1-\varepsilon_d/\varepsilon_\infty)$. Depending on the ratio $\varepsilon_d/\varepsilon_\infty$, this term has attractive or repulsive character.

The wave function $\phi_0(r,\theta)$ and the energy E_0 of the ground state in the absence of the impurity are given by Ref. [41]

$$\phi_0(r,\theta) = \left(\frac{m\omega_0}{\pi\hbar}\right)^{\frac{3}{4}} \exp\left\{-\frac{m\omega_0}{2\hbar}\left[r^2 + 2\frac{eFr}{m\omega_0^2}\cos\theta + \left(\frac{eF}{m\omega_0^2}\right)^2\right]\right\}, E_0 = \frac{3}{2}\hbar\omega_0 - \frac{e^2F^2}{2m\omega_0^2}. \tag{3}$$

The variational envelope wave functions $\psi_{nl}(r,\theta,\varphi)$ associated with a different impurity ground and excited states in the QD can be labeled for convenience by their bulk hydrogenic limits, namely, $1s$, $2s$, $2p_x$, etc., and taken as the product of the electron ground state wave function ϕ_0 in the dot without impurity, and the hydrogen-like wave functions Γ_{nl} that correspond to different impurity ground and excited (nl) states, i.e. [42–44],

$$\psi_{nl}(r,\theta,\varphi) = N_{nl}\phi_0(r,\theta)\Gamma_{nl}(r,\theta,\varphi\{\lambda_{nl}\}), \tag{4}$$

where N_{nl} are the normalization constants and