Physica E 75 (2016) 174–180

Contents lists available at ScienceDirect

Physica E

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

Influence of the image charge effect on the hydrogen-like impurity-bound polaron in a spherical quantum dot in the presence of an electric field

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HIGHLIGHTS

- Image charges reduce the binding energies of 1s-, 2s-like states.
- Image charges don't allow the occurrence of 2p-like bound states.
- Phonon contribution in ground energy is 36.9% at $F = 5\mathrm{kV/cm}$, $\hbar\omega_0 = 5\mathrm{meV}$.

ARTICLE INFO

Article history:
Received 21 July 2015
Received in revised form
5 September 2015
Accepted 15 September 2015
Available online 16 September 2015

Keywords:
Quantum dot
Hydrogen-like impurity
Polaron
Image charge effect
Electric field

ABSTRACT

We have investigated the influence of an external electric field on the binding energies and polaronic shifts of the ground and some first few excited states of a hydrogenic impurity in a spherical quantum dot by taking into account the image charge effect. By using Landau–Pekar variational method the general analytical expression is obtained for the impurity bound-polaron energies. It has been numerically identified the conditions (electric field, nominal radius of quantum dot, etc.) in which the bound-polaron states can be existence in GaAs quantum dot. We have shown that the polaronic shifts in the binding energy of 1s-like state are the same in cases with and without image charge effect while they for 2s-like state are not coincide and have different monotonic behavior versus confinement potential. Electron–phonon interaction lifts the degeneracy of the 2px-, 2py-, and 2pz-like states of a donor impurity and reduces their binding energies.

1. Introduction

The rapid advances in nanotechnology have allowed controlling the electronic, optical and magnetic phenomena in quantum dot (QD) systems through the modern grown and fabrication techniques. To develop novel nano-devices, e.g., light emitting diodes [1], single photon sources [2–4], solar cells [5] and infrared photodetectors [6–8], understanding of the carrier–phonon interaction, and the effects of the applied electric and magnetic fields on physical properties of low-dimensional semiconductor structures is prerequisite. The measurements of the optical (magneto-photoluminescence [9], resonant photoluminescence [10] and photoluminescence excitation [11]) spectra of self-assembled InAs/GaAs QDs reveal a remarkably high probability of phonon assisted transitions.

The electronic energy states and therefore the electrical, optical and transport properties of QDs are affected drastically by the presence of impurities. Therefore the understanding of impurity effects in QDs is one of the most important problems in semiconductor nanophysics because the presence of impurities can alter dramatically the performance of quantum devices. The application of an electric or magnetic fields can provide much valuable information about the confined hydrogen atoms. Recently, within the quasi-one-dimensional effective potential model and effective mass approximation, there have been calculated the ground and the first 9 excited-state binding energies (BEs) of a hydrogen-like donor impurity in a rectangular QD in the presence of electric field [12]. A detailed variational calculation of the BEs of hydrogenic impurities in a cubic [13] and in a rectangular parallelepiped-shaped quantum dot [14] as a function of both the impurity position and an applied electric field has also been carried out. The BE of an on-center and off-center shallow hydrogen-like impurity in a spherical semiconductor QD with a parabolic confinement as a function of the radius and the intensity of an applied electric

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http://dx.doi.org/10.1016/j.physe.2015.09.021
1386-9477/

field have been investigated by the variational method [15,16] and the nondegenerate and degenerate perturbation approach [17,18].

Since QD's are usually manufactured from polar materials, the electron–LO phonon interaction must be taken into account for reliable description. Longitudinal optical and transverse optical phonons confined in QDs and interface-optical phonons localized in the vicinity of QD/matrix and wetting layer/matrix interfaces were observed by means of Raman spectroscopy in asymmetric GaAs/InAs/AlAs QD structures [19]. Analogous Raman spectra reveal the InAs-like LO phonon response related to the InGaAs/GaAs QD structures [20]. There have recently been carried out a considerable number of theoretical studies on electron–phonon effect on impurity energies in QDs in the presence of external fields (see Refs. [21–28] and references therein). We have theoretically investigated the influence of electric and magnetic fields as well as electron-polar optical phonon interaction on an electron bound to a Coulomb impurity in a cylindrical QD [21–23]. It has been analyzed the interplay between the confinement effects due to applied fields, quantum-size confinements, and the electron–phonon coupling on the impurity BE. The BE of the hydrogen-like impurity state in a spherical QD under an external electric field has been calculated by taking into account the interactions of an electron with both the confined longitudinal optical phonons and the surface optical phonons [24]. Kumar et al. [25] have investigated the effect of longitudinal optical phonon field on the ground state and low lying-excited state energies of a hydrogen-like impurity in a $Zn_{1-x}Cd_xSe/ZnSe$ strained QD for various Cd content using the Aldrich–Bajaj effective potential. The ground state of bound polaron in a weakly prolate ellipsoidal QD in the presence of an external electric field has been investigated by Shi and Yan [26] within the effective-mass approximation by using a variational method in the framework of perturbation theory. They have also studied the effects of electric field and size on the electron–phonon interaction with an on-center impurity in a $Zn_{1-x}Cd_xSe/ZnSe$ spherical QD, taking into account the interactions with confined, half-space and surface optical phonons [27,28].

The electronic states in nanostructures can be significantly changed because of image charges which arise due to the mismatch of the dielectric constant at the surface. Therefore, they are a relevant issue in the study of electrostatic interactions in low-dimensional systems [29–34]. To our knowledge, there has been no report of the image charge effect (ICE) on the ground and first few excited-state binding energies of a hydrogen-like donor impurity in a spherical quantum dot in the presence of an electric field. The theoretical description of the behavior of a hydrogen-like polaronic states in a QD in the presence of an electric field will lead to a better understanding of the properties of a spherical QD systems. This is the subject of this paper. We follow a variational approach in the effective mass approximation and assume the impurity to be located on the center of the QD.

2. Theory

For our theoretical modeling, the quantum dot is assumed to have a spherical form and is made of a polar semiconductor materials (specified by the static and high frequency dielectric constants ε_0 and ε_∞) embedded in a matrix with a dielectric constant ε_d. In the presence of an electric field, $\boldsymbol{F}$, the basic Hamiltonian for the single conduction-band electron coupled to an on-center located donor impurity and interacting with the LO-phonon field can be written within the effective-mass approximation as

$$H = H_e + H_{ph} + H_{int}. \tag{1}$$

The first term is the electronic Hamiltonian which in spherical coordinates is given by.

$$H_e = -\frac{\hbar^2}{2m^*}\nabla^2 + \frac{1}{2}m^*\omega_0^2 r^2 + |e|Fr\cos\theta + V_c(r) \tag{2}$$

where m^* is the electronic effective mass in the QD, F is the intensity of the electric field applied along the z-direction, ω_0 is the parabolic confinement strength and can be chosen as $\omega_0 = \hbar/2m^*R^2$, R is the nominal value of the dot radius. $V_c(r)$ is the electrostatic potential energy for the electron motion inside the sphere and is given by [35,30]

$$V_c(r) = -\frac{e^2}{\varepsilon_\infty r} + \sum_{l=0}^{\infty}\alpha_l\left(\frac{r}{R}\right)^{2l}\frac{e^2}{2R}, \tag{3}$$

where

$$\alpha_l = \left(\frac{1}{\varepsilon_d} - \frac{1}{\varepsilon_\infty}\right)\frac{\varepsilon_d(l+1)}{\varepsilon_\infty l + \varepsilon_d(l+1)}. \tag{4}$$

The first term in Eq. (3) is the screened Coulomb potential; the second describes a weak electric field directed to the center of the dot. The last term in Eq. (3) constitutes the image charge potential arising in the QD due to the difference in dielectric constants inside and outside the dot.

The phonon Hamiltonian H_{ph} in Eq. (1) is written as [36–38]

$$H_{ph} = \sum_{s,\sigma}\hbar\omega_{s\sigma}a_{s\sigma}^+a_{s\sigma}, \tag{5}$$

where $\sigma = 1$ and $\sigma = 2$ denote the bulk-type and the interface-type optical phonon modes, respectively. The index s is given by $n = 1, 2, \cdots,\ l = 0, 1, 2, \cdots,\ m = 0, \pm 1, \pm 2, \cdots, \pm l$ for the bulk-type phonon and $l = 1, 2, \cdots,\ m = 0, \pm 1, \pm 2, \cdots, \pm l$ for the interface-type phonon. $a_{s\sigma}^+(a_{s\sigma})$ is the creation (annihilation) operator of the $(s\sigma)$ phonon mode. The energy for the bulk-type LO phonon is equal to the bulk LO phonon energy $\hbar\omega_{LO}$, being independent of the index s. The interface phonon energy is given by

$$\hbar\omega_{s2} = \left[\frac{\varepsilon_d + (\varepsilon_d + \varepsilon_0)l}{\varepsilon_d + (\varepsilon_d + \varepsilon_\infty)l}\right]^{1/2}\hbar\omega_{TO} \tag{6}$$

where ω_{TO} is the transverse optical phonon frequency related to ω_{LO} by well-known Lyddane–Sachs–Teller relation $\omega_{LO}^2/\omega_{TO}^2 = \varepsilon_0/\varepsilon_\infty$.

The electron–phonon interaction Hamiltonian H_{int} in Eq. (1) depends on the coordinates of both impurity and electron, reflecting the fact that both of them, being charged, interact with phonons. By means of Platzman's canonical transformation [39], we can eliminate the contribution to the total electron energy from the impurity–LO-phonon interaction. As a result, the Hamiltonian of the system now takes the form [30]

$$H = H_e + H_x + H_{ph} - \sum_{s,\sigma}V_{s\sigma}\left[S_{s\sigma}(r,\theta,\varphi)a_{s\sigma} + S_{s\sigma}^*(r,\theta,\varphi)a_{s\sigma}^+\right], \tag{7}$$

where

$$H_x = \left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right)\frac{e^2}{r}\left(1 - \frac{r}{R}\right), \tag{8}$$

$$S_{s1}(r,\theta,\varphi) = \begin{cases} j_l(\mu_{nl}r)Y_{lm}(\theta,\varphi) & (r \le R), \\ 0 & (r > R), \end{cases} \tag{9}$$

$$S_{s2}(r,\theta,\varphi) = \begin{cases} (r/R)^l\, Y_{lm}(\theta,\varphi) & (r \le R), \\ (R/r)^{l+1}\, Y_{lm}(\theta,\varphi) & (r > R), \end{cases} \tag{10}$$

$$V_{s1}(r) = \left(\frac{4\pi e^2\hbar\omega_{LO}}{\mu_{nl}^2 j_{l+1}^2(\mu_{nl})R}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right)\right)^{1/2}, \tag{11}$$