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Hydrogenic impurity bound polaron in a cylindrical quantum dot in an electric field

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Abstract

The influence of electric field on the ground-state energy of a polaron, bound to a hydrogenic impurity in a cylindrical quantum dot is investigated. The results illustrate the competing effects of the quantum confinement, the electric-field confinement, and the Coulomb interaction.

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Keywords: Quantum dot; Electric field; Bound polaron

1. Introduction

The rapid developments in the field of semiconductor nanotechnology and the potential device application in recent years have attracted great attention to quantum dot (QD) systems. To develop novel devices, e.g., flash memories, tunneling-injection quantum dot lasers and optical detector structures, understanding of the carrier-phonon interaction [1], and the effects of the applied electric field on physical properties of low-dimensional semiconductor structures [2] is a prerequisite. Recent measurements [3–7] of the optical (photoluminescence, magneto-photoluminescence, resonant photoluminescence and photoluminescence excitation) spectra of self-assembled InAs/GaAs quantum dots reveal a remarkably high probability of phonon-assisted transitions. The application of an electric field in the heterostructure growth direction raises the polarization of the carrier distribution and the energy shift of the quantum states [8–12]. Such effects introduce considerable changes in the transition energy spectrum of carriers, which may be used to control and modulate the intensity output of optoelectronic devices.

The polaronic effect has become the main subject in these studies because the electron–phonon interaction is enhanced by the geometric confinement, which makes the polaronic effects obvious [13]. Therefore, one of the recent interests in the area of quantum dots has been to explore the electron–phonon interaction effects on the energies of electron states. A number of authors [14–25] have investigated in this connection the ground and some excited state polaronic properties of several semiconductor quantum dots.

A number of studies have focused on the influence of electron–phonon interactions on the impurity properties in a QD [26–33]. Xie and Chen have investigated the phonon contribution to the binding energy (BE) of the on-center and off-center impurities in a spherical quantum dot [26]. The binding energy and dipole moment of a hydrogenic impurity confined in a quantum dot with the shape of spherical cap are calculated by Yuan et al. [27]. Recently, Charrour et al. [28,29], and Wang et al. [30] calculated the influence of the coupling between the electron and ion with the confined LO, top-surface and side-surface phonon modes on the binding energy of an on-centre donor impurity in a cylindrical QD embedded in a dielectric matrix. The adiabatic variational method was used to calculate the bound polaron and the so-called donor-like exciton bind-

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ing energy shift in nanocrystals [31,32]. The influence of the electron–phonon coupling on the properties of a negatively charged donor center confined in a semiconductor spherical quantum dot embedded in a glass matrix was studied by Szafran et al. [33].

Polaronic effect becomes more pronounced also in the presence of external electric and magnetic fields. A lot of work has been devoted to the study of magnetic field effects in QDs [34–39]. Chen et al. [34] have studied the thickness dependence of the binding energy of an impurity bound polaron in a parabolic QD in presence of a magnetic field by the second-order perturbation theory. Resonant shallow donor magnetopolaron effect in a GaAs/AlGaAs quantum dot in high magnetic fields is investigated by variational treatment by Zhu et al. [35]. Using an exact numerical diagonalization scheme, the low-lying spectrum of a magnetopolaron quantum dot with a confined parabolic potential in the presence of a Coulomb impurity have been studied by Lee et al. [36]. Kandemir et al. [37] have calculated the polaronic effects for an electron confined in an anisotropic QD in presence of magnetic field. A unitary transformation scheme to diagonalize the Frölich Hamiltonian describing an impurity magnetopolaron confined in 3D parabolic QD potential has developed in [38]. The polaronic correction to the ground-state energy of an electron confined in a cylindrical quantum dot (CQD) subject to electric and magnetic fields along the growth axis has been investigated by Wang et al. [39].

To the best of our knowledge, the impurity bound electronic states in QD has not been considered in presence of both—applied electric field and electron-LO phonon (ELOP) coupling. In this Letter, we consider this problem for the semiconductor QD embedded in a dielectric medium, assuming an infinite-confinement potential. Binding energy and polaronic shift calculations were performed as function of the impurity positions, the electric field and the QD sizes. The results illustrate the competing effects of the spatial confinement, the confinement effects due to applied electric field and the electron coupling with the polar-optical phonon. The variational procedure [40] in the framework of adiabatic approximation has been used. This Letter is organized as follows: in Section 2 we present the theoretical model with calculations of the hydrogenic impurity ground-state binding energy and its polaronic shift. In Section 3 the numerical results for the ground-state binding energy of an impurity and polaronic correction to this state are analyzed. In Section 4, we present our conclusions.

2. Theory

For our theoretical modeling, the quantum dot is assumed to have a cylindrical form and is made of a polar semiconductor materials surrounded by another kind of polar crystal. In the presence of an electric field $\vec{F}$ applied in the axial direction, the basic Hamiltonian for the single conduction-band electron coupled to a hydrogenic impurity and interacting with the LO-phonon field can be written within the effective-mass approximation as

$$H = H_{\mathrm{e}} + H_{\mathrm{ph}} + H_{\mathrm{e\text{–}ph}}. \tag{1}$$

The first term is the electronic Hamiltonian given by

$$H_{\mathrm{el}} = -\frac{\hbar^2}{2m}\nabla^2 + V(\rho, z) + |e|Fz - \frac{e^2}{\varepsilon_0\sqrt{(\vec{\rho}-\vec{\rho}_i)^2 + (z-z_i)^2}}, \tag{2}$$

where m is the effective mass of the electron, F is the value of the electric field applied along the z axis, $(\vec{\rho}, z)$ and $(\vec{\rho}_i, z_i)$ are the electron and impurity position vectors, respectively. ε_0 is the static dielectric constant. The confining potential has the form:

$$V(\rho, z) = \begin{cases} 0, & \rho < R, \text{ and } |z| < d/2, \\ \infty, & \rho \geqslant R, \text{ or } |z| \geqslant d/2, \end{cases} \tag{3}$$

where R and d are the cylindrical dot radius and length, respectively.

The second term is the phonon Hamiltonian

$$H_{\mathrm{ph}} = \sum_{\vec{q}} \hbar\omega_{\mathrm{LO}} a_{\vec{q}}^{+} a_{\vec{q}}, \tag{4}$$

where $a_{\vec{q}}^{+}$ $(a_{\vec{q}})$ is the creation (annihilation) operator of the longitudinal optical bulk phonon with wave vector $\vec{q}$ and frequency ω_{LO}.

The third term is the electron phonon interaction Hamiltonian

$$H_{\mathrm{el\text{–}ph}} = \sum_{\vec{q}} \bigl(V_{\vec{q}} \exp(i\vec{q}\vec{r}) a_{\vec{q}} + V_{\vec{q}}^{*} \exp(-i\vec{q}\vec{r}) a_{\vec{q}}^{+}\bigr), \tag{5}$$

where

$$V_{\vec{q}} = -\frac{i\hbar\omega_{\mathrm{LO}}}{q}\left(\frac{4\pi\alpha}{\Omega}\right)^{1/2}\left(\frac{\hbar}{2m\omega_{\mathrm{LO}}}\right)^{1/4}, \tag{6}$$

with

$$\alpha = \left(\frac{e^2}{2\hbar\omega_{\mathrm{LO}}}\right)\left(\frac{2m\omega_{\mathrm{LO}}}{\hbar}\right)^{1/2}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right). \tag{7}$$

In order to calculate the ground-state energy of the hydrogenic impurity in a quantum dot with an applied electric field the trial wave function can be written as

$$\Phi(\vec{r}, \lambda) = \Phi_0(\vec{\rho}, z) \exp\bigl[-\lambda\sqrt{(\vec{\rho}-\vec{\rho}_i)^2 + (z-z_i)^2}\bigr], \tag{8}$$

where $\exp[-\lambda\sqrt{(\vec{\rho}-\vec{\rho}_i)^2 + (z-z_i)^2}]$ is the hydrogenic variational wave function with parameter λ, and $\Phi_0(\vec{\rho}, z)$ is the ground-state eigenfunction of the Hamiltonian (2) when the hydrogenic impurity is absent. The function $\Phi_0(\vec{\rho}, z)$ is given by [9]

$$\Phi_0(\vec{\rho}, z) = \begin{cases} J_0(\eta) Z(\zeta), & \rho < R, \text{ and } |z| < d/2, \\ 0 & \rho \geqslant R, \text{ or } |z| \geqslant d/2, \end{cases} \tag{9}$$

where $J_0(\eta)$ is the ordinary Bessel function of order zero, and $Z(\zeta)$ is a linear combination of Airy functions:

$$Z(\zeta) = Bi(+)Ai(\zeta) - Ai(+)Bi(\zeta). \tag{10}$$

The arguments of the Bessel and Airy functions are

$$\eta = \kappa_{10}\rho/R \tag{11}$$

and

$$\zeta = a_c \frac{z}{d} - \frac{E_0 - (\kappa_{10} a^*/R)^2}{\omega_c}, \tag{12}$$

where κ_{10} is the first zero of the Bessel function, $\omega_c = (|e|Fa_B^*/Ry^*)^{2/3}$ and $a_c = (\omega_c)^{1/2} d/a_B^*$. a_B^* is the effective Bohr radius and Ry^* is the effective Rydberg energy. In Eq. (10)

$$Ai(\pm)\big[Bi(\pm)\big] = Ai[Bi]\left(\pm a_c/2 - \frac{E_0 - (\kappa_{10} a^*/R)^2}{\omega_c}\right), \tag{13}$$

and E_0 is the dimensionless eigenvalue of Hamiltonian (2) without hydrogenic impurity. It is obtained as the first root of the transcendental equation:

$$Bi(+)Ai(-) - Ai(+)Bi(-) = 0. \tag{14}$$

The expectation value of the energy of the Hamiltonian H_{el} is given by

$$E(\lambda) = \big\langle \Phi(\vec{r},\lambda) \big| H_{\mathrm{el}} \big| \Phi(\vec{r},\lambda) \big\rangle / \big\langle \Phi(\vec{r},\lambda) \big| \Phi(\vec{r},\lambda) \big\rangle. \tag{15}$$

The binding energy $E_b(x_i, y_i)$ for the impurity is defined as the ground-state energy of the system without Coulomb interaction, minus the ground-state energy in the presence of electron-hydrogenic impurity interaction

$$E_b(x_i, y_i) = E(\lambda = 0) - E(\lambda_0), \tag{16}$$

where λ_0 is the value of λ, which minimizes $E(\lambda)$. Expression for $E(\lambda)$ in a closed form is presented in [9].

In the framework of the adiabatic approximation we can write the total wave function of the electron–phonon system as the product of an electronic wave function $\Phi(\vec{\rho}, z)$ and a phonon part.

$$|\Psi\rangle = \Phi(\vec{\rho}, z) U |0\rangle, \tag{17}$$

where $|0\rangle$ is the vacuum state for phonons. This implies that the phonon field experiences a static distribution of electronic charge and there is no correlation between the instantaneous position of the electron and the induced polarization field. In QDs this situation can be realized in the following cases: (i) when the radius of the QD is small so that the quantum confinement increases the electron speed (ii) when the electron–phonon interaction is so strong that electron self-localization occurs, i.e., fast electron oscillations; (iii) when the electron-impurity interaction is so strong that the electron becomes localized around the impurity [30,31].

The unitary displacement transformation operator is given by

$$U = \exp\left(\sum_{\vec{q}} \big(f_{\vec{q}} a_{\vec{q}}^{+} - f_{\vec{q}}^{*} a_{\vec{q}}\big)\right). \tag{18}$$

The function $f_{\vec{q}}$ and the parameter λ are determined by minimizing the expected value of the Hamiltonian, $E_{\mathrm{el-ph}}(f_{\vec{q}}, \lambda) = \langle \Psi | H | \Psi \rangle / \langle \Psi | \Psi \rangle$. The following relations hold for the transformations:

$$U^{-1} a_{\vec{q}} U = a_{\vec{q}} + f_{\vec{q}} \quad \text{and} \quad U^{-1} a_{\vec{q}}^{+} U = a_{\vec{q}}^{+} + f_{\vec{q}}^{*}. \tag{19}$$

Then we obtain the expected value of the transformed Hamiltonian of the system

$$\begin{aligned} &E_{\mathrm{el-ph}}(f_{\vec{q}}, \lambda) \\ &\quad = E(\lambda) + \sum_{\vec{q}} \hbar\omega_{\mathrm{LO}} |f_{\vec{q}}|^2 \\ &\qquad + \sum_{\vec{q}} V_{\vec{q}} \frac{\langle \Phi(\vec{r},\lambda) | \exp(i\vec{q}\vec{r}) | \Phi(\vec{r},\lambda) \rangle}{\langle \Phi(\vec{r},\lambda) | \Phi(\vec{r},\lambda) \rangle} f_{\vec{q}} \\ &\qquad + \sum_{\vec{q}} V_{\vec{q}}^{*} \frac{\langle \Phi(\vec{r},\lambda) | \exp(-i\vec{q}\vec{r}) | \Phi(\vec{r},\lambda) \rangle}{\langle \Phi(\vec{r},\lambda) | \Phi(\vec{r},\lambda) \rangle} f_{\vec{q}}^{*}. \end{aligned} \tag{20}$$

From the variation condition

$$\frac{\delta E_{\mathrm{e-ph}}(f_{\vec{q}}, \lambda)}{\delta f_{\vec{q}}} = 0, \tag{21}$$

we obtain

$$f_{\vec{q}} = -\frac{V_{\vec{q}}^{*}}{\hbar\omega_{\mathrm{LO}}} \frac{\langle \Phi(\vec{r},\lambda) | \exp(-i\vec{q}\vec{r}) | \Phi(\vec{r},\lambda) \rangle}{\langle \Phi(\vec{r},\lambda) | \Phi(\vec{r},\lambda) \rangle}. \tag{22}$$

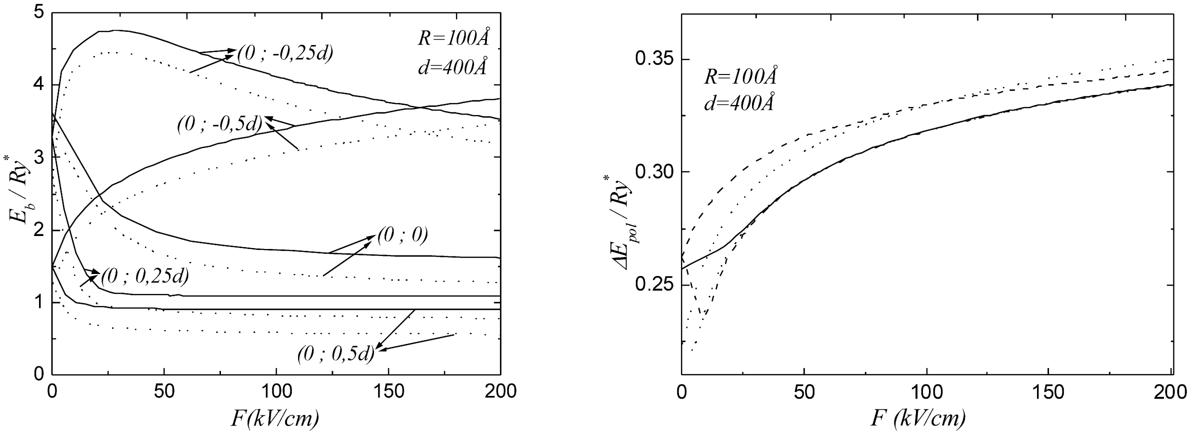
Substituting Eq. (22) into Eq. (20), the bound electron's ground state energy in a quantum dot with an applied electric field in the presence of electron–LO phonon interaction is obtained as

$$\begin{aligned} &E_{\mathrm{el-ph}}(\lambda) \\ &\quad = E(\lambda) - \sum_{\vec{q}} \frac{|V_{\vec{q}}|^2}{\hbar\omega_{\mathrm{LO}}} \left| \frac{\langle \Phi(\vec{r},\lambda) | \exp(-i\vec{q}\vec{r}) | \Phi(\vec{r},\lambda) \rangle}{\langle \Phi(\vec{r},\lambda) | \Phi(\vec{r},\lambda) \rangle} \right|^2. \end{aligned} \tag{23}$$

3. Numerical results and discussion

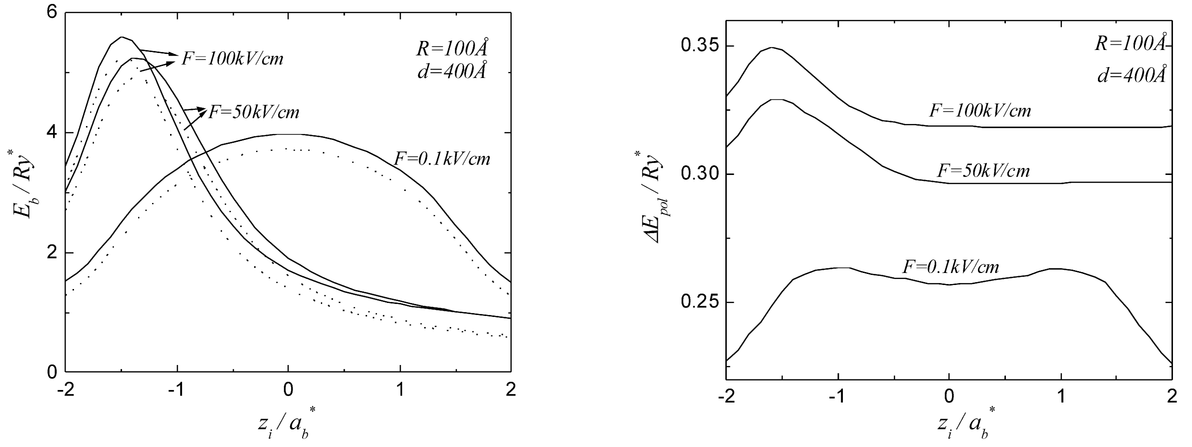
To calculate the bound polaron energy spectrum in CQD with electric field, we carry out numerical integration in Eq. (23). In the calculations we use the following parameter values for GaAs [41]: $\varepsilon_0 = 12.83$, $\varepsilon_\infty = 10.9$, $\hbar\omega_{\mathrm{LO}} = 36.7$ meV, and electron–phonon coupling strength $\alpha = 0.0681$.

The aim of our numerical calculations is to clarify the role of effective confinement on the polaronic shifts of BE. The electron effective confinement is a result of competing action of three effects: (i) spatial quantum confinement, (ii) electron-impurity Coulomb interaction, and (iii) electric-field confinement. To see the effect of Stark confinement, we show in Fig. 1 the variation of the ground-state BE of a hydrogenic impurity (a), and the polaronic shifts of the BE due to ELOP interaction (b) as a function of the electric field, at various symmetric positions of an impurity on CQD axis. Solid lines in Fig. 1(a) correspond to the impurity binding energy with ELOP interaction. For comparison, in this figure we also show the results obtained by Duque et al. [9] without ELOP interaction (dotted lines). Note that for on-center impurity the BE shift increases with field intensity, whereas BE decreases. This is caused by the effective confinement, which in spite of the electron-impurity Coulomb interaction strength decrease increases due to the Stark confinement strengthening. Both the Stark confinement and the Coulomb interaction between the electron and the hydrogenic impurity increase, with the increase of the electric field for



(a) (b)

Fig. 1. Reduced binding energy E_b/Ry^* (a) with (solid lines) and without (dotted lines) ELOP interaction, and reduced polaronic shifts of binding energy $\Delta E_{\text{pol}}/Ry^*$ (b) as a function of the electric field for different impurity positions.



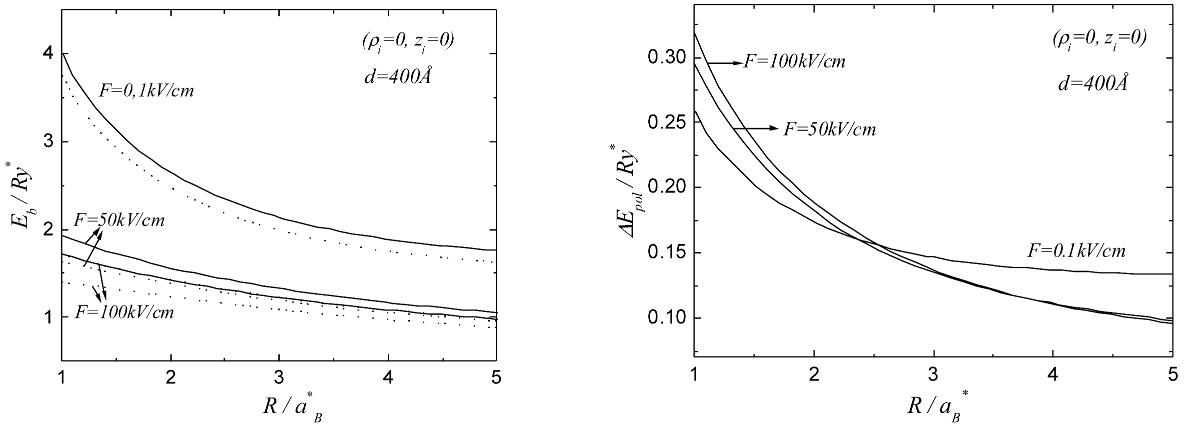
(a) (b)

Fig. 2. Reduced binding energy (a) with (solid lines) and without (dotted lines) ELOP interaction, and reduced polaronic shifts of binding energy (b) as a function of the impurity position along the CQD axis at different values of electric field.

impurity positions $(0; -0.25d)$ and $(0; -0.5d)$, as the electric field forces the electron to approach the impurity. As a consequence, the curves of BE shift in this case are placed higher than the curves with $(0; 0)$ position of impurity. Note that the curves of BE shift cross at $F = 100$ kV/cm, for impurities at $(0; -0.25d)$ and $(0; -0.5d)$. It means that for larger electric fields the electron is closer to the impurity position $(0; -0.5d)$. The BE shift ΔE_{pol} as a function of electric field has a minima. The presence of minima can be explained, taking into account that with the increase of electric field, the Coulomb interaction weakens as the field removes electron from impurity, and then the effective confinement increases because of the electron confinement increase in the electric field. The merging of the BE shift curves, for positions of an impurity $(0; 0)$, $(0; 0.25d)$ and $(0; 0.5d)$, at large values of an electric field, testifies that the effective confinement basically is determined by the electric field. For CQD with $d = 4a_B^*$ and $R = a_B^*$, the contribution of ELOP interaction to BE for $z_i = 0.25d$ ($z_i = 0.5d$) is about 7.8% (15%) for $F = 0$, and increases to about 29.5% (37.5%) as electric field increases to $F = 200$ kV/cm, while in the situation in which the impurity is located at $z_i = -0.25d$ ($z_i = -0.5d$), the contribution changes from 7.8% (13%) to 9.7% (9%). These results show that the electric field leads to a significant increase in the polaronic correction to the ground state binding energy in QD.

In Fig. 2 we display the BE and BE shift as a function of an impurity position along the CQD axial direction, for different values of applied electric field. Obviously, the peaks of the BE shifts, just as the BE peaks, are displaced in opposite to the electric field direction and have different from the BE peak positions. Indeed, for the electric field $F = 100$ kV/cm (50 kV/cm) the BE has a maximum at $z_i = -1.5d$ ($z_i = -1.4d$) while the maximum of the BE shift is at $z_i = -1.6d$ ($z_i = -1.5d$). Such discrepancy again testifies for the increase of the influence of polaronic effect on BE energy with the electron effective confinement strengthening. In difference to the BE, the polaronic correction is not dependent on the impurity position for the electric field $F = 100$ kV/cm (50 kV/cm) when $z_i > -0.1d$ ($z_i > 0$). It means that at these conditions the electric field plays a main role in the polaronic effect.

The BE of the on-center hydrogenic impurity with and without the ELOP interaction and the polaronic shift as a function



(a) (b)

Fig. 3. Reduced binding energy (a) with (solid lines) and without (dotted lines) ELOP interaction, and reduced polaronic shifts of binding energy (b) of on-center impurity as a function of CQD radius at different values of electric field.

of radius of the CQD for different values of the electric field are presented in Fig. 3. As expected, the BE, as well as the polaronic shift of the BE decreases with the increase of the CQD radius, due to the decrease of the electron quantum confinement. The contribution of ELOP interaction to BE for $d = 4a_B^*$ and $F = 100$ kV/cm (50 kV/cm) is about 18.5% (15.4%) for the CQD radius $R = a_B^*$, and decreases to about 9.8% (9.3%) as radius increases to $R = 5a_B^*$. At comparatively weak electric field ($F = 0.1$ kV/cm) the contribution of the ELOP interaction increases from 6.4% to about 7.6%, when radius changes in the above mentioned range. As seen in this figure, the dot radius dependence of the polaronic shift of the BE becomes slower with the decrease of the electric field. The crossing of the curves in Fig. 3(b), may be explained as follows: for large values of the CQD radius quantum confinement does not play a dominant role, and the effective confinement is determine by the interplay of Stark confinement and electron–hydrogenic impurity interaction. Therefore in stronger electric fields due to the larger displacement of the electron from the impurity the effective confinement decreases, and thus the BE shift is smaller. For small values of the CQD radius quantum confinement plays a dominant role, and the effective confinement is determined by the interplay of Stark and quantum confinements. Thus in stronger electric fields the effective confinement increases, which brings to the increase of the BE shift.

4. Conclusions

We have first presented a systematic study of the ground-state binding energy of a hydrogenic impurity in cylindrical quantum dot subjected to external electric field and ELOP interaction. The results of the polaronic effects on the binding energy are obtained as functions of the applied electric field as well as of the impurity position and the radius of QD. The interplay between the confinement effects due to the applied electric field, spatial confinement and Coulomb interaction on the binding energy is analyzed. We show that the polaronic shift of the binding energy increases with the enhancement of the effective confinement. The results of numerical calculations show also that the influence of the ELOP interaction on the BE depends strongly on the impurity position, electric field and dot size. The correction of the binding energy due to electron coupling with the polar-optical phonon for the same cases can reach values up to 37.5%. This aspect must be taken into account in the interpretation of optical phenomena related to hydrogenic impurities in which the effect of an applied electric field competes with the spatial quantum confinement.

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