Bound polaron in a spherical quantum dot: Strong electron-phonon coupling case

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The effect of the electron-phonon interaction on an electron bound to an impurity in a spherical quantum dot embedded in a nonpolar matrix is studied theoretically. The adiabatic variational method is used to calculate the polaron energy shift. General analytical results are obtained for small and large dots for different impurity positions. Numerical calculations were performed for ZnSe quantum dots of different radii. It is shown that (1) the interaction with interface phonons is absent when the impurity is in the center of the dot, reaches its maximum when the impurity is close to the boundary, and decreases in value if the impurity is on the interface; (2) unlike the interaction with bulk-type LO phonons, the interaction with interface phonons is negligible in small dots but gives a considerable contribution to the energy in the large dots provided the impurity is located near the dot's boundary.

I. INTRODUCTION

In recent years quantum dot (QD) systems have attracted considerable attention due to the interesting quantum-mechanical phenomena associated with them and their potential applications to electronic and optoelectronic devices.[1,2] In these systems electronic states are subject to a strong three-dimensional (3D) confinement effect arising from the mismatch in the band gaps of the materials. The electron–LO-phonon coupling also has different features from that in the bulk, namely, there is a strong increase of its strength with reduction of dimensionality (from 3D in the bulk to 0D in the QD), and there also exist bulk and interface [surface optical (SO)] types of phonon.[3]

As in the bulk case, polaron corrections are also present for the electron confined in the QD, and they change the electronic properties significantly. This effect was studied earlier for the case of a free polaron in a spherical QD using variational techniques[4–7] and within second-order perturbation theory.[8–11]

The study of impurity states in these materials is important since the impurities greatly affect both electronic and optical properties of QD's. Since the impurity can be located, in principle, anywhere in the dot, it is necessary to study the dependence of all relevant physical quantities on its position. The polaron effect on the so-called donorlike exciton in nanocrystals can also be treated within the framework of the models applied to the free polaron case.[5] A recent experimental study of the luminescence in AgCl nanocrystals[12] indicates that a compact, heavy hole can be trapped at different lattice sites, causing changes in peak positions in the observed spectra when it tunnels or hops toward the center of the nanocrystal.

In the present work we describe the electron-phonon interaction in a spherical QD for the case of an electron bound to a hydrogenlike impurity (or donorlike exciton with a heavy hole) located at some point within the dot. The calculation of the polaron ground state (GS) energy is performed within the framework of the effective mass approximation, i.e., assuming that all characteristic lengths of the problem are large compared to the lattice constant.[13] The electron-phonon interaction is treated within the adiabatic approximation, which, despite its obvious limitations[14] and due to its relative mathematical simplicity, allows one to obtain detailed information about the properties of the electron-phonon coupling.

Recently the binding energy of a hydrogenlike impurity in a spherical QD has been studied[5,13–17] theoretically. In Refs. 13–16 the dependence of the binding energy of the ground and several excited electronic states on the location of the impurity was investigated using variational calculations. It was found, in particular, that the binding energy of the ground state has a maximum when the impurity is positioned in the center of the dot and decreases with its shift from the center. In Refs. 5 and 17 the influence of the electron-phonon interaction on the binding energy was considered in the strong coupling (adiabatic) case. However, no analysis of the dependence of the bulk and SO modes on the size of the dot was provided.

This paper is organized in the following way. In Sec. II the adiabatic variational model for an electron in a spherical QD interacting with bulk and interface LO phonons is described. In Sec. III the general behavior of the bound polaron in small and large QD's is analyzed. Then the dependence of the polaron energy and the electron-phonon interaction energies on the impurity position is studied numerically for QD's of several arbitrary radii.

II. MODEL

A. Hamiltonian

Let us consider an electron that is perfectly confined in a sphere with radius R and is interacting with LO phonons. A hydrogenlike impurity is located at the position $\mathbf{r}_0$ (the center of the sphere is taken as the origin). In the effective mass approximation the Hamiltonian of the system is given by

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

Here the electronic part is given by

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$$H_e = \frac{\mathbf{p}^2}{2m} + V_{QD}(\mathbf{r}) + V_C(\mathbf{r},\mathbf{r}_0), \tag{2}$$

where $\mathbf{p}$ and $\mathbf{r}$ are the momentum and coordinate of the electron, $V_{QD}(\mathbf{r})$ is the confinement potential of the QD,

$$V_{QD}(\mathbf{r}) = \begin{cases} 0, & r < R \\ \infty, & r > R, \end{cases} \tag{3}$$

and the electrostatic potential energy $V_C(\mathbf{r},\mathbf{r}_0)$ for the electron motion inside the sphere is[18]

$$V_C(\mathbf{r},\mathbf{r}_0) = -\frac{e^2}{\varepsilon_\infty |\mathbf{r}-\mathbf{r}_0|} + \sum_{l=0}^{\infty} \alpha_l \left(\frac{r}{R}\right)^{2l} \frac{e^2}{2R}$$
$$- \sum_{l=0}^{\infty} \alpha_l \frac{e^2}{R} \left(\frac{rr_0}{R^2}\right)^l P_l(\cos\theta), \tag{4}$$

where

$$\alpha_l = \left(\frac{1}{\varepsilon_d} - \frac{1}{\varepsilon_\infty}\right) \frac{\varepsilon_d(l+1)}{\varepsilon_\infty l + \varepsilon_d(l+1)} \tag{5}$$

and P_l is a Legendre polynomial. The first term in Eq. (4) is the screened Coulomb potential, the second describes a weak electric field directed to the center of the dot (the point of the highest dielectric stabilization), and the last one is a polarization term giving the interaction with the surface polarization charge. These last two terms constitute the image charge potential arising in the QD due to the difference in dielectric constants inside and outside the dot.

The LO phonon Hamiltonian H_{ph} is written as

$$H_{ph} = \sum_s \hbar \omega a_s^\dagger a_s. \tag{6}$$

The electron-phonon interaction Hamiltonian H_{int} is given within the well-known Fröhlich continuum model adapted for this particular physical situation of an electron in a spherical environment (specified by the static and high-frequency dielectric constants ε_0 and ε_∞) embedded in a matrix with a dielectric constant ε_d. H_{int} depends on the coordinates of both impurity and electron, reflecting the fact that both of them, being charged, interact with phonons:

$$H_{int} = \sum_{j=1,2} \sum_s V_{js} [\{S_{js}(\mathbf{r}) - S_{js}(\mathbf{r}_0)\} a_{js} + \text{H.c.}], \tag{7}$$

where

$$S_{1s}(\mathbf{r}) = j_l(\mu_{nl}r/R) Y_{lm}(\theta,\varphi), \tag{8}$$

$$S_{2s}(\mathbf{r}) = (r/R)^l Y_{lm}(\theta,\varphi). \tag{9}$$

Here 1 and 2 denote the bulk-type and interface- (or surface-) type phonons, respectively. The index s is given by $n = 1,2,\ldots, l = 0,1,2,\ldots, m = 0,\pm 1,\ldots$ for the bulk phonon and $l = 1,2,\ldots, m = 0,\pm 1,\ldots$ for the surface (SO) phonon. For SO modes the lowest value of l is 1 since the state with $l = 0$ does not interact with this type of phonon (the electric field causing the polarization is equal to zero.[7])

The electron-phonon coupling coefficients are given by

$$V_{1s} = \sqrt{\frac{4\pi\hbar\omega_{LO}e^2}{\mu_{nl}^2 j_{l+1}^2(\mu_{nl})R} \frac{1}{\varepsilon^*}}, \tag{10}$$

$$V_{2s} = \frac{\varepsilon_\infty \sqrt{l}}{l\varepsilon_\infty + (l+1)\varepsilon_d} \omega_{LO} \sqrt{\frac{2\pi\hbar e^2}{\omega_l R} \frac{1}{\varepsilon^*}}, \quad \frac{1}{\varepsilon^*} = \frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}, \tag{11}$$

where ω_{LO} is the frequency of the bulk LO phonon and the eigenfrequencies of the SO modes ω_l depend on the quantum number l as follows:

$$\omega_l^2 = \frac{\varepsilon_d + (\varepsilon_d + \varepsilon_0)l}{\varepsilon_d + (\varepsilon_d + \varepsilon_\infty)l} \omega_{TO}^2. \tag{12}$$

The values of μ_{nl} are the roots of the spherical Bessel function $j_l(\mu_{nl}) = 0$ of order l, and $Y_{lm}(\theta,\varphi)$ are the spherical harmonics.

B. Variational procedure

As is usually done for the bulk bound polaron, first it is necessary to eliminate the contribution to the total electron energy from the impurity–LO-phonon interaction. This can be achieved by means of a first canonical transformation[19] whose effect is to displace the equilibrium position of the ions:

$$U = \exp\left\{\sum_{j=1,2} \sum_s [V_{js}^* S_{js}(\mathbf{r}_0) a_{js} + \text{H.c.}]\right\}. \tag{13}$$

Apart from the nonphysical divergent term arising from the use of the point-charge model, the effect of this displacement on the lattice polarization leads to the following electron-impurity "exchange" interaction (the term electron-impurity exchange interaction used here was first proposed in Ref. 5):

$$H_x = \sum_s \left[\left\{ |V_{1s}|^2 j_l\left(\mu_{nl}\frac{r_0}{R}\right) j_l\left(\mu_{nl}\frac{r}{R}\right) \right. \right.$$
$$\left. \left. + |V_{2s}|^2 \left(\frac{rr_0}{R^2}\right)^l \right\} Y_{lm}^*(\theta_0,\varphi_0) Y_{lm}(\theta,\varphi) + \text{H.c.} \right]. \tag{14}$$

When the impurity is located in the center of the QD ($r_0 = 0$), it is easy to obtain[5] that

$$H_x = \left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right) \frac{e^2}{r} \left(1 - \frac{r}{R}\right), \tag{15}$$

which partially compensates the electron-impurity Coulomb interaction. Note that only when $R \to \infty$ does this energy coincide with the corresponding value for the bulk case.

The Hamiltonian of the system now takes the form

$$H = H_e + H_x + H_{ph} - \sum_{j=1,2} \sum_s V_{js} [S_{js}(\mathbf{r}) a_{js} + \text{H.c.}], \tag{16}$$

where the symbols 1 and 2 again denote contributions from the bulk LO and surface LO phonons.

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 $\psi(\mathbf{r})$ and a phonon part $|\chi\rangle$. 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 QD's this situation can be realized in the following three cases: (1) when the radius of the QD is small so that the quantum confinement increases the kinetic energy of the electron and, as a result of this, the distance between adjacent energy levels; (2) when the electron-phonon interaction is so strong that electron self-localization occurs, i.e., fast electron oscillations; (3) when the electron-impurity interaction is so strong that the electron becomes localized around the impurity.

Within the adiabatic approximation, the effect of the electron-phonon interaction is to displace further the equilibrium positions of the ions. This can be achieved by performing another two linear shift canonical transformations corresponding to the interaction with bulk ($j=1$) and interface ($j=2$) phonon modes:

$$U_j = \exp\left\{\sum_s \left[f_{js}a_{js}+\text{H.c.}\right]\right\},\tag{17}$$

where the parameters f_{js} are to be determined variationally. With these transformations taken into account, the total wave function of the system is given by the product

$$|\Psi\rangle = U_1 U_2 |\psi(\mathbf{r})\rangle|0\rangle,\tag{18}$$

where $|0\rangle$ is the phonon ground state.

The subsequent minimization of the expectation energy value

$$E_{tot} = \langle\Psi|H|\Psi\rangle\tag{19}$$

with respect to the variational parameters f_{js} leads to the following standard expressions for them:

$$f_{1s} = -V_{1s}\frac{\langle\psi|S_{1s}(\mathbf{r})|\psi\rangle}{\hbar\omega_{LO}},\tag{20}$$

$$f_{2s} = -V_{2s}\frac{\langle\psi|S_{2s}(\mathbf{r})|\psi\rangle}{\hbar\omega_l}.\tag{21}$$

Choosing the electronic part of the trial function in the form

$$|\psi(\mathbf{r})\rangle = N\frac{\sin(\pi r/R)}{r}e^{-\gamma|\mathbf{r}-\mathbf{r}_0|},\tag{22}$$

with N as a normalization constant and γ as a variational parameter indicating the degree of spatial correlation between the electron and the impurity, after some calculations we can find E_{tot} as a functional of γ:

$$E_{tot} = \langle\psi|H_e+H_x|\psi\rangle - \sum_s \hbar\omega_{LO}|V_{1s}|^2|f_{1s}|^2$$

$$- \sum_s \hbar\omega_l|V_{2s}|^2|f_{2s}|^2.\tag{23}$$

The energy of the bound polaron can be found by minimizing E_{tot} with respect to γ. In the following calculations we will pay special attention to the following quantities: the binding energy of the polaron (polaron energy shift), which is determined as the difference between the total energy of the polaron and the ground state energy of the electron confined in the QD without the impurity present,

$$E = E_{tot} - \frac{\hbar^2}{2m}\left(\frac{\pi}{R}\right)^2,\tag{24}$$

and contributions to the total energy from electron–bulk-phonon ($E^{(b)}$) and electron–SO-phonon ($E^{(s)}$) interactions,

$$E^{(b)} = -\sum_s \hbar\omega_{LO}|V_{1s}|^2|f_{1s}|^2,\tag{25}$$

$$E^{(s)} = -\sum_s \hbar\omega_l|V_{2s}|^2|f_{2s}|^2.\tag{26}$$

III. ANALYSIS AND CALCULATIONS

A. Electron-phonon coupling in a small quantum dot

Let us consider first the case of the small QD with $R \ll a_B$, where a_B is the Bohr radius of the effective mass electron. In this case the kinetic energy of the electron will predominate and the interaction energy may be regarded as a perturbation to the free moving electron in the QD. This indicates that, in order to obtain the leading term of the energy E_0, we can put $\gamma=0$ in the electronic wave function (22), thus making it the eigenfunction of the unperturbed Hamiltonian. After some calculations, the final result for this term in the polaron binding energy can be cast in the following form:

$$E_0 = E_{C0} - E_{x0} + E_0^{(b)} + E_0^{(s)},\tag{27}$$

where the first term E_{C0} representing the potential energy of the electron in the QD, the "exchange" energy E_{x0}, and the interactions with bulk $E_0^{(b)}$ and interface $E_0^{(s)}$ phonons are equal to

$$E_{C0} = \frac{e^2}{\varepsilon_\infty R}\left[F\left(\frac{2\pi r_0}{R}\right) + \frac{1}{2}\left(\frac{\varepsilon_\infty}{\varepsilon_d}-1\right) - \frac{\varepsilon_\infty}{2}\sum_{n=1}^{\infty}\frac{\alpha_l}{\pi^{2l+1}}J_l\right],\tag{28}$$

$$E_{x0} = \frac{e^2}{\varepsilon^* R}\left[F\left(\frac{2\pi r_0}{R}\right)-1\right],\tag{29}$$

$$E_0^{(b)} = -C\frac{e^2}{\varepsilon^* R},\tag{30}$$

$$E_0^{(s)} = 0, \tag{31}$$

with

$$J_l = \int_0^\pi dx \, \sin^2(x) x^{2l}. \tag{32}$$

The function $F(x)$ is given by [Cin(x) is the integral cosine]

$$F(x) = 1 - \frac{\sin(x)}{x} + \text{Cin}(2\pi) - \text{Cin}(x) \tag{33}$$

and the coefficient $C = [1 - \text{Si}(2\pi) + \text{Si}(4\pi)/2]/2 = 0.3931$. In order to obtain the expressions (29) and (30) above, summation over the roots of the Bessel function $j_0(x)$ was performed and then the resulting two-dimensional integrals were evaluated. It should be mentioned that Eqs. (29)–(31) are the same as given in Ref. 5 (with $\alpha = 0$), but written in a closed analytical form.

The contribution to the electron-phonon interaction energy from the spatial correlation has a small but nonetheless finite value even when $R \to 0$. This was calculated separately for two impurity positions in the quantum dot: (1) the impurity is in the center of the dot and (2) the impurity is located close to the dot's boundary. To evaluate these corrections the terms with the smallest values of the orbital quantum number ($l = 0$, $n = 1$ for bulk and $l = 1$ for interface phonons) were taken into account. This can be justified by the fact that in a small QD the distance between adjacent levels is large enough to provide a negligible mixing of states with higher values of l with the ground state; in other words, in this case the deviation of the function (22) from spherical symmetry is small and the maximum input to the energy will be given by the matrix elements with lowest lying states. Neglecting exchange energy terms for the case $r_0 \to R$ and image charge effects to simplify the consideration, after elementary but somewhat tedious calculations we can obtain the asymptotic values for $E_1^{(b)}$ and $E_1^{(s)}$ in the form

$$E_1^{(b)} = \begin{cases} -[0.0418 - 0.034(1 - \varepsilon_\infty/\varepsilon_0)]\dfrac{e^2}{\varepsilon^* a_B}, & r_0 = 0, \tag{34} \\ \\ -0.0061\dfrac{e^2}{\varepsilon^* a_B} - 0.033(R - r_0)\dfrac{e^2}{\varepsilon^* R^2}, & r_0 \to R, \end{cases} \tag{35}$$

$$E_1^{(s)} = -[0.0016 + 0.0022(R - r_0)/R]$$

$$\times \frac{e^2 R}{\varepsilon^* a_B^2} \frac{\varepsilon_0 \varepsilon_\infty}{(\varepsilon_0 + 2\varepsilon_d)(\varepsilon_\infty + 2\varepsilon_d)}, \quad r_0 \to R. \tag{36}$$

From these results the following conclusions can be drawn: the binding energy has a maximum when the impurity is located in the center of the dot and decreases with change in the position of the impurity away from the center [see Eq. (27)]. The electron–LO-phonon interaction is largely independent of the impurity's position in the dot and also reaches its maximum (in absolute value) in the center of the QD [Eqs. (30), (34), and (35)]. It should also be mentioned that the interaction energy with bulk phonons increases when $R \to 0$ [Eq. (30)], while the electron–SO-phonon interaction approaches zero in this limit [Eq. (36)]. This means that even in the small dot polaron corrections arising from the bulk phonons will always be present and should be taken into account when calculating the electron binding energies. The gradual decrease of $E^{(s)}$ obtained here can be explained as follows. The smaller the dot, the smaller the impact of the spatial correlation between the electron and impurity on the behavior of the electron since the trial wave function (22) becomes spherically symmetrical. This means that the corresponding matrix elements in Eq. (26) for interaction energies will also approach zero for all nonzero values of l. This explanation also implies that the interaction with SO phonons is always absent in the adiabatic limit when the impurity is in the center of the quantum dot.

On the contrary, the situation is quite different near the boundary of the QD. In that region $E_1^{(s)}$ has a nonzero value and increases (in absolute value) with the shifting of the impurity away from the boundary [see Eq. (36)], reaching its maximum inside the dot. This can be understood by noting that when the impurity is on the surface, then the electron is localized only on one side of it. When the impurity is moved away from the surface, the electron can ''leak'' behind it and become effectively closer to the interface, thus increasing the interaction with SO modes. Such behavior of the electron–SO-phonon interaction energy is quite different from the results reported for a GaAs-Al$_{0.3}$Ga$_{0.7}$As quantum well,[20] where it was found that this energy increases with decrease of the well width, has a nonzero value when the impurity is in the center of the well, and reaches its maximum for the impurity located on the boundary.

B. Large quantum dot

In this case the electron is localized in a small region of the quantum dot. Provided that the impurity is located far from the boundary of the dot and the radius of the electron localization is much smaller than the dot's radius, the electronic wave function (22) reduces to the form usually adopted for the description of the GS of the bulk bound polaron:[21]

$$|\psi(\mathbf{r})\rangle = \left(\frac{\gamma^3}{\pi}\right)^{1/2} e^{-\gamma r}. \tag{37}$$

Then for sufficiently large values of γ in a large QD the matrix elements in Eq. (23) can be easily evaluated (only the interaction with bulk phonons contributes to the energy) and yield the following result for the polaron energy:

$$E_{tot} = \frac{\hbar^2}{2m} \frac{\gamma^2}{4} - \frac{e^2}{\varepsilon_0} \frac{\gamma}{2} - \frac{5}{16} \frac{e^2}{\varepsilon^*} \frac{\gamma}{2}. \tag{38}$$

Minimization of this equation with respect to γ immediately leads to the polaron energy E_{tot} and electron–LO-interaction energy $E^{(b)}$ given by
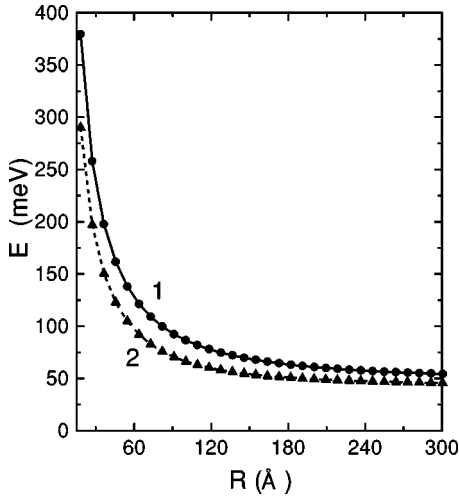
FIG. 1. Dependence of the polaron binding energy E on the radius of the quantum dot R ($r_0=0$): curve 1, with image charge potential; curve 2, without it. Dots represent calculated values; the curves are a guide to the eye.

$$E_{tot} = -\frac{me^4}{2\hbar^2 \varepsilon_0^2}\left[1 + \frac{5}{16}\frac{\varepsilon_0}{\varepsilon^*}\right]^2, \qquad (39)$$

$$E^{(b)} = -\frac{5}{16}\frac{me^4}{2\hbar^2 \varepsilon_0 \varepsilon^*}\left[1 + \frac{5}{8}\frac{\varepsilon_0}{8\varepsilon^*}\right], \qquad (40)$$

which are the well-known expressions for a system with strong electron-phonon coupling in the bulk.[21]

C. Results of numerical calculations

Numerical calculations have been carried out for ZnSe using the following material parameters:[17] $\varepsilon_0=8.33$, $\varepsilon_\infty=5.9$, $\varepsilon_d=2.25$, $m=0.171m_0$, and $\hbar\omega_{LO}=38.49$ meV.

The dependence of the polaron binding energy defined by Eq. (24) on the radius of the quantum dot for the case of $r_0=0$ is shown in Fig. 1 for potentials with (curve 1) and without (curve 2) image charge effects. The upward shift of the binding energy is quite noticeable. In the next figure (Fig. 2) the dependence of the electron–LO-phonon interaction for the same case of the impurity positioned in the center of the dot is shown. It is seen that for small radii this energy diverges (in inverse proportion to the radius of the dot; see Sec. III A), reaches a minimum value around $R=100$ Å, and then gradually approaches the bulk value for large values of R. Such behavior is analogous to that obtained earlier.[5,17]

To study the dependence of all interesting physical quantities on the impurity position in various quantum dots, calculations for three radii (20, 100, 300 Å) of the dot were performed (Figs. 3–6).

Figures 3(a)–3(c) show the polaron binding energy [Fig. 3(a), curve 1] and the electron–LO-phonon [Fig. 3(b)] and electron–SO-phonon [Fig. 3(c)] interaction energies evaluated as functions of the impurity position r_0 in the QD with $R=20$ Å. Curve 2 in Fig. 3(a) is the corresponding result of the approximate calculations using Eq. (27) of Sec. III A; it slightly underestimates the exact values, probably due to the
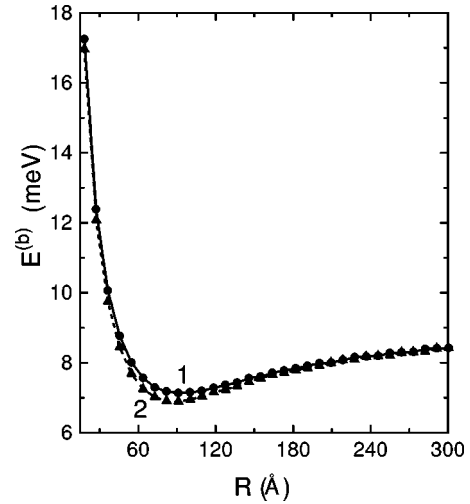

FIG. 2. Electron-phonon interaction energy as a function of the radius of the quantum dot R ($r_0=0$): curve 1, with image charge potential; curve 2, without it.

fact that the radius of the dot is of the order of (not smaller than) the Bohr radius for ZnSe. Nevertheless, it is clear that even for this radius the approximate results agree with numerical data quite favorably. From Figs. 3(b) and 3(c) it may be concluded that the interaction with phonons (with SO modes in particular) is quite small and weakly dependent on the position of the impurity as demonstrated in Sec. III A.

The calculations for the QD with radius 100 Å were performed to show the situation when both the kinetic energy and the Coulomb interaction determine the behavior of the electron in the QD. It is seen that the binding energy [Fig. 4(a)] and the absolute value of the interaction energy with bulk phonons [Fig. 4(b), curve 1] are decreased in comparison with the values obtained for the QD with $R=20$ Å. However, the absolute value of the electron–SO-phonon interaction energy [Fig. 4(b), curve 2] is greater for this size of dot. The observed behavior of this quantity is also different from that reported in Ref. 17 in the vicinity of the interface: instead of approaching a constant value as reported in Ref. 17, it decreases after reaching a maximum around $r_0/R \approx 0.8$. This behavior also corroborates the results of the analytical consideration of Sec. III A.

In the case of a 300 Å quantum dot the results converge to those valid for the bulk, namely, the binding energy and the electron-phonon interaction approach the values given by Eqs. (39) and (40), respectively, for most positions of the impurity in the dot [Figs. 5(a) and 5(b)] and then decrease sharply around $r_0/R \approx 0.9$. The value of $E^{(s)}$ [Fig. 5(c)] is greater than for the two other QD's studied here (around 30% of $E^{(b)}$) and again exhibits a gradual increase in absolute value with the displacement of the impurity from the center and then a sharp roll-off near the boundary of the dot. This is different from the results[6] for an electron in a spherical QD and an exciton in a QD[22] where it was found that interactions with SO phonons yield only small corrections for all values of the dot radius and electron-phonon coupling strength. It should also be remarked here that the decrease in
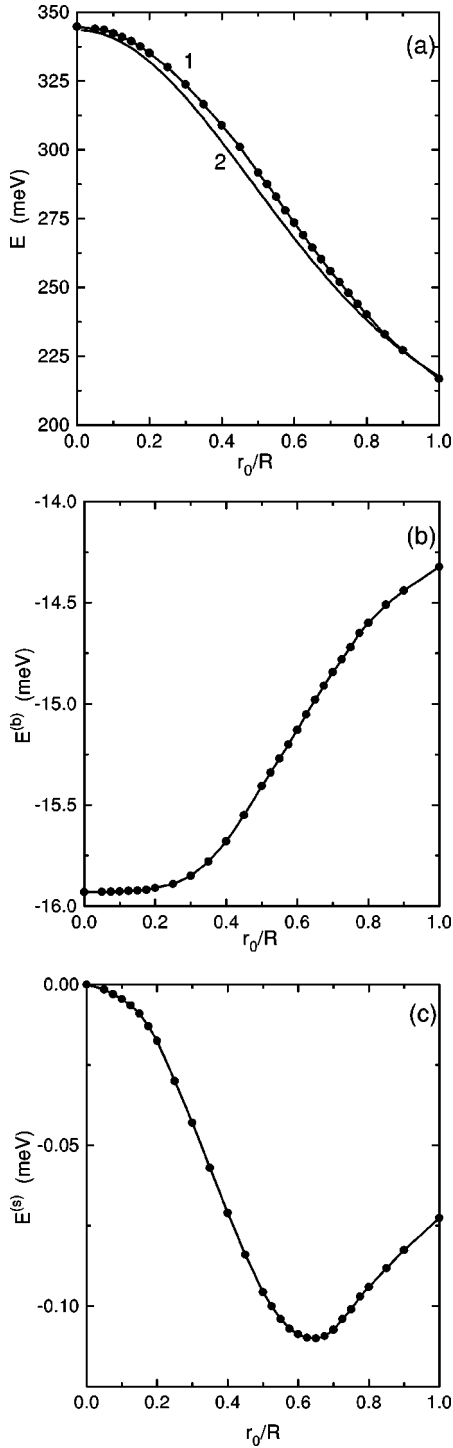
FIG. 3. (a) The dependence of the polaron binding energy on the impurity position for a QD with $R = 20$ Å (curve 1); curve 2, the same as curve 1 but using Eq. (27). (b) The electron–bulk-phonon interaction energy as a function of the impurity position for $R = 20$ Å. (c) The electron–SO-phonon interaction energy vs the impurity position.

coupling with SO modes occurs in all dots studied at a distance from the interface approximately equal to the Bohr radius for ZnSe.

Finally, we also plotted the value of the parameter γ corresponding to the minimum of the total energy (23) for all
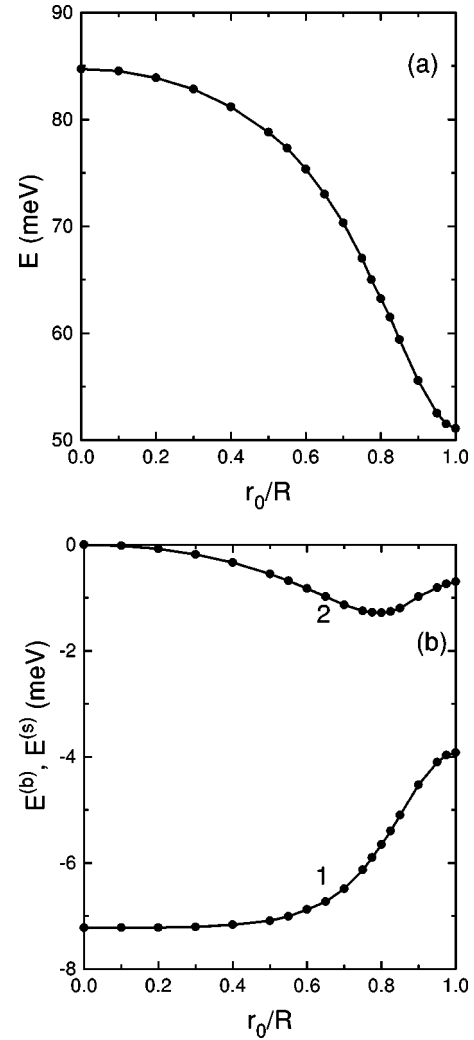

FIG. 4. (a) The dependence of the polaron binding energy on the impurity position for a QD with $R = 100$ Å. (b) The electron–bulk-phonon (curve 1) and electron–SO-phonon (curve 2) interaction energies as functions of the impurity position for $R = 100$ Å.

three quantum dots as a function of the impurity position (Fig. 6). It is clear that, unlike all other energy quantities, this parameter reaches its maximum away from the center of the QD and decreases when the impurity approaches the boundary. This means that maximum localization of the electron occurs away from the center of the dot, probably due to reflection from the nearest boundary (the electron is affected by that boundary). The value of this parameter also increases when the dot becomes larger so that the situation becomes similar to the bulk case. The ratio of γ for $r_0 = 0$ and for $r_0 = R$ for the largest dot (curve 3) is approximately equal to 2, which is reminiscent of the so called bound surface polaron,[23] where the trial wave function is usually taken to be the $2p$ state for the impurity on the surface and $1s$ when it is located in the bulk of the material.[24]

IV. CONCLUDING REMARKS

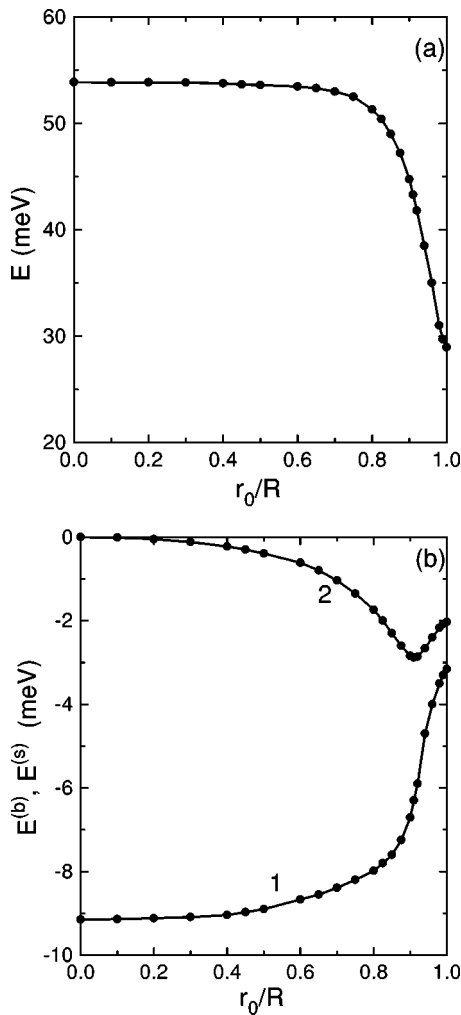The effect of the electron interaction with LO phonons is discussed for an electron bound to a hydrogenlike impurity

FIG. 5. (a) The same as in Fig. 4(a) but for a QD with $R = 100$ Å. (b) The same as in Fig. 4(b) but for $R = 100$ Å.

FIG. 6. Dependence of the variational parameter γ on the impurity position for three QD's: curve 1, $R = 20$ Å; curve 2, $R = 100$ Å; curve 3, $R = 300$ Å.

confined in a spherical quantum dot embedded in a nonpolar matrix. Both bulk and SO phonons were taken into account when calculating the binding energy of the electron. The adiabatic variational method was used to treat the electron-phonon interaction. Strictly speaking, this method gives valid results only for small quantum dots when the effects of quantum confinement predominate. Nevertheless, the use of this approach allowed us to obtain some general analytical results
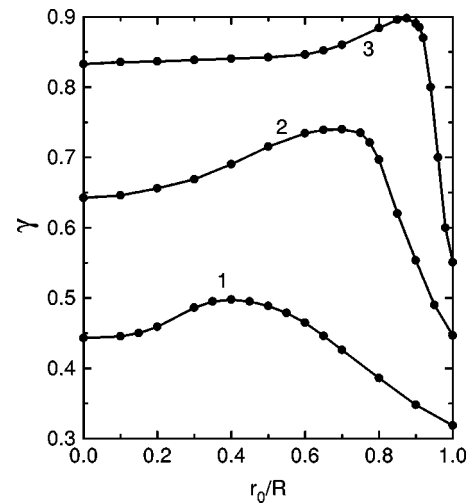
for small dots, showing that here, unlike in quantum wells, the interaction with SO phonons reaches its maximum away from the boundary of the dot and is equal to zero when the impurity is in the center. Results of numerical calculations show that the electron–SO-phonon interaction depends strongly on the dot size: it is negligible in small dots and amounts to up to 30% of the interaction with bulk phonons in large QD's.

To conclude, we mention several remaining problems closely related to the present work. The most obvious extension of the present approach would be the incorporation in the variational scheme of the terms pertinent to the intermediate-coupling case as was performed earlier,[6,22] on the basis of which general properties of the electron-phonon interaction in the spherical QD could be investigated. The realistic case of imperfect electron confinement in the QD (finite value of the potential barrier at the interface) should also be studied, taking into account the frequent situation when the LO phonons are present not only in the dot but also within the barrier (such as for CuCl in a NaCl crystal).

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