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Bound polarons in quantum dot quantum well structures*

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The problem of bound polarons in quantum dot quantum well (QDQW) structures is studied theoretically. The eigenfrequencies of bulk longitudinal optical (LO) and surface optical (SO) modes are derived in the framework of the dielectric continuum approximation. The electron–phonon interaction Hamiltonian for QDQW structures is obtained and the exchange interaction between impurity and LO-phonons is discussed. The binding energy and the trapping energy of the bound polaron in CdS/HgS QDQW structures are calculated. The numerical results reveal that there exist three branches of eigenfrequencies of surface optical vibration in the CdS/HgS QDQW structure. It is also shown that the binding energy and the trapping energy increase as the inner radius of the QDQW structure decreases, with the outer radius fixed, and the trapping energy takes a major part of the binding energy when the inner radius is very small.

Keywords: bound polaron, quantum dot, quantum well
PACC: 6320K, 7320D, 7138

1. Introduction

In recent decades, quantum dot (QD) systems have attracted considerable attention due to their associated interesting quantum mechanical phenomena and potential applications.[1−13] Among these systems, a new kind of QD structure, called a quantum dot quantum well (QDQW) structure, has been fabricated and studied.[7−13] The QDQW structure can be formed by coating a core composed of a semiconductor with a large energy gap as the QD, and a thin shell layer composed of another semiconductor with a small energy gap as the quantum well (QW) of the structure. The QDQW structure is commonly embedded in a nonpolar medium such as water, glass, etc. Thus, the conduction electron will be confined in the QW.

It is well known that electron–phonon (e–p) interaction is an important factor influencing the physical properties of polar semiconductors, especially in low-dimensional systems. Wendler[1] studied the phonon modes in a QW and gave an e–p interaction Hamiltonian. Klein *et al* [2] discussed the e–p interaction in a polar semiconductor spherical QD. Marini *et al* [3] considered an exciton–phonon interaction in a polar semiconductor QD. Melnikov and Fowler[4] investigated the bound polaron in a spherical QD. Tkach *et al* [9] studied the exciton–phonon interaction in a QDQW system and obtained the phonon modes. Zhang *et al* [10] explored the phonon modes in QDQW and gave the e–p interaction Hamiltonian. All these studies were carried out in the framework of the standard dielectric continuum approximation presented in Refs.[14–16]. It has been proven that the bulk longitudinal optical (LO) modes and the interface or surface optical (SO) modes obtained from the dielectric continuum model are consistent with those obtained from other approaches.[17−19] Because of the simplicity and efficiency of this model, we use it to study the bound polaron in QDQW structures.

In the present paper, we consider a QDQW structure where a spherical core with radius R_1, composed of a semiconductor with dielectric constant ε_1, is surrounded by a thin spherical shell with outer radius R_2, composed of another semiconductor with dielectric constant ε_2. The QDQW structure is embedded in a nonpolar insulating medium with dielectric constant $\varepsilon_{\rm d}$. We investigate the e–p interaction in an ideal QDQW structure, where the electrons are confined in the thin spherical shell completely. The remainder

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of the present paper is organized as follows. In Section 2, we study the LO modes and the SO modes in QDQW structures and derive the eigenfrequencies of these modes. In Section 3, we discuss the e–p interaction and give an interaction Hamiltonian. In Section 4, we examine the exchange interaction between impurity and LO phonons. In Section 5, we consider the polaron effect on an electron confined in the well of QDQW structures. In Section 6, we give the main conclusions drawn from the present study.

2. Vibration eigenmodes of QDQW structures

In the case of polar interaction, the relevant modes are only the LO and the SO modes. To derive the eigenfrequencies of LO and SO modes from the dielectric continuum model, we start from the standard equations

$$\boldsymbol{D} = \varepsilon_2 \boldsymbol{E} = \boldsymbol{E} + 4\pi \boldsymbol{P}, \tag{1}$$

$$\boldsymbol{E} = -\nabla\phi, \tag{2}$$

and

$$\nabla \cdot \boldsymbol{D} = 0, \tag{3}$$

where $\boldsymbol{D}$, $\boldsymbol{E}$, $\boldsymbol{P}$, and ϕ are the electric displacement vector, the electric field, the polarization density, and the electric potential, respectively. From Eqs.(1)–(3) we obtain

$$\varepsilon_2 \Delta\phi = 0. \tag{4}$$

There exist two possibilities in Eq.(4). One is $\varepsilon_2 = 0$ and the other is $\Delta\phi = 0$. Since the dielectric constant is given by

$$\varepsilon_2 = \varepsilon_{\infty 2} \frac{\omega^2 - \omega_{\mathrm{LO2}}^2}{\omega^2 - \omega_{\mathrm{TO2}}^2}, \tag{5}$$

where ω_{LO2} and ω_{TO2} are the eigenfrequencies of the LO and TO phonons of the shell material respectively, and they are related by

$$\frac{\omega_{\mathrm{LO2}}^2}{\omega_{\mathrm{TO2}}^2} = \frac{\varepsilon_{02}}{\varepsilon_{\infty 2}}, \tag{6}$$

where ε_{02} and $\varepsilon_{\infty 2}$ are the static dielectric constant and high frequency dielectric constant of the shell material respectively. The case $\varepsilon_2 = 0$ corresponds to the internal LO modes. The boundary conditions, the continuity of ϕ and the normal component of $\boldsymbol{D}$ in the interface, imply that ϕ vanishes outside the spherical shell and in its surface. From the boundary conditions, we choose eigenfunctions in the spherical shell with the following form:

$$N_{ln} g_l(kr) Y_{lm}(\theta, \varphi), \tag{7}$$

and

$$g_l(kr) = n_l(kR_1) j_l(kr) - j_l(kR_1) n_l(kr), \tag{8}$$

where $j_l(x)$ and $n_l(x)$ are the spherical Bessel function and spherical Neumann function of order l ($l = 0, 1, 2, 3 \ldots$), Y_{lm} (θ, φ) are the spherical harmonic functions with $m = 0, \pm 1, \ldots \pm l$, and k is the constant that is chosen such that $g_l(kR_2) = 0$. If x_n is the nth zero value of $g_l(x) = 0$, then $k_{ln} = x_n / R_2$.

It can be shown that the components of expression (8) are orthogonal to each other, namely

$$\int_{R_1}^{R_2} g_l(kr) g_l(k'r) r^2 \mathrm{d}r = 0, (k \neq k'). \tag{9}$$

The normalization constant is given by

$$N_{ln}^{-2} = \int_{R_1}^{R_2} g_l^2(k_{ln} r) r^2 \mathrm{d}r. \tag{10}$$

Thus we can obtain the polarization potential as follows:

$$\phi(\boldsymbol{r}) = \sum N_{ln} \phi_{lmn} g_l(k_{ln} r) Y_{lm}(\theta, \varphi), \tag{11}$$

and the inverse transform is given by

$$\phi_{lmn} = \int \phi(\boldsymbol{r}) N_{ln} g_l(k_{ln} r) Y_{lm}^*(\theta, \varphi) \mathrm{d}\boldsymbol{r}. \tag{12}$$

The second possibility, i.e. $\Delta\phi = 0$, will give us the SO modes. The possible solutions are

$$\phi(\boldsymbol{r}) = r^l Y_{lm}(\theta, \varphi), \quad \text{for} \quad r < R_1, \tag{13a}$$

$$\phi(\boldsymbol{r}) = (A_l r^l + B_l r^{-l-1}) Y_{lm}(\theta, \varphi), \quad \text{for} \quad R_1 < r < R_2, \tag{13b}$$

and

$$\phi(\boldsymbol{r}) = C_l r^{-l-1} Y_{lm}(\theta, \varphi), \quad \text{for} \quad r > R_2, \tag{13c}$$

with $l = 1,\ 2,\ 3 \ldots$, $m = 0,\ \pm 1,\ \ldots \pm l$.

From the boundary conditions of the electric potential and the electric displacement vector we have

$$R_1^l = A_l R_1^l + B_l R_1^{-l-1}, \tag{14a}$$

$$C_l R_2^{-l-1} = A_l R_2^l + B_l R_2^{-l-1}, \tag{14b}$$

$$\varepsilon_1 l R_1^{l-1} = \varepsilon_2 [A_l l R_1^{l-1} - B_l (l+1) R_1^{-l-2}], \tag{14c}$$

and

$$\varepsilon_d (l+1) C_l R_2^{-l-2} = -\varepsilon_2 [A_l l R_2^{l-1} - B_l (l+1) R_2^{-l-2}], \tag{14d}$$

with

$$\varepsilon_1 = \varepsilon_{\infty 1} \frac{\omega^2 - \omega_{\mathrm{LO1}}^2}{\omega^2 - \omega_{\mathrm{TO1}}^2}, \tag{15}$$

where $\omega_{\rm LO1}$ and $\omega_{\rm TO1}$ are the eigenfrequencies of the LO and TO phonons of the core material respectively, and they are related by

$$\frac{\omega_{\rm LO1}^2}{\omega_{\rm TO1}^2} = \frac{\varepsilon_{01}}{\varepsilon_{\infty 1}}, \tag{16}$$

where ε_{01} and $\varepsilon_{\infty 1}$ are the static dielectric constant and the high frequency dielectric constant of the core material, respectively.

From expression (14) we have

$$A_l = \frac{(l+1)+l\varepsilon_1/\varepsilon_2}{2l+1}, \tag{17a}$$

$$B_l = \frac{l(1-\varepsilon_1/\varepsilon_2)}{2l+1}R_1^{2l+1}, \tag{17b}$$

$$C_l = \frac{(l+1)+l\varepsilon_1/\varepsilon_2}{2l+1}R_2^{2l+1} + \frac{l(1-\varepsilon_1/\varepsilon_2)}{2l+1}R_1^{2l+1}. \tag{17c}$$

and

$$\begin{aligned}&\varepsilon_{\rm d}(l+1)\big\{\left[(l+1)\varepsilon_2+l\varepsilon_1\right]R_2^{2l+1}\\&+l(\varepsilon_2-\varepsilon_1)R_1^{2l+1}\big\}\\&+\varepsilon_2 l\big\{\left[(l+1)\varepsilon_2+l\varepsilon_1\right]R_2^{2l+1}\\&-(l+1)(\varepsilon_2-\varepsilon_1)R_1^{2l+1}\big\}=0.\end{aligned} \tag{18}$$

It is noted that when $R_1 = 0$, for a QD structure with radius R_2, expression (18) changes into $\varepsilon_2 = -\varepsilon_{\rm d}(l+1)/l$, which is consistent with that in Ref.[2]. Also, it is found from expression (18) that the eigenfrequencies of the SO modes are dependent on radii R_1 and R_2, in contrast to the case of QD structure, in which the eigenfrequencies of the SO modes are dependent only on l.

We have calculated the eigenfrequencies of the SO modes for a CdS/HgS QDQW structure embedded in water.[9] The material parameters used in the calculation are listed in Table 1.

Table 1. Values of the physical parameters used in the computation.[9] Energy is in units of meV and mass is electron rest mass.

materials	$m_{\rm b}$	$\hbar\omega_{\rm LO}$	$\hbar\omega_{\rm TO}$	ε_0	ε_∞	$\varepsilon_{\rm d}$
CdS	0.2	57.2	44.5	9.1	5.5	
HgS	0.036	27.8	22.0	18.2	11.36	
H_2O	1					1.78

The result is shown in Table 2. It can be seen that there are three branches of SO modes for the CdS/HgS QDQW structure. The 1st branch is under the TO phonon frequency of HgS, the 2nd branch is between the LO phonon frequency of HgS and the TO phonon frequency of CdS, and the 3rd branch is between the TO phonon frequency and the LO phonon frequency of CdS.

Table 2. The three branches of eigenfrequencies of SO modes at $\gamma = 0.4$ ($\gamma = R_1/R_2$) for a CdS/HgS QDQW structure. $\hbar\omega$ is in units of meV.

l	1	2	3	∞
$\hbar\omega_{l1}$	17.19	17.57	18.01	19.32
$\hbar\omega_{l2}$	32.06	32.51	32.94	33.26
$\hbar\omega_{l3}$	46.34	47.16	47.43	48.53

3. Interaction between electron and phonons

We start from the well-known Born–Huang equations

$$\ddot{\boldsymbol{w}} = b_{11}\ddot{\boldsymbol{w}} + b_{12}\boldsymbol{E}, \tag{19}$$

and

$$\boldsymbol{P} = b_{21}\boldsymbol{w} + b_{22}\boldsymbol{E}, \tag{20}$$

with

$$b_{11} = -\omega_{\rm LO2}^2, \tag{21a}$$

$$b_{12} = b_{21} = \left[(\varepsilon_{02}-\varepsilon_{\infty 2})/4\pi\right]^{1/2}\omega_{\rm TO2}, \tag{21b}$$

and

$$b_{22} = (\varepsilon_{\infty 2}-1)/4\pi. \tag{21c}$$

For LO modes, we have

$$\boldsymbol{D} = \boldsymbol{E} + 4\pi\boldsymbol{P} = 0. \tag{22}$$

Substituting expression (22) into expression (20), yields

$$\boldsymbol{E} = -(4\pi)^{1/2}\left(\frac{1}{\varepsilon^*}\right)^{1/2}\omega_{\rm LO2}\boldsymbol{w}, \tag{23}$$

where

$$\frac{1}{\varepsilon^*} = \frac{1}{\varepsilon_{\infty 2}} - \frac{1}{\varepsilon_{02}}. \tag{24}$$

This implies that

$$\nabla\phi = (4\pi)^{1/2}\left(\frac{1}{\varepsilon^*}\right)^{1/2}\omega_{\rm LO2}\boldsymbol{w}. \tag{25}$$

For a given mode (l, m), we start with

$$\boldsymbol{w} = \boldsymbol{w}_0 N_{ln}\nabla[g_l(k_{ln})Y_{lm}(\theta,\varphi) + \text{H.c.}]. \tag{26}$$

The kinetic energy density is

$$U_k = \frac{1}{2}\dot{w}^2, \tag{27}$$

and the total energy will be obtained by integrating U_k over the spherical shell, using Green's first identity

$$\int_V \nabla\phi\cdot\nabla\psi \mathrm{d}V = \int_V \phi\,\nabla^2\psi \mathrm{d}V + \int_S \phi\frac{\partial\psi}{\partial n}\mathrm{d}S. \quad (28)$$

In the present case, $\phi = \psi = N_{ln}g_l(k_{ln}r)Y_{lm}(\theta,\varphi)$ and $\phi(R_1) = \phi(R_2) = 0$, so that the integral value at the surface vanishes. After introducing the annihilation and creation operators, a_{lm} and a^+_{lm}, the standard Hamiltonian can be written as

$$H_{ph} = \hbar\omega_{\mathrm{LO}2}[a^+_{lm}a_{lm} + \frac{1}{2}]. \quad (29)$$

For mode (l,m), we thus obtain

$$\boldsymbol{w}(\boldsymbol{r}) = \left[\frac{\hbar N^2_{ln}}{2\omega_{\mathrm{LO}2}k^2_{ln}}\right]^{1/2} \times \{a_{lm}\nabla[g_l(k_{ln}r)Y_{lm}(\theta,\varphi)] + \mathrm{H.c.}\}. \quad (30)$$

From expressions (25) and (30), we obtain the electric potential

$$\phi(\boldsymbol{r}) = \left[\frac{2\pi\hbar\omega_{\mathrm{LO}2}N^2_{ln}}{k^2_{ln}\varepsilon^*}\right]^{1/2} \times [a_{lm}g_l(k_{ln}r)Y_{lm}(\theta,\varphi) + \mathrm{H.c.}]. \quad (31)$$

Considering all the LO modes, we obtain the final result

$$\phi(\boldsymbol{r}) = \sum V_{lmn}[a_{lm}g_l(k_{ln}r)Y_{lm}(\theta,\varphi) + \mathrm{H.c.}], \quad (32)$$

and

$$V_{lmn} = \left[\frac{2\pi\hbar\omega_{\mathrm{LO}2}N^2_{ln}}{k^2_{ln}\varepsilon^*}\right]^{1/2}. \quad (33)$$

The Hamiltonian of electron–LO–phonon interaction is

$$H' = \sum V^L_{lmn}[a_{lm}g_l(k_{ln}r)Y_{lm}(\theta,\varphi) + \mathrm{H.c.}], \quad (34)$$

with

$$V^L_{lmn} = -\left[\frac{2\pi\hbar\omega_{\mathrm{LO}2}\mathrm{e}^2N^2_{ln}}{k^2_{ln}\varepsilon^*}\right]^{1/2}. \quad (35)$$

It is noted that for a QD structure, the eigenfunction of expression (8) will be $g_l(kr) = j_l(kr)$, and $N_l^{-2} = (R_2^3/2)j^2_{l+1}(kR_2)$, thus we have $V^L_{lmn} = [4\pi\hbar\omega_{\mathrm{LO}2}\mathrm{e}^2/k^2_{ln}\varepsilon^*R_2^3j^2_{l+1}(kR_2)]^{1/2}$, which is equivalent to the result in Refs.[3,4].

Now we come to discuss the SO modes. For this case, we have

$$\boldsymbol{E} + 4\pi\boldsymbol{P} = \varepsilon(\omega_{l\alpha})\boldsymbol{E}, \quad (36)$$

where $\alpha = 1$, 2 and 3 refer to the nth branch of the SO modes. Substituting expression (36) into expression (20) yields

$$\boldsymbol{E} = \sqrt{4\pi}\frac{\varepsilon_{\infty 2}}{\varepsilon(\omega_{l\alpha}) - \varepsilon_{\infty 2}}\left(\frac{1}{\varepsilon^*}\right)^{1/2}\omega_{\mathrm{LO}2}\boldsymbol{w}. \quad (37)$$

The relation corresponding to expression (23) is then

$$\nabla\phi = -\sqrt{4\pi}\frac{\varepsilon_{\infty 2}}{\varepsilon(\omega_{l\alpha}) - \varepsilon_{\infty 2}}\left(\frac{1}{\varepsilon^*}\right)^{1/2}\omega_{\mathrm{LO}2}\boldsymbol{w}. \quad (38)$$

For a given mode (l,m), we now start from

$$\boldsymbol{w} = \boldsymbol{w}_0\nabla[(A_lr^l + B_lr^{-l-1})Y_{lm}(\theta,\varphi) + \mathrm{H.c.}], \quad (39)$$

and also use Green's first identity to calculate the energy. But this time it is the volume integral value that vanishes. We introduce the annihilation and creation operators $b_{\alpha lm}$ and $b^+_{\alpha lm}$ for SO-phonons; the relative displacement can be written as

$$\boldsymbol{w} = \left[\frac{2\pi\hbar N_S^2}{\omega_{l\alpha}}\right]^{1/2}\left[b_{\alpha lm}\nabla\left(A_lr^l + B_lr^{-l-1}\right) \times Y_{lm}(\theta,\varphi) + \mathrm{H.c.}\right], \quad (40)$$

with

$$\begin{aligned} N_S^{-2} = {} & 4\pi R_2^2[A_llR_2^{l-1} - B_l(l+1)R_2^{-l-2}] \\ & \times [A_lR_2^l + B_lR_2^{-l-1}] \\ & - 4\pi R_1^2[A_llR_1^{l-1} - B_l(l+1)R_1^{-l-2}] \\ & \times [A_lR_1^l + B_lR_1^{-l-1}]. \end{aligned} \quad (41)$$

Then the electric potential can be written as

$$\phi = \frac{\sqrt{4\pi}\varepsilon_{\infty 2}}{\varepsilon(\omega_{l\alpha}) - \varepsilon_{\infty 2}}\left(\frac{1}{\varepsilon^*}\right)^{1/2}\omega_{\mathrm{LO}2}\left(\frac{2\pi\hbar N_S^2}{\omega_{l\alpha}}\right)^{1/2} \times \left[b_{\alpha lm}\left(A_lr^l + B_lr^{-l-1}\right)Y_{lm}(\theta,\varphi) + \mathrm{H.c.}\right]. \quad (42)$$

The Hamiltonian of the electron–SO–phonon interaction is given by

$$H'' = \sum\left[V^S_{\alpha lm}b_{\alpha lm}\left(A_lr^l + B_lr^{-l-1}\right) \times Y_{lm}(\theta,\varphi) + \mathrm{H.c.}\right], \quad (43)$$

and

$$V^S_{\alpha lm} = -\frac{\sqrt{4\pi}\varepsilon_{\infty 2}\omega_{\mathrm{LO}2}}{\varepsilon(\omega_{l\alpha}) - \varepsilon_{\infty 2}}\left(\frac{1}{\varepsilon^*}\right)^{1/2}\left(\frac{2\pi\hbar N_S^2e^2}{\omega_{l\alpha}}\right)^{1/2}. \quad (44)$$

It is noted that our conclusion is applicable to the case of a QD structure. Let $R_1 = 0$, it becomes the situation for the spherical QD with radius R_2. The

coefficient of electron–SO–phonon interaction then becomes

$$V_{\alpha lm}^{S}=\frac{\sqrt{l}\varepsilon_{\infty 2}\omega_{\mathrm{LO2}}}{\varepsilon_d+l(\varepsilon_d+\varepsilon_{\infty 2})}\left(\frac{1}{\varepsilon^*}\right)^{1/2}\left(\frac{2\pi\hbar e^2}{\omega_{l\alpha}R_2}\right)^{1/2}. \tag{45}$$

The present result is identical to those in Refs.[3, 4].

4. Interaction between impurity and LO phonons

The study of impurity states is important, for the impurities greatly affect both electronic and optical properties of QDQW structures. So we consider the case where the impurity (positively charged centre) is located in the centre of the spherical core and the electron is confined in the spherical shell completely. The Hamiltonian of the system is given as

$$H=H_{\mathrm{e}}+H_{\mathrm{ph}}+H'+H''-\sum[V_{lmn}^{L}g_l(0)Y_{00}(\theta,\varphi)a_{lm}+\mathrm{H.c.}]. \tag{46}$$

The first term on the right-hand side in expression (46) is the Hamiltonian of the electron in a 'vacant' (without phonons) QDQW structure and can be described as

$$H_{\mathrm{e}}=\frac{p^2}{2m_{\mathrm{b}}}+V_w+\frac{\mathrm{e}^2}{\varepsilon_{\infty 2}r}, \tag{47}$$

with

$$V_w=\begin{cases}0, & R_1<r<R_2\\ \infty, & r<R_1, r>R_2\end{cases}. \tag{48}$$

The second term on the right-hand side in expression (46) is the phonon Hamiltonian

$$H_{\mathrm{ph}}=\sum\hbar\omega_{\mathrm{LO2}}a_{lm}^{+}a_{lm}+\sum\hbar\omega_{l\alpha}b_{\alpha lm}^{+}b_{\alpha lm}. \tag{49}$$

In expression (46), H' and H'' are the interaction Hamiltonians of electron–LO–phonon and electron–SO–phonon, which are given in expressions (34) and (43), respectively.

The last term on the right-hand side in expression (46) describes the interaction between the impurity and the LO phonons. This contribution can be eliminated by means of a first canonical transformation,[20] whose function is to displace the equilibrium position of the ions

$$U=\exp\left\{\sum V_{lmn}^{L}[g_l(k_{ln}r)Y_{lm}(\theta,\varphi)a_{lm}+\mathrm{H.c.}]\right\}. \tag{50}$$

Apart from the nonphysical divergent term arising from the use of the point-charge model, the effect of this displacement on lattice polarization leads to the following exchange interaction:

$$H_x=\sum\frac{|V_{lmn}^{L}|^2}{\hbar\omega_{\mathrm{LO2}}}g_l(0)Y_{00}[g_l(k_{ln}r)Y_{lm}(\theta,\varphi)+\mathrm{H.c.}]. \tag{51}$$

After straightforward summation, we obtain

$$H_x=\frac{e^2}{\varepsilon^* r}\left(1-\frac{r-R_1}{R_2-R_1}\right). \tag{52}$$

In the present situation, the impurity is located in the centre of the spherical QD structure. The SO phonons make no contribution to the exchange interaction, so we consider only impurity–LO–phonon interaction. Note that when $R_1=0$, expression (52) becomes the expression for the QD structure.[3,4]

5. Bound polarons in QDQW structures

Now we discuss an electron confined in the well of a QDQW structure, completely interacting with the positively charged centre and the phonons as well. The effective Hamiltonian of the system is given by

$$H=H_{\mathrm{e}}+H_x+H_{\mathrm{ph}}+H'+H''. \tag{53}$$

Within the adiabatic approximation, the effect of the e–p interaction is to displace the equilibrium positions of the ions. This can be achieved by performing a canonical transformation corresponding to the bulk and the surface modes

$$U=\exp\left[\sum(f_{lmn}a_{lm}+\mathrm{H.c.})+\sum(f_{\alpha lm}b_{\alpha lm}+\mathrm{H.c.})\right], \tag{54}$$

where the parameters f_{lmn} and $f_{\alpha lm}$ will be determined by using the variational technique later. The total wave function of the system is given by the product

$$\Psi=U\,|\psi\rangle\,|0\rangle, \tag{55}$$

where $|0\rangle$ is the zero-phonon state, and $|\psi\rangle$ is an electronic wavefunction.

In order to describe the electronic ground state using the variational technique, we choose the trial wavefunction as follows:

$$\psi(r)=N\frac{\sin(k(r-R_1))}{kr}\mathrm{e}^{-\beta k\,r}, \tag{56}$$

where β is the variational parameter, and $k = \pi/(R_2 - R_1)$ that is obtained from the boundary condition $\psi(R_2) = 0$. After some calculations we obtain the total energy of the system

$$E = E_k + E_p + E_{\rm I}. \tag{57}$$

The first term on the right-hand side in expression (57) is the kinetic energy of the electron, expressed as

$$E_k = \frac{\hbar^2 k^2}{2m_{\rm b}}(1+\beta^2). \tag{58}$$

The second term on the right-hand side in expression (57) is the potential energy, given by

$$E_p = \langle\psi| - \frac{{\rm e}^2}{\varepsilon_{\infty 2} r} + H_x|\psi\rangle = \boldsymbol{E}_1 + \boldsymbol{E}_2 \tag{59}$$

with

$$E_1 = -\frac{{\rm e}^2 k}{\varepsilon_{02}} \frac{4\beta(1+\beta^2)}{{\rm e}^{-2\beta k R_1} - {\rm e}^{-2\beta k R_2}} I_1, \tag{60a}$$

$$E_2 = -\frac{{\rm e}^2 k}{\pi\varepsilon^*} \frac{4\beta(1+\beta^2)}{{\rm e}^{-2\beta k R_1} - {\rm e}^{-2\beta k R_2}} I_2, \tag{60b}$$

and

$$I_1 = \int_0^\pi \frac{{\rm d}x}{x + kR_1} \sin^2 x\, {\rm e}^{-2\beta(x+kR_1)}, \tag{61a}$$

$$I_2 = \int_0^\pi \frac{x{\rm d}x}{x + kR_1} \sin^2 x\, {\rm e}^{-2\beta(x+kR_1)}. \tag{61b}$$

The last term on the right-hand side in expression (57) is the e–p interaction energy expressed as

$$E_{\rm I} = \langle 0|\langle\psi|U^{-1}(H_{\rm ph} + H' + H'')U|\psi\rangle|0\rangle. \tag{62}$$

Solving equations $\partial E_{\rm I}/\partial f_{lmn} = 0$ and $\partial E_{\rm I}/\partial f_{\alpha lm} = 0$, one can obtain the following parameters f_{lmn} and $f_{\alpha lm}$:

$$f_{lmn} = -V^L_{lmn} \frac{F_{lmn}}{\hbar\omega_{\rm LO2}} \tag{63a}$$

and

$$f_{\alpha lm} = -V^S_{\alpha lm} \frac{F_{\alpha lm}}{\hbar\omega_{l\alpha}}, \tag{63b}$$

with

$$F_{lmn} = \langle\psi|g_l(k_{ln}r)Y_{lm}(\theta,\varphi)|\psi\rangle, \tag{64a}$$

and

$$F_{\alpha lm} = \langle\psi|(A_l r^l + B_l r^{-l-1})Y_{lm}(\theta,\varphi)|\psi\rangle. \tag{64b}$$

Substituting expressions (34), (43), (49), (63) and (64) into expression (62), we have

$$E_{\rm I} = -\sum \frac{|V^L_{lmn}|^2 |F_{lmn}|^2}{\hbar\omega_{\rm LO2}} - \sum \frac{|V^S_{\alpha lm}|^2 |F_{\alpha lm}|^2}{\hbar\omega_{l\alpha}}. \tag{65}$$

Using expressions (56) and (65) yields

$$E_{\rm I} = -\frac{{\rm e}^2 k}{\varepsilon^*} \frac{4^3\beta^2(1+\beta^2)^2}{({\rm e}^{-2\beta k R_1} - {\rm e}^{-2\beta k R_2})^2} \sum_{n=1}^{\infty} \frac{I_n^2}{n^2}, \tag{66}$$

where

$$I_n = \int_0^\pi \frac{{\rm d}x}{x + kR_1} \sin^2(x)\sin(nx) \times \exp[-2\beta(x + kR_1)]. \tag{67}$$

The binding energy of the bound polaron can be determined by

$$E_b = \frac{\hbar^2}{2m}\left(\frac{\pi}{\Delta R}\right)^2 - E, \tag{68}$$

with

$$\Delta R = (1-\gamma)R_2. \tag{69}$$

The CdS/HgS QDQW structure is numerically investigated. The material parameters used in the calculation are listed in Table 1, and $R_2 = 100$Å (1 Å=0.1 nm). The dependence of the polaron binding energy on the spherical shell width is shown in Fig.1. The width of shell is described by the parameter γ. Figure 2 shows the trapping energy, determined by $E_{\rm tr} = |E_{\rm I}|$, as a function of the parameter γ. It can be seen that the binding energy and the trapping energy increase as R_1 decreases, with the outer radius fixed, and the trapping energy takes a major part of the binding energy when R_1 is very small.

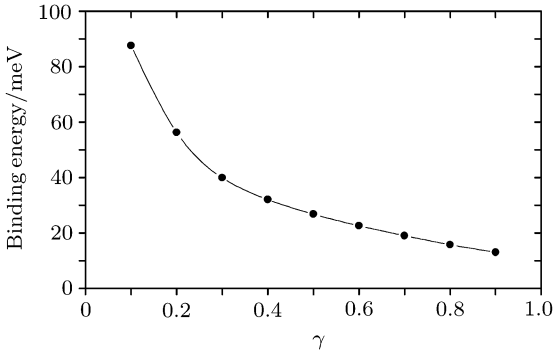


Fig.1. Binding energy of a bound polaron as a function of the parameter γ.

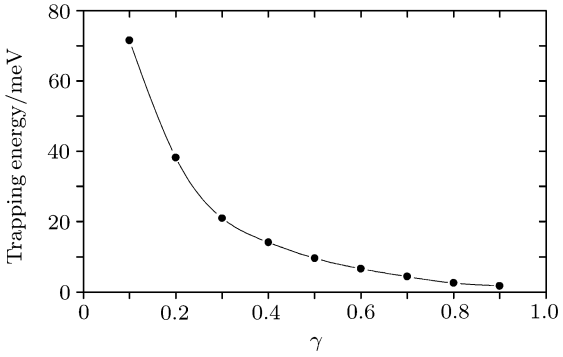


Fig.2. Trapping energy of a bound polaron as a function of the parameter γ.

6. Conclusions

We have investigated the bound polaron in quantum dot quantum well (QDQW) structures. The eigenfrequencies of bulk longitudinal optical (LO) and surface optical (SO) modes are derived in the framework of the dielectric continuum approximation. The eigenfrequencies of the SO mode for CdS/HgS QDQW structures are calculated. It is found that there exist three branches of eigenfrequencies of SO modes and the eigenfrequency is dependent on mode order and ratio between the inner radius and the outer radius of the QDQW structure. By quantizing the vibration eigenmodes, we have obtained the electron–phonon interaction Hamiltonian and the exchange interaction between impurity and LO-phonons for the QDQW structures. The binding energy and the trapping energy of the bound polaron in QDQW structures are calculated. It is shown that the binding energy and the trapping energy increase as the inner radius of the QDQW structure decreases, with the outer radius fixed, and the trapping energy takes a major part of the binding energy when the inner radius is very small.

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