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## Electron-phonon effects on Stark shifts of bound polarons in quantum dot quantum well nanostructures

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### ABSTRACT

Electron-phonon effects on Stark shifts of bound polarons in quantum dot quantum well nanostructures are studied theoretically by using a variational approach. The binding energy of the hydrogenic impurity state is calculated by taking the interaction of an electron with both the longitudinal optical phonons and the surface optical phonons into account. The interaction between impurity and longitudinal optical phonons has also been considered to obtain the binding energy of bound polarons. The numerical results for a CdS/HgS quantum dot quantum well nanostructure show that the Stark shift obviously increases as the core radius increases with the outer radius of spherical shell fixed and the electron-phonon effects give significant corrections to the binding energy. © 2010 Trade Science Inc. - INDIA

### INTRODUCTION

During the past few years, there has been considerable interest in investigating quantum dots (QD) both experimentally and theoretically<sup>[1-8]</sup>. Since 1993, a new kind of QD structure, called quantum dot quantum well (QDQW) nanostructure, has been fabricated and studied<sup>[9-17]</sup>. The semiconductor materials usually used to synthesize QDQW nanostructures are CdS/HgS, ZnSe/CdSe, CdS/PbS, etc. The material with a smaller bulk band gap(shell material, such as HgS) is embedded between a core with a larger bulk band gap(core material, such as CdS) and a nonpolar medium(such as water), so the material with the smaller bulk band gap acts as a shell material for the electron and hole as well as the phonon in the polar crystal. The QDQW nanostructures display quite interesting physical properties and appear to have promising perspectives in the

streaming progress of nanostructured device technology.

The electron-phonon interaction plays an important role in determining the physical properties of QDQW nanostructures. A previous work<sup>[13]</sup> studied the electron-phonon interaction in a QDQW nanostructure and calculated the ground state and excited state electron energy levels using the dielectric continuum approach. Interesting results concerning the dependence of polaronic corrections with the QDQW nanostructure size are analyzed. Schrier et al.<sup>[14]</sup> considered the electronic nanostructures of CdS/CdSe/CdS QDQWs by large-scale pseudopotential local density approximation. Their calculation found that the wave functions, eigenvalues, Coulomb interaction, and exciton energy change according to the sizes of the core, well, and shell. The authors have recently derived the electron-phonon interaction Hamiltonian for QDQW

nanostructures and calculated the binding energy and the trapping energy of the bound polarons in CdS/HgS QDQW nanostructures<sup>[17]</sup>.

The application of an external electric field in the low-dimensional quantum system, induces both a polarization of the carrier distribution and an energy shift of the quantum states. This property has significant effect on optoelectronic devices. The quantum-confined Stark effects have been extensively investigated for both QWs<sup>[18-20]</sup>, and QDs<sup>[21-26]</sup>. Huangfu et al.<sup>[24]</sup> studied the bound polaron in a spherical quantum dot structure under an electric field. They calculated the binding energy of the hydrogenic impurity state and found that the polaron effects give significant corrections to the binding energy and its Stark shift. However, up to now, only a few authors have investigated the polaron problem in QDQW nanostructures and the electron-phonon effects on Stark shifts for QDQW nanostructures have rarely been studied.

In this paper, electron-phonon effects on Stark shifts of bound polarons in QDQW nanostructures are studied theoretically by using a variational approach. The binding energy of the hydrogenic impurity state is calculated by taking the interaction of an electron with both the bulk longitudinal optical phonons and the surface optical phonons into account. The exchange interaction between impurity states and longitudinal optical phonons has also been considered to obtain the binding energy of the bound polaron. The numerical calculations for CdS/HgS QDQW nanostructure embedded in water have been carried out. The results reveal that the electron-phonon effects give significant corrections to the Stark shift. Electron-phonon contribution to the binding energy decreases significantly with increasing the electric-field strength. It is also found that the binding energy increase as the core radius of the QDQW nanostructure decreases while the outer radius of the shell is fixed.

## THEORY

We consider an electron confined in the well of a QDQW nanostructure, completely interacting with the positively charged centre and the phonons in an external electric field along the z-direction. The Hamiltonian of the system is given as

$$\mathbf{H} = \mathbf{H}_e + \mathbf{H}_{ph} + \mathbf{H}_x + \mathbf{H}' + \mathbf{H}'' \quad (1)$$

The first term in Eq.(1) is the Hamiltonian of the electron in a 'vacant'(without phonons) QDQW nanostructure and can be described as,

$$\mathbf{H}_e = \frac{\mathbf{p}^2}{2m_b} + \mathbf{V}(\mathbf{r}) - \frac{e^2}{\epsilon_\infty r} + e\mathbf{F}r \cos \theta \quad (2)$$

where  $m_b$  and  $e$  are the electron effective mass and charge, and  $\epsilon_\infty$  is the high-frequency dielectric constant of the shell material.  $r$  is the distance between the electron and the impurity site.  $F$  is the electric field intensity and  $\theta$  is the angle between the position vector and the electric field.  $V(r)$  is the confining potential of the QDQW nanostructure and is given by

$$\mathbf{V}(\mathbf{r}) = \begin{cases} 0, R_1 < r < R_2 \\ \infty, r < R_1, r > R_2 \end{cases} \quad (3)$$

where  $R_1$  and  $R_2$  are the radii of the spherical core and spherical shell.

The second term in Eq. (1) is the phonon Hamiltonian

$$\mathbf{H}_{ph} = \sum \mathbf{h}\omega_{LO} \mathbf{a}_{lm}^+ \mathbf{a}_{lm} + \sum \mathbf{h}\omega_{\alpha} \mathbf{b}_{\alpha lm}^+ \mathbf{b}_{\alpha lm} \quad (4)$$

where  $\mathbf{a}_{lm}^+$  ( $\mathbf{a}_{lm}$ ) is the creation(annihilation) operator for the confined LO phonons with frequency  $\omega_{LO}$ .  $\mathbf{b}_{\alpha lm}^+$  ( $\mathbf{b}_{\alpha lm}$ ) is the corresponding operator for SO phonons with frequency  $\omega_{\alpha}$  and  $\alpha = 1, 2$  and 3 refer to the  $n^{\text{th}}$  branch of the SO modes, which are given in Ref.<sup>[17]</sup>.

The last three terms in Eq. (1) describe the interaction Hamiltonian, reflecting the fact that both the impurity and the electron interact with phonons and can be written as<sup>[17]</sup>,

$$\mathbf{H}_x = \frac{e^2}{\epsilon^* r} \left( 1 - \frac{r - R_1}{R_2 - R_1} \right) \quad (5)$$

$$\mathbf{H}' = \sum \mathbf{V}_{nlm}^L [\mathbf{a}_{lm} \mathbf{g}_l(\mathbf{k}_n \mathbf{r}) \mathbf{Y}_{lm}(\theta, \phi) + \mathbf{H.c.}] \quad (6)$$

and

$$\mathbf{H}'' = \sum \mathbf{V}_{\alpha lm}^S [\mathbf{b}_{\alpha lm} (\mathbf{A}_1 \mathbf{r}^l + \mathbf{B}_1 \mathbf{r}^{l-1}) \mathbf{Y}_{lm}(\theta, \phi) + \mathbf{H.c.}] \quad (7)$$

where

$$\frac{1}{\epsilon^*} = \frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0} \quad (8)$$

$\epsilon_0$  is the static dielectric constant of the shell material, and

$$\mathbf{g}_l(\mathbf{k}_n \mathbf{r}) = n_l(\mathbf{k}_n \mathbf{R}_1) j_l(\mathbf{k}_n \mathbf{r}) - j_l(\mathbf{k}_n \mathbf{R}_1) n_l(\mathbf{k}_n \mathbf{r}) \quad (9)$$

where  $j_l(x)$  and  $n_l(x)$  are the spherical Bessel function and spherical Neumann function of order  $l$  ( $l = 0, 1, 2,$

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3...).  $Y_{lm}(\theta, \phi)$  are the spherical harmonic functions with  $m = 0, \pm 1, \dots, \pm l$ . The constants  $k_{nl}$  are chosen so that  $g_{nl}(k_{nl}R_2) = 0$ . If  $x_n$  is the  $n^{\text{th}}$  zero of equation  $g_1(x) = 0$ , then  $k_{nl} = x_n/R_2$ .

The electron-phonon coupling coefficients are given by

$$V_{nlm}^L = -\left[\frac{2\pi\hbar\omega_{LO}e^2N_{nl}^2}{k_{nl}^2\epsilon^*}\right]^{\frac{1}{2}} \quad (10)$$

and

$$V_{\alpha lm}^S = -\frac{\sqrt{4\pi\epsilon_\infty\omega_{LO}}}{\epsilon(\omega_{l\alpha}) - \epsilon_\infty}\left(\frac{1}{\epsilon^*}\right)^{\frac{1}{2}}\left(\frac{2\pi\hbar N_s^2 e^2}{\omega_{l\alpha}}\right)^{\frac{1}{2}} \quad (11)$$

where  $N_{nl}$  and  $N_s$  are the normalization constants of eigenfunctions of longitudinal optical phonons and the surface optical phonons, respectively.

Within the adiabatic approximation, the effect of the electron-phonon interaction is to displace the equilibrium positions of the ions. This can be achieved by performing a canonical transformations corresponding to the bulk and the surface modes.

$$U = \exp\left[\sum\left(a_{nlm}^+ f_{nlm}^* - H.c.\right) + \sum\left(b_{\alpha lm}^+ f_{\alpha lm}^* - H.c.\right)\right] \quad (12)$$

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

$$|\Psi\rangle = U|\psi\rangle|0\rangle \quad (13)$$

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

In order to describe the electronic ground state by means of variational technique, we chose the trial wave function as follows.

$$|\psi\rangle = N\frac{\sin k(\mathbf{r} - \mathbf{R}_1)}{r}e^{-\beta kr}e^{-\mu k r \cos\theta} \quad (14)$$

where  $N$  is the normalization constant,  $\beta$  and  $\mu$  are

variational parameters, and  $\mathbf{k} = \frac{\pi}{\mathbf{R}_2 - \mathbf{R}_1}$  is obtained

from the boundary condition  $\psi(R_2) = 0$ . After some calculations we obtain the total energy of the system

$$E = E_k + E_p + E_1 \quad (15)$$

The first term in Eq. (15) is kinetic energy of the electron, and

$$E_k = \left\langle \psi \left| -\frac{\hbar^2 \nabla^2}{2m_b} \right| \psi \right\rangle$$

$$= -\frac{\pi N^2 \hbar^2}{m_b} \int_{R_1}^{R_2} \left[ \sin^2 k(\mathbf{r} - \mathbf{R}_1) e^{-2k r(\beta - \mu)} \left( -\frac{k\mu}{2r} + \frac{1}{2r^2} - \frac{k\beta}{r} + \frac{\beta}{2\mu r^2} + \frac{k\beta^2}{2\mu r} - \frac{k}{2\mu r} \right) \right.$$

$$\left. + \sin^2 k(\mathbf{r} - \mathbf{R}_1) e^{-2k r(\beta + \mu)} \left( -\frac{k\mu}{2r} - \frac{1}{2r^2} - \frac{k\beta}{r} - \frac{\beta}{2\mu r^2} - \frac{k\beta^2}{2\mu r} + \frac{k}{2\mu r} \right) \right.$$

$$\left. + \cos k(\mathbf{r} - \mathbf{R}_1) \sin k(\mathbf{r} - \mathbf{R}_1) e^{-2k r(\beta - \mu)} \left( \frac{k}{r} - \frac{1}{2\mu r^2} - \frac{k\beta}{\mu r} \right) \right.$$

$$\left. + \cos k(\mathbf{r} - \mathbf{R}_1) \sin k(\mathbf{r} - \mathbf{R}_1) e^{-2k r(\beta + \mu)} \left( \frac{k}{r} + \frac{1}{2\mu r^2} + \frac{k\beta}{\mu r} \right) \right] dr \quad (16)$$

The second term in Eq. (15) is the potential energy given by

$$E_p = \left\langle \psi \left| -\frac{e^2}{\epsilon_\infty r} + H_x + eFr \cos\theta \right| \psi \right\rangle = E_1 + E_2 + E_3 \quad (17)$$

with

$$E_1 = -\frac{\pi e^2 N^2}{\epsilon_0 \mu k} \int_{R_1}^{R_2} \frac{\sin^2 k(\mathbf{r} - \mathbf{R}_1)}{r^2} e^{-2\beta kr} (e^{2\mu kr} - e^{-2\mu kr}) dr \quad (18)$$

$$E_2 = -\frac{\pi e^2 N^2}{\epsilon^* \mu k} \int_{R_1}^{R_2} \frac{r - \mathbf{R}_1}{R_2 - \mathbf{R}_1} \frac{\sin^2 k(\mathbf{r} - \mathbf{R}_1)}{r^2} e^{-2\beta kr} (e^{2\mu kr} - e^{-2\mu kr}) dr \quad (19)$$

and

$$E_3 = 2\pi e FN^2 \int_{R_1}^{R_2} \left[ \sin^2 k(\mathbf{r} - \mathbf{R}_1) e^{-2k r(\beta - \mu)} \left( -\frac{1}{2\mu k} + \frac{1}{4\mu^2 k^2 r} \right) + \sin^2 k(\mathbf{r} - \mathbf{R}_1) e^{-2k r(\beta + \mu)} \left( -\frac{1}{2\mu k} - \frac{1}{4\mu^2 k r} \right) \right] dr \quad (20)$$

The last term in Eq. (15) is the electron-phonon interaction energy given by

$$E_1 = \langle 0 | \langle \psi | U^{-1} (H_{ph} + H' + H'') U | \psi \rangle | 0 \rangle \quad (21)$$

Solving the minimum equation  $\partial E_1 / \partial f_{nlm} = 0$  and  $\partial E_1 / \partial f_{\alpha lm} = 0$ , one can obtain the parameters  $f_{nlm}$  and  $f_{\alpha lm}$  as follows,

$$f_{nlm} = -V_{nlm}^L \frac{F_{nlm}}{\hbar \omega_{LO}} \quad (22a)$$

$$f_{\alpha lm} = -V_{\alpha lm}^S \frac{F_{\alpha lm}}{\hbar \omega_{l\alpha}} \quad (22b)$$

with

$$F_{nlm} = \langle \psi | g_l(\mathbf{k}_l, \mathbf{r}) Y_{lm}(\theta, \phi) | \psi \rangle \quad (23a)$$

$$F_{\alpha lm} = \langle \psi | (A_l r^l + B_l r^{l-1}) Y_{lm}(\theta, \phi) | \psi \rangle \quad (23b)$$

Substituting Eqs. (4), (6), (7), (22), (23) into Eq. (21), we have

$$E_l = -\sum \frac{|V_{nlm}^L|^2 |F_{nlm}|^2}{\hbar \omega_{LO}} - \sum \frac{|V_{\alpha lm}^S|^2 |F_{\alpha lm}|^2}{\hbar \omega_{\alpha}} \quad (24)$$

The binding energy of the bound polaron can be defined by

$$E_b = E_{\text{free}} - E \quad (25)$$

The corresponding Hamiltonian for a free polaron is written as

$$H_{\text{free}} = \frac{\mathbf{p}^2}{2m_b} + V(\mathbf{r}) + H_{\text{ph}} + H' + H'' + eF r \cos \theta \quad (26)$$

We choose the trial wave function

$$|\Psi'\rangle = U |\psi'\rangle |0\rangle \quad (27)$$

with the trial wave function for the electron

$$|\psi'\rangle = N \frac{\sin k(\mathbf{r} - \mathbf{R}_1)}{r} e^{-\lambda k r \cos \theta} \quad (28)$$

where  $\lambda$  is variational parameter. The ground-state energy of the free polaron can be obtained by a variational procedure.

$$E_{\text{free}} = \min_{\lambda} \frac{\langle \Psi' | H_{\text{free}} | \Psi' \rangle}{\langle \Psi' | \Psi' \rangle} \quad (29)$$

## NUMERICAL RESULTS AND DISCUSSION

The binding energies of bound polarons in the CdS/HgS QDQW nanostructure with an applied electric field have been computed numerically by the variational approach and the results are illustrated in figure 1-4. The material parameters used in the calculation are listed in TABLE 1.

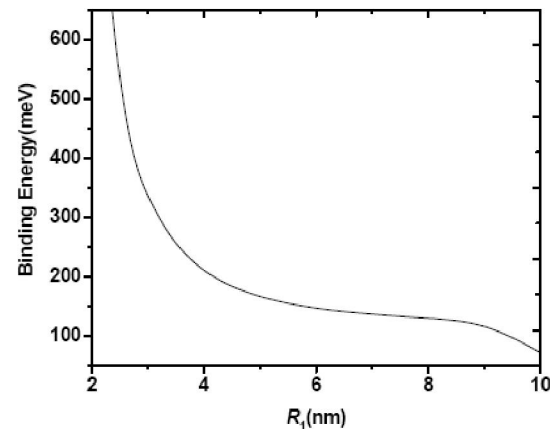
**TABLE 1 : Values of the physical parameters used in the computations<sup>[17]</sup>. Energies are measured in meV and masses in the electron rest mass**

Materials	$m_b$	$\hbar \omega_{LO}$	$\hbar \omega_{TO}$	$\epsilon_0$	$\epsilon_\infty$	$\epsilon_d$
CdS	0.2	57.2	44.5	9.1	5.5	
HgS	0.036	27.8	22.0	18.2	11.36	
H <sub>2</sub> O	1					1.78

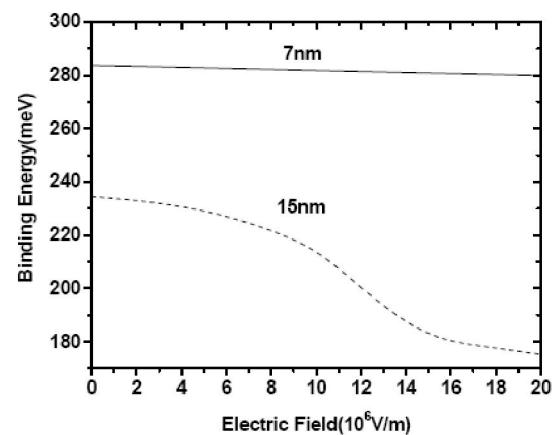
The binding energy of bound polaron as a function of the spherical core radius in CdS/HgS QDQW

nanostructure with the outer radius of spherical shell  $R_2=15\text{nm}$  at the electric field  $F=5 \times 10^6\text{V/m}$  is plotted in figure 1. It is clearly seen that the binding energy of a bound polaron decreases when the core radius increases. This is due to the fact that the well-width is reduced with the increasing core radius when the outer radius of spherical shell is fixed.

To clearly understand the influences of the electron field on the binding energy of bound polaron, we have also plotted the curves of the binding energy of a bound polaron as functions of the electric field in the CdS/HgS QDQW nanostructure for outer radii of spherical shells  $R_2=7\text{nm}$  and  $15\text{nm}$  in figure 2, respectively. It is found that the binding energy of a bound polaron decreases monotonously with increasing the electric-field intensity. The Stark shifts are considerably enhanced



**Figure 1 : Binding energy of a bound polaron as a function of the spherical core radius  $R_1$  in the CdS/HgS QDQW nanostructure with the outer radius of spherical shell  $R_2=15\text{nm}$  at the electric field  $F=5 \times 10^6\text{V/m}$**



**Figure 2 : Binding energies of a bound polaron with the spherical core radius  $R_1=3.5\text{nm}$  as functions of the electric field in the CdS/HgS QDQW nanostructure for the outer radii of spherical shells  $R_2=7\text{nm}$  and  $15\text{nm}$ , respectively**

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when the outer radius of spherical shell becomes larger. For example, the binding energies are reduced by 25.3% for the outer radius of spherical shell  $R_2=15\text{nm}$ , but only 1.2% for  $R_2=7\text{nm}$ , as an electric field of  $F=20\times 10^6\text{V/m}$  is supplied.

Figures 3 and 4 illustrate the Stark shifts and contribution of the electron-phonon interaction to the binding energies of a bound polaron as functions of the core radius in the CdS/HgS QDQW nanostructure with the outer radius of spherical shell fixed at 15nm, respectively. It is shown that Stark shift obviously increases with increasing core radius. The contribution of the electron-phonon interaction to the binding energies decreases with increasing core radius and the polaron effect is un-negligible.

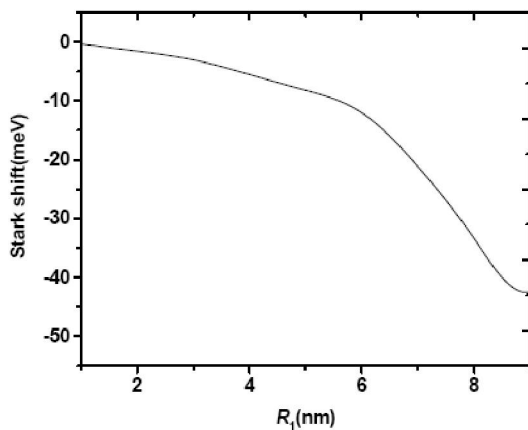


Figure 3 : Stark shift of a bound polaron as a function of the spherical core radius  $R_1$  in the CdS/HgS QDQW nanostructure with the outer radius of spherical shell  $R_2=15\text{nm}$  at the electric field  $F=5\times 10^6\text{V/m}$

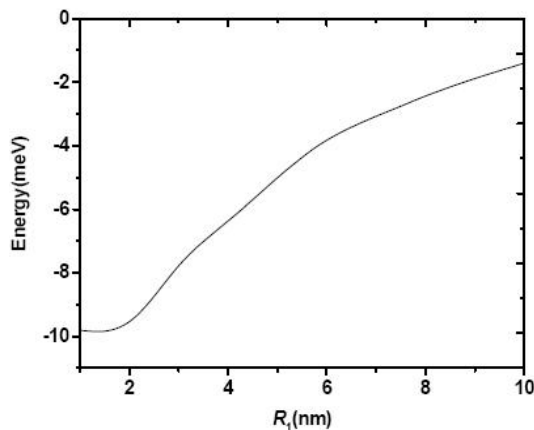


Figure 4 : The electron-phonon interaction to the binding energy of a bound polaron as a function of the spherical core radius  $R_1$  in the CdS/HgS QDQW nanostructure with the outer radius of spherical shell  $R_2=15\text{nm}$  at the electric field  $F=5\times 10^6\text{V/m}$

## CONCLUSIONS

In conclusion, we have studied theoretically the electron-phonon effects on Stark shifts of bound polarons in the quantum dot quantum well nanostructure by using a variational approach. The binding energy of the hydrogenic impurity state is calculated by taking the interaction of an electron with both the longitudinal optical phonons and the surface optical phonons into account. The interaction between impurity and longitudinal optical phonons has also been considered to obtain the binding energy of bound polarons. The numerical results for a CdS/HgS quantum dot quantum well nanostructure show that the binding energy of the bound polaron decrease monotonously with increasing core radius and the electric-field intensity, respectively. Stark shift obviously increases with increasing core radius, while the contribution of the electron-phonon interaction to the binding energies decreases with increasing core radius, and the polaron effect is un-negligible.

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