Vol 14 No 11, November 2005
1009-1963/2005/14(11)/2314-06
Chinese Physics
© 2005 Chin. Phys. Soc.
and IOP Publishing Ltd

On the binding energies of excitons in polar quantum well structures in a weak electric field*

Wu Yun-Feng(吴云峰)[a], Liang Xi-Xia(梁希侠)[a]†, and K. K. Bajaj[b]

[a] *Department of Physics, Inner Mongolia University, Hohhot 010021, China*

[b] *Department of Physics, Emory University, Atlanta, GA 30322, USA*

(Received 16 May 2005; revised manuscript received 27 June 2005)

The binding energies of excitons in quantum well structures subjected to an applied uniform electric field by taking into account the exciton longitudinal optical phonon interaction is calculated. The binding energies and corresponding Stark shifts for III–V and II–VI compound semiconductor quantum well structures have been numerically computed. The results for GaAs/AlGaAs and ZnCdSe/ZnSe quantum wells are given and discussed. Theoretical results show that the exciton–phonon coupling reduces both the exciton binding energies and the Stark shifts by screening the Coulomb interaction. This effect is observable experimentally and cannot be neglected.

Keywords: quantum confined stark effects, exciton, quantum well
PACC: 7320D, 6320K, 7135, 3260S

1. Introduction

Much attention has been paid recently to optical properties of heterostructures, such as superlattices, quantum wells, etc., due to the fact that these systems offer a promising class of materials for a variety of opto-electronic device applications.[1−5] Since excitonic effects play an important role in optical phenomena in semiconductor materials, the behaviour of excitons in quantum wells (QWs) has been extensively investigated both theoretically and experimentally. The stability of excitons in an external electric field is particularly important for designing new types of high-speed electro-optical devices.

In Refs.[6–8] electric-field-induced excitonic absorption peaks in QW structures were observed and found to shift significantly to lower energies accompanied by some broadening. This phenomenon is attributed to the fact that the applied electric field perpendicular to the well plane pushes the electrons and holes towards opposite sides of the layers and thus reduces the exciton binding energies and the transition energies. This phenomenon is often referred to as quantum-confined Stark effect (QCSE).[6] Some authors have calculated the electric field dependence of the exciton binding energy without taking into account the exciton–phonon interaction.[9−13] On the other hand, the effects of the electron–phonon (e–p) interaction on the exciton binding energies in QWs have also been investigated by using various theoretical methods.[14−19] Different conclusions were drawn for the e–p effect enhancing or reducing of the exciton binding energy. Generally, it is understood that the e–p interaction causes a decrease in the exciton binding energy. A few effective interaction potentials between an electron and a hole in the longitudinal optical (LO) phonon field in a QW were derived and used to calculate the exciton binding energies.[17−19] However, to our knowledge, the effect of e–p interaction on the exciton binding energy in QW structures in an external electric field has not been studied yet.

In this paper, a variational method is used to investigate the binding energies and the Stark shift of excitons in QWs by including the effect of optical phonons in an external electric field. An effective electron–hole potential has been used to take into ac-

*Project supported in part by the National Natural Science Foundation of China (Grant No 10164003) and the Natural Science Foundation of Inner Mongol of China (Grant No 200408020101).
†Corresponding author. E-mail: xxliang@imu.edu.cn

count their interactions with the optical phonon field. Numerical calculations for several III–V and II–VI compound QWs have been performed. The results for $GaAs/Al_{0.3}Ga_{0.7}As$ and $Zn_{0.69}Cd_{0.31}Se/ZnSe$, as examples, are given. And the effects of the electron–phonon interaction on the binding energy and Stark effects of excitons are discussed.

2. Hamiltonian

Let us consider an exciton consisting of an electron and a hole confined completely in a polar QW of width $2d$ in the presence of a uniform weak electric field perpendicular to the interface of the well. The origin of the coordinate system is set at the centre of the well. The well material is confined in the range $|z| \leq d$ and the barrier material in the spaces $|z| > d$. The electron and the hole are coupled together to form an exciton by an attractive Coulomb potential. Both of them also interact with the LO-phonon field.

Within the framework of the effective mass approximation and taking into account the exciton–phonon field coupling, the system Hamiltonian can be written as

$$\begin{aligned} H =& \frac{P_{\mathrm{R}}^2}{2M_{\parallel}} + \frac{P_{\rho}^2}{2\mu_{\parallel}} + \frac{P_{\mathrm{e}z}^2}{2m_{\mathrm{e}}} + \frac{P_{\mathrm{h}z}^2}{2m_{\mathrm{h}\perp}} + V(z_{\mathrm{e}}) + V(z_{\mathrm{h}}) \\ & - \frac{e^2}{\varepsilon_{\infty}\sqrt{(z_{\mathrm{e}} - z_{\mathrm{h}})^2 + \rho^2}} \\ & + H_{\mathrm{F}} + H_{\mathrm{ph}} + H_{\mathrm{ex-ph}}. \end{aligned} \tag{1}$$

Here $\boldsymbol{R}$ is the mass-centre coordinate and $\boldsymbol{\rho} = \boldsymbol{\rho}_{\mathrm{e}} - \boldsymbol{\rho}_{\mathrm{h}}$ the relative coordinate of the electron–hole system in $x - y$ plane. $\boldsymbol{P}_{\mathrm{R}}$ and $\boldsymbol{P}_{\rho}$ are respectively the corresponding centre of mass and relative momenta. $M_{\parallel}$ and $\mu_{\parallel}$ are the total mass and the reduced mass in the $x - y$ plane respectively, given by

$$M_{\parallel} = m_{\mathrm{e}} + m_{\mathrm{h}\parallel}, \quad \mu_{\parallel} = \frac{m_{\mathrm{e}} m_{\mathrm{h}\parallel}}{m_{\mathrm{e}} + m_{\mathrm{h}\parallel}}, \tag{2}$$

where $m_{\mathrm{e}\parallel}$ and $m_{\mathrm{h}\parallel}$ are respectively the masses of the electron and hole in $x - y$ plane and $m_{\mathrm{e}\perp}$ and $m_{\mathrm{h}\perp}$ are the masses along the z-direction. We have assumed that the mass of the electron is isotropic, i.e. $m_{\mathrm{e}\parallel} = m_{\mathrm{e}\perp} = m_{\mathrm{e}}$. The hole masses $m_{\mathrm{h}\perp}$ and $m_{\mathrm{h}\parallel}$ are determined from the Kohn–Luttinger parameters γ_1 and γ_2 as[9,20]

$$\frac{1}{m_{\mathrm{h}\perp}} = \frac{1}{m_0}(\gamma_1 - 2\gamma_2), \tag{3a}$$

$$\frac{1}{m_{\mathrm{h}\parallel}} = \frac{1}{m_0}(\gamma_1 + \gamma_2), \tag{3b}$$

where m_0 is the free electron mass.

Since our attention is focused on the bound state of the exciton, the centre of mass momentum $\boldsymbol{P}_{\mathrm{R}}$ will be omitted hereafter. The infinitely deep potential well approximation will be used for the confining potentials V_{e} and V_{h} of the electron and the hole respectively, i.e.

$$V_{\mathrm{e,h}} = \begin{cases} \infty, & |z_{\mathrm{e,h}}| > d, \\ 0, & |z_{\mathrm{e,h}}| \leq d. \end{cases} \tag{4}$$

The electric field energy H_{F} of the electron–hole system in the external field F is given by

$$H_{\mathrm{F}} = eF(z_{\mathrm{e}} - z_{\mathrm{h}}). \tag{5}$$

The last term in Eq.(1) is related to the exciton–phonon interaction, which influences the exciton binding energies by screening the Coulomb potential. This effect will be taken into account by using an effective potential derived by Aldrich *et al* which has been verified to be quite efficient to calculate the exciton binding energies in QW structures.[18,19] To do so, the Hamiltonian (1) can be rewritten as

$$H = H_{\mathrm{e}} + H_{\mathrm{h}} + H_{\mathrm{F}} + H_{\mathrm{ex}}, \tag{6}$$

where

$$H_{\mathrm{e}} = -\frac{\hbar^2}{2m_{\mathrm{e}}^*}\frac{\partial^2}{\partial z_{\mathrm{e}}^2} + V_{\mathrm{e}}(z_{\mathrm{e}}) - \alpha_{\mathrm{e}}\hbar\omega_{\mathrm{LO}}, \tag{7a}$$

and

$$H_{\mathrm{h}} = -\frac{\hbar^2}{2m_{\mathrm{h}\perp}^*}\frac{\partial^2}{\partial z_{\mathrm{h}}^2} + V_{\mathrm{h}}(z_{\mathrm{h}}) - \alpha_{\mathrm{h}}\hbar\omega_{\mathrm{LO}}. \tag{7b}$$

Here m_{e}^* and $m_{\mathrm{h}\perp}^*$ are the polaron masses of the electron and the hole along the z-direction and are given respectively by

$$m_{\mathrm{e}}^* = \frac{1 + \alpha_{\mathrm{e}}/12}{1 - \alpha_{\mathrm{e}}/12} m_{\mathrm{e}}, \tag{8a}$$

and

$$m_{\mathrm{h}\perp}^* = \frac{1 + \alpha_{\mathrm{h}}/12}{1 - \alpha_{\mathrm{h}}/12} m_{\mathrm{h}\perp}, \tag{8b}$$

where α_{e} and α_{h} are respectively the electron- and the hole-bulk LO-phonon coupling constants and are given by

$$\alpha_{\mathrm{e}} = \frac{m_{\mathrm{e}} e^2}{\hbar^2 u_{\mathrm{e}} \bar{\varepsilon}}, \quad \alpha_{\mathrm{h}} = \frac{m_{\mathrm{h}} e^2}{\hbar^2 u_{\mathrm{h}} \bar{\varepsilon}}, \tag{8c}$$

with

$$u_{\mathrm{e}} = \left(\frac{2m_{\mathrm{e}}\omega_{\mathrm{LO}}}{\hbar}\right)^{1/2}, \qquad u_{\mathrm{h}} = \left(\frac{2m_{\mathrm{h}}\omega_{\mathrm{LO}}}{\hbar}\right)^{1/2},$$
$$\frac{1}{\bar{\varepsilon}} = \frac{1}{\varepsilon_{\infty}} - \frac{1}{\varepsilon_0}. \tag{8d}$$

It should be noted that the hole mass we used in (8c) and (8d) is chosen as the average isotropic mass.

The last term in Eq.(1), $H_{\rm ex}$ includes the exciton motion in $x-y$ plane and the effective interaction potential between the electron and the hole

$$H_{\rm ex} = -\frac{\hbar^2}{2\mu*}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}\right) + V_{\rm eff}(r). \quad (9)$$

Here $\rho = [(x_{\rm e}-x_{\rm h})^2 + (y_{\rm e}-y_{\rm h})^2]^{1/2}$ is the distance between the electron and the hole, and μ^* is the reduced mass of the exciton in the $x-y$ plane, given by

$$\mu^* = \frac{m_{\rm e}^* m_{\rm h\|}^*}{m_{\rm e}^* + m_{\rm h\|}^*}. \quad (10)$$

$V_{\rm eff}(r)$ is the effective electron–hole interaction potential including the phonon effects and can be written, following Antonelli *et al*,[18,19] as

$$V_{\rm eff}(r) = -\frac{e^2}{\varepsilon_0 r} - \frac{e^2}{2\bar{\varepsilon}}\left[\left(\frac{1}{r}-\varsigma_{\rm e}\right)\mathrm{e}^{-u_{\rm e}r} + \left(\frac{1}{r}-\varsigma_{\rm h}\right)\mathrm{e}^{-u_{\rm h}r}\right], \quad (11)$$

where

$$\varsigma_{\rm e} = \frac{u_{\rm e}}{\{1+\alpha_{\rm e}/[4(1+\alpha_{\rm e}/12)^2]\}(1+\alpha_{\rm e}/12)}, \quad (11a)$$

and

$$\varsigma_{\rm h} = \frac{u_{\rm h}}{\{1+\alpha_{\rm h}/[4(1+\alpha_{\rm h}/12)^2]\}(1+\alpha_{\rm h}/12)}, \quad (11b)$$

$r = [(z_{\rm e}-z_{\rm h})^2 + \rho^2]^{1/2}$ is the distance between the electron and the hole.

3. Variational treatment

We use a variational method to calculate the ground state energy of the exciton. The trial wavefunction can be chosen as[7,9,10]

$$|\psi\rangle = |z_{\rm e}\rangle|z_{\rm h}\rangle|\rho\rangle, \quad (12)$$

where

$$|z_{\rm e,h}\rangle = \begin{cases} N_{\rm e,h}\cos\dfrac{\pi z_{\rm e,h}}{2d}\exp\left[-\beta_{\rm e,h}\left(\dfrac{z_{\rm e,h}}{2d}+\dfrac{1}{2}\right)\right] & |z_{\rm e,h}| \le d, \\ 0 & |z_{\rm e,h}| > d, \end{cases} \quad (13)$$

describes the electron (e) and the hole (h) wavefunction confined in the well. $N_{\rm e}$ and $N_{\rm h}$ are the normalization constants which depend on the parameters $\beta_{\rm e}$ and $\beta_{\rm h}$, respectively and are given by

$$N_{\rm e,h}^2 = \frac{2\beta_{\rm e,h}(\beta_{\rm e,h}^2+\pi^2)}{d\pi^2(1-\mathrm{e}^{-2\beta_{\rm e,h}})}. \quad (13a)$$

Here we consider the case where the applied electric field is weak and the exciton is un-dissociated.[21] The wavefunction of the exciton in the $x-y$ plane $|\rho\rangle$ is then chosen as

$$|\rho\rangle = (\lambda/\sqrt{2\pi})\mathrm{e}^{-\lambda\rho/2}, \quad (14)$$

where λ, $\beta_{\rm e}$ and $\beta_{\rm h}$ are all the variational parameters and will be determined by minimizing the expectation values of the Hamiltonian (1).

Consequently the ground-state energy of the exciton can be calculated by the following minimizing equation

$$E_{\rm g} = \min_{\lambda,\beta_{\rm e},\beta_{\rm h}}\langle\psi|H|\psi\rangle. \quad (15)$$

The binding energy of the exciton may then be obtained by subtracting the ground state energy from the free electron–hole pair $E_{\rm free}$

$$E_{\rm B} = E_{\rm free} - E_{\rm g}. \quad (16)$$

By dropping the free motions of the electron and the hole in the $x-y$ plane, the corresponding electron–hole pair Hamiltonian is written as

$$H_{\rm free} = H_{\rm e} + H_{\rm h} + H_{\rm F}. \quad (17)$$

Choosing the trial wavefunction as

$$|f\rangle = |z_{\rm e}\rangle|z_{\rm h}\rangle, \quad (18)$$

the energy of the free electron–hole pair can be calculated by

$$E_{\rm free} = \min_{\beta_{\rm e},\beta_{\rm h}}\langle f|H_{\rm free}|f\rangle. \quad (19)$$

The stark shifts of the exciton binding energy is determined as

$$\Delta E_{\rm B} = E_{\rm B}(F) - E_{\rm B}(F=0). \quad (20)$$

4. Numerical results and discussion

The calculations for the values of the binding energies of the heavy-hole excitons for III–V and II–VI compound QW systems are performed numerically. The results for $GaAs/Al_{0.3}Ga_{0.7}As$ and $Zn_{0.69}Cd_{0.31}Se/ZnSe$ QWs are shown in Figs.1–3. The parameters used in the calculations are listed in Table 1.

Table 1. Values of the physical parameters used in the computations. Energies are measured in meV and masses in units of the mass of a free electron.

	ε_0	ε_∞	$\hbar\omega_{\rm LO}$	γ_1	γ_2	m_1
$GaAs/Al_{0.3}Ga_{0.7}As$	12.5	10.9	35.2	6.93	2.15	0.067
$Zn_{0.69}Cd_{0.31}Se/ZnSe$[a)]	8.7	5.73	31.7	2.45	0.61	0.14

[a)] Ref. [22, 23, 24]

In Fig.1 we plot the values of the binding energies of heavy-hole excitons in the $GaAs/Al_{0.3}Ga_{0.7}As$ and $Zn_{0.69}Cd_{0.31}Se/ZnSe$ QWs as a function of half well width d. As expected, the exciton binding energies increase monotonically with decreasing well-width from the bulk (3D) values for very large widths, and to the 2D values, namely, 4 times the 3D value for the case of $F = 0$ (see Fig.1(a)), for very thin wells. The values of the exciton binding energies with the exciton-LO-phonon interaction are lower than those without, for both the III–V and II–VI compound QWs as respectively shown in Figs.1(a) and 1(b). Phonon contribution to the reduction of the exciton binding energies for the ZnCdSe/ZnSe system is much bigger (by an order of magnitude) than that for GaAs/AlGaAs QW because of the stronger polarity of the II–VI compounds. The exciton–phonon interaction reduces the exciton binding energy by screening the Coulombic potential by LO phonons. It is also seen clearly by comparing the results for F =5 and 0kV/cm in Fig.1(a) that the external electric field reduces the binding energy and will cause a Stark shift. It is well known that the electron is pushed against the direction of the applied field while the hole along the field so that the binding of the excitons is weakened due to the reduced overlap of the two wavefunctions. Furthermore, the influence of the e–p interaction on the Stark shift can be found clearly for GaAs/AlGaAs QW in Fig.1(a), in which the reduction of the exciton binding energy from F =0 to 5.0kV/cm with phonon contribution is lower than that without phonons. However, the effect is negligible for the ZnCdSe/ZnSe system due to the large binding energy as in Fig.1(b). To illustrate the effect of Stark shift, the electric field dependence of the exciton binding energies will be illustrated in the following figures.

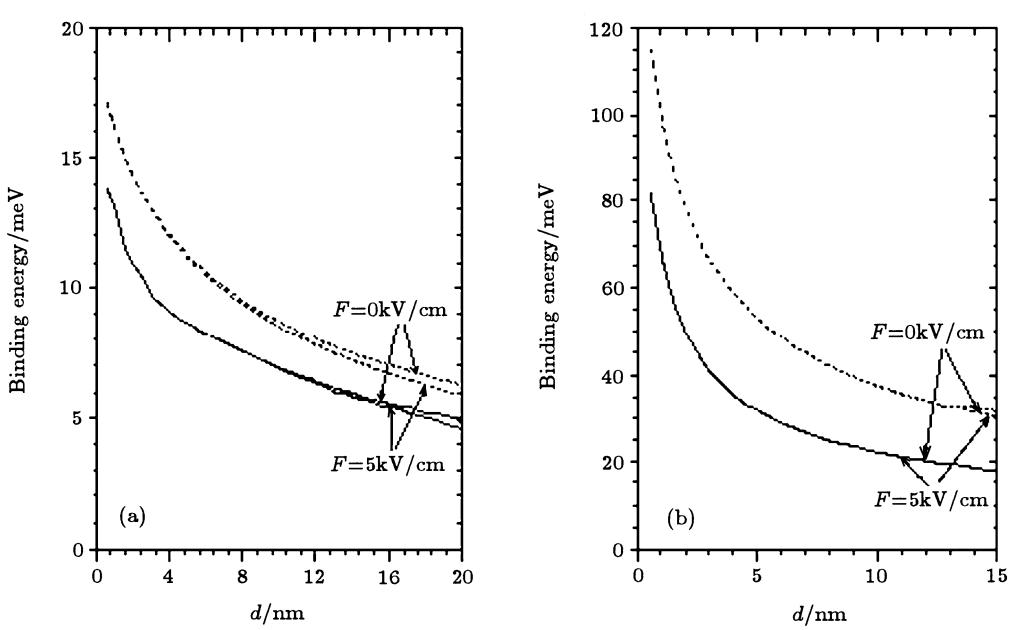


Fig.1. Values of the binding energies of heavy-hole excitons as a function of half-well-width d without (dotted lines) and with (solid lines) exciton–phonon interaction for (a) $GaAs/Al_{0.3}Ga_{0.7}As$ QW and (b) $Zn_{0.69}Cd_{0.31}Se/ZnSe$ QW for two different values of the electric field F=0 and 5.0kV/cm.

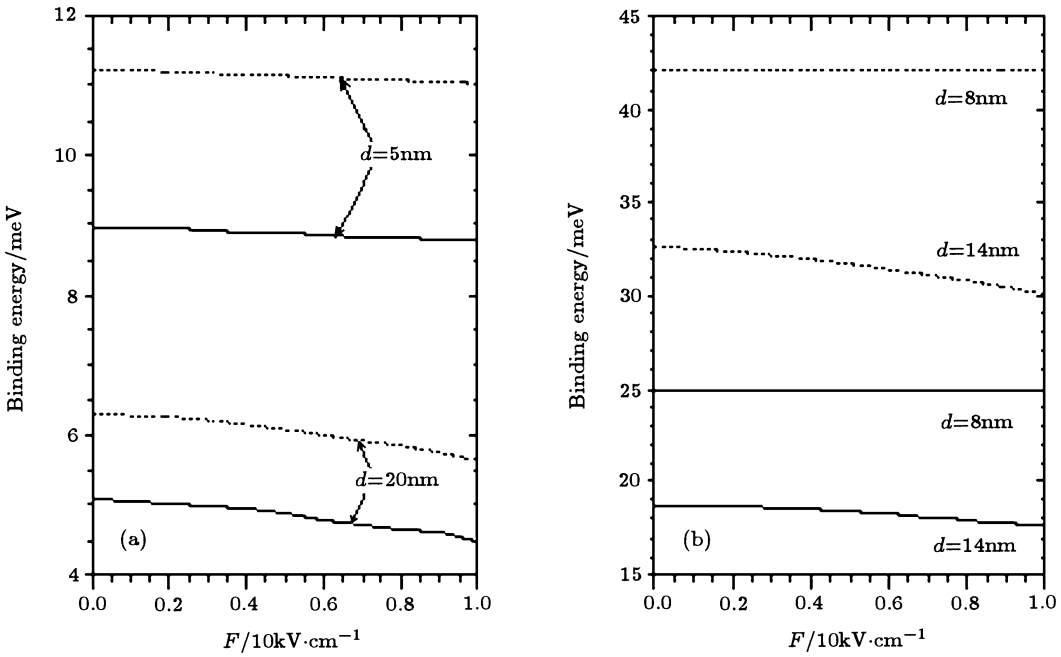


Fig.2. Exciton binding energies with (solid) and without (dotted) LO-phonons as functions of the electric field in (a) GaAs/$Al_{0.3}Ga_{0.7}As$ QWs of the well width d= 5 and 20nm, (b) $Zn_{0.69}Cd_{0.31}Se$/ZnSe QWs of d=8 and 14nm.

The numerical results of the electric field dependence of the binding energy of heavy-hole excitons are shown in Fig.2 for the GaAs/$Al_{0.3}Ga_{0.7}As$ QWs of the well width d=5 and 20nm and for the $Zn_{0.69}Cd_{0.31}Se$/ZnSe QWs of d=8 and 14nm. One can see from the figures that the binding energies of excitons decrease significantly with increasing electric field strength for the wide well case, whereas the decrease is not significant for narrow wells, because the electron and hole cannot be pulled apart so far due to the confinement by the two closed barriers. Another interesting feature is seen in Fig.2, namely, the slopes of the curves for the binding energies without LO-phonon effect are steeper than those with phonon contribution for both the systems. It is clear that the exciton–phonon interaction introduces a depolarized field and reduces the macroscopic electric field, so that the QCSE is weakened.

To clearly see the influence of the e–p interaction on the Stark shifts, we have plotted in Fig.3 the exciton binding energy shifts (the Stark effect) with and without phonons as functions of the electric field for the above mentioned systems. It is found again that the phonon field screens and reduces the Stark shifts for both the systems, and the screening increases rapidly with the electric field as well as the well-width. Moreover, the screening depends sensitively on the e–p coupling strength. As is shown in Fig.3, the e–p screening in the ZnCdSe/ZnSe system is much stronger than that in the GaAs/AlGaAs system because of stronger polarity. In the wide well-width (d=14nm) case, the e–p coupling around 3/5 reduces the Stark shift of the exciton at F=10kV/cm. Therefore, the e–p coupling plays an important role in the QCSE and cannot be neglected, especially for the II–VI polar semiconductor QW systems.

In conclusion, we have presented a theoretical investigation of the effect of exciton-LO-phonon coupling on exciton binding energies in a polar quantum well in the presence of an applied weak electric field perpendicular to the well layer. The results show that the exciton-LO-phonon interaction reduces the Stark shift of the exciton binding energy. This effect depends on both the well-width and the polarity of the materials. It cannot be neglected for wider wells, particularly in II–VI compound systems. We have used an infinite-deep well approximation in the calculations. The formulation is valid for the considered weak field and not very narrow well case, due to the fact that the exciton is not dissociated by the electric field and also the probability of the particles penetrating into the barrier regions is very small in the two

QWs considered above. Although our calculation can give reliable theoretical results in the two-dimensional limit, it should not be compared directly with the experimental data without appropriate modifications.

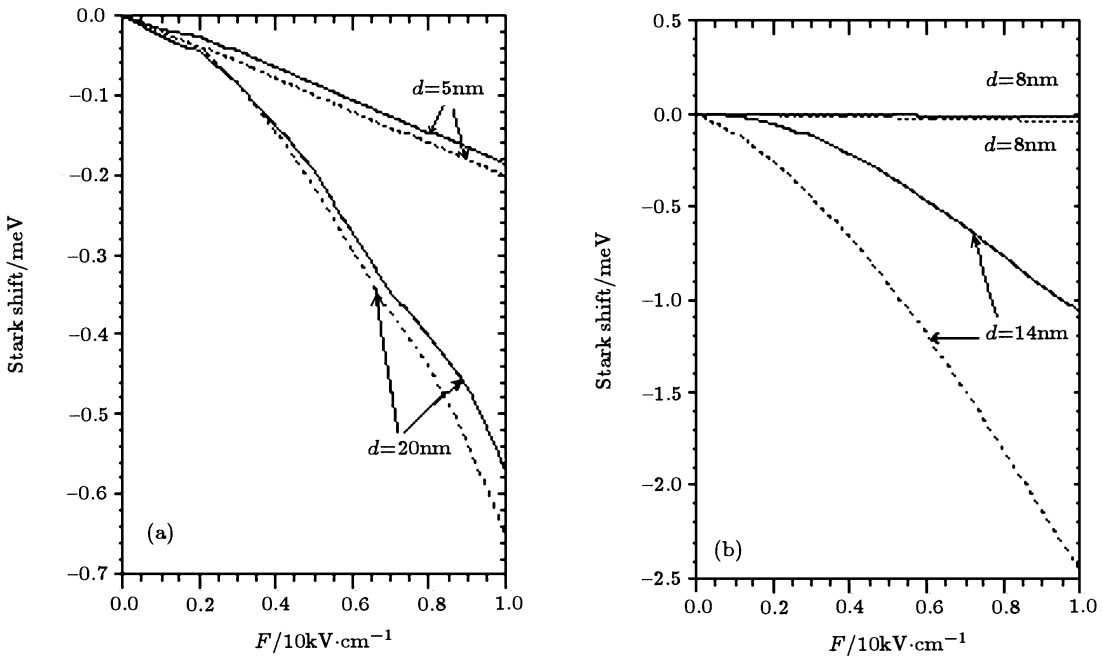


Fig.3. Exciton binding energy shifts with (solid) and without (dotted) LO-phonons as functions of the electric field in (a) GaAs/$Al_{0.3}Ga_{0.7}As$ QWs of the well width d=5 and 20nm, (b) $Zn_{0.69}Cd_{0.31}Se$/ZnSe QWs of d=8 and 14nm.

References

[1] Goldenberg B, Zook J D and Ulmer R J 1993 *Appl. Phys. Lett.* **62** 381
Nakamura S, Senoh M and Mukai T 1993 *Appl. Phys. Lett.* **62** 2390

[2] Zhang A Z, Zhang P, Duan S Q, Zhao X G and Liang J Q 2001 *Chin. Phys.* **10** 537

[3] Bastard G, Mendez E E, Chang L L and Esaki L 1982 *Phys. Rev.* B **26** 1974

[4] Greene R L and Bajaj K K 1983 *Solid State Commun.* **45** 831

[5] Chemla D S, Damen T C, Miller D A B, Gossard A C and Wiegmann W 1983 *Appl. Phys. Lett.* **42** 864

[6] Miller D A B, Chemla D S, Damen T C, Gossard A C, Wiegmann W, Wood T H and Burrus C A 1984 *Phys. Rev. Lett.* **53** 2173

[7] Miller D A B, Chemla D S, Damen T C, Gossard A C, Wiegmann W, Wood T H and Burrus C A 1985 *Phys. Rev.* B **32** 1043

[8] Collins R T, Vinã L, Wang W I, Chang L L, Esaki L, Klitzing K V and Ploog K 1987 *Phys. Rev.* B **36** 1531

[9] Brum J A and Bastard G 1985 *Phys. Rev.* B **31** 3893

[10] Bastard G, Mendez E E, Chang L L and Esaki L 1983 *Phys. Rev.* B **28** 3241

[11] Zhu B F 1988 *Phys. Rev.* B **38** 13316

[12] Tokuda Y, Kanamoto K and Tsukada N 1990 *Appl. Phys. Lett.* **56** 166

[13] Li Z H, Yu T J, Yang Z J, Feng Y C, Zhang G Y, Guo B P and Niu H B 2005 *Chin. Phys.* **14** 830

[14] Diganiet M H and Hipolito O 1987 *Phys. Rev.* B **35** 4507

[15] Matsuura M 1988 *Phys. Rev.* B **37** 6977

[16] Zheng R S and Matsuura M 1997 *Phys. Rev.* B **56** 2058

[17] Pollmann J and Büttner H 1975 *Solid State Commun.* **17** 1171

[18] Aldrich C and Bajaj K K 1977 *Solid State Commun.* **22** 157

[19] Antonelli A, Cen J and Bajaj K K 1996 *Semicond. Sci. Technol.* **11** 74

[20] Senger R T and Bajaj K K 2003 *Phys. Rev.* B **68** 205314

[21] Bastard G 1988 *Interface, Quantum Wells and Superlattices* (New York: Plenum) p189

[22] Hoscher H W, Nohe A and Uihlein C 1985 *Phys. Rev.* B **31** 2379

[23] Pellegrini V, Atanasov R, Tredicucci A, Beltram F, Amzulini C, Sorba L, Vanzetti L and Franciosi A 1995 *Phys. Rev.* B **51** 5171

[24] Cingolani R, Prete P, Greco D, Gilugno P V, Lomascolo M, Rinaldi R, Calcagnile L, Vanzetti L, Sorba L and Franciosi A 1995 *Phys. Rev.* B **51** 5176