

Phonon effect on exciton binding energies in cylindrical quantum wires in the presence of an electric field

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(Received April 12, 2010)

We have determined the effects of the electron-phonon and hole-phonon interactions on the binding energies of excitons in cylindrical quantum wires in the presence of an external electric field. The exciton binding energies of several III-V and II-VI compound semiconductor quantum wire structures have been calculated as functions of the electric fields and the transverse dimension of the quantum wires. Theoretical results show that the exciton-phonon coupling reduces both the exciton binding energies and the Stark shifts by screening the Coulomb interaction; thus, the exciton-phonon coupling is significant and cannot be neglected.

PACS numbers: 73.21.Hb, 71.35.-y, 63.20.kk

I. INTRODUCTION

The behavior of excitons in quantum wires has been extensively investigated, both experimentally [1] and theoretically [2–19]. Brown *et al.* [2] studied the ground-state energies of an exciton in a cylindrical quantum wire (CQW) for both infinite and finite potential wells and found that the binding energy increases with a decrease in the well width in the case of the quantum wire with the infinite confining potential well, whereas it reaches a certain peak value and then decreases to the value of the barrier material surrounding the wire in the case of the finite confining potential well. Xia *et al.* [3] theoretically investigated the exciton states in isolated and semi-isolated quantum wires with circular cross sections and indicated that the binding energies in quantum wires are approximately ten times larger than those in quantum wells. Some authors have discussed exciton states in type-II quantum wires, where the electrons and holes are confined separately in distinct regions [4, 5]. Studies on the bi-exciton states in low-dimensional systems have also been carried out [6–8].

Electron-phonon interaction plays an important role in low-dimensional systems, and it has been attracting considerable attention [10–14]. Degani *et al.* adopted a variational solution to study the binding energies of the excitons in rectangular quantum wires [11]; they used a bulk-phonon approximation. Sheng *et al.* studied the effect of the electron (hole)-surface-optical (SO)-phonon coupling on the excitonic ground states in a CQW [12, 13] and indicated that the effect of the electron-SO-phonon coupling on the exciton binding energy is not as significant as that in the case of three-dimensional or two-dimensional systems,

even though the electron-SO-phonon coupling is very strong in quantum wires. Escorcia *et al.* discussed the polaronic exciton in quantum wires by using the Aldrich-Bajaj effective potential for Wannier excitons [14].

The optical properties of quantum wires can undergo significant changes when an electric field is applied perpendicular to the wires. This effect is called the quantum-confined Stark effect, and it has been extensively studied in the past few years [15–19]. Kasapoglu calculated the exciton binding energies and interband optical absorptions in GaAs quantum wires in an electric field by using the effective-mass approximation and a variational approach [16]. Chang and Xia investigated the exciton quantum-confined Stark effects on an exciton in V-shaped GaAs/Al_xGa_{1-x}As quantum wires and found blue shifts when the electric field was applied in the growth direction [17]. However, to the best of our knowledge, there are few studies on the effect of exciton–phonon coupling on the exciton binding energies in quantum wire structures in the presence of an external electric field.

In the study described in this paper, we adopted a variational solution to investigate the binding energies and the Stark shift of an exciton in a CQW with an infinite potential well. The exciton–phonon interactions were considered by taking into account both the confined bulk longitudinal optical (LO) and interface optical (IO) phonons in the calculations. The effects of the exciton–phonon couplings on the binding energies and Stark effects are discussed for several III-V and II-VI compound CQWs.

II. THEORY

Let us consider a polar semiconductor CQW that has a circular cross section of radius R and whose wire axis is in the z -direction; the CQW is surrounded by a nonpolar material. An external electric field is applied perpendicular to the wire axis. We adopt the effective-mass approximation and assume that the well has a sharp boundary and that the exciton wave function is confined wholly to the well. The Fröhlich-like electron–phonon Hamiltonian derived by Wang and Lei [20], who discussed the confined phonon modes for a CQW in the continuum dielectric approximation, is used to describe the exciton–phonon coupling.

The Hamiltonian of an exciton–phonon system in an external electric field can be written as

$$H = H_{\text{ex}} + H_{\text{F}} + H_{\text{ph}} + H_{\text{ex-ph}}. \quad (1)$$

In a cylindrical coordinate system, where the coordinate origin is chosen at the center of the cross section perpendicular to the wire, the exciton Hamiltonian H_{ex} can be written

as

$$\begin{aligned}
H_{\text{ex}} = & -\frac{\hbar^2}{2m_e} \left(\frac{\partial^2}{\partial r_e^2} + \frac{1}{r_e} \frac{\partial^2}{\partial r_e^2} + \frac{1}{r_e^2} \frac{\partial^2}{\partial r_e^2} \right) + V_e(r_e) \\
& -\frac{\hbar^2}{2m_{\perp h}} \left(\frac{\partial^2}{\partial r_h^2} + \frac{1}{r_h} \frac{\partial^2}{\partial r_h^2} + \frac{1}{r_h^2} \frac{\partial^2}{\partial r_h^2} \right) + V_h(r_h) \\
& -\frac{\hbar^2}{2\mu_{\parallel}} \frac{\partial^2}{\partial z^2} - \frac{\hbar^2}{2M_{\parallel}} \frac{\partial^2}{\partial Z^2} - \frac{e^2}{\varepsilon_{\text{infly}} \sqrt{z^2 + |\vec{r}_e - \vec{r}_h|^2}},
\end{aligned} \tag{2}$$

where $\varphi_e(\varphi_h)$ is the pole angle of the two-dimensional projection $\mathbf{r}_e(\mathbf{r}_h)$ of the electron (hole) position vector in the cross section. Z and z are the mass-center and relative coordinates of the exciton, respectively, and M_{\parallel} and μ_{\parallel} are their corresponding masses along the z -direction; they are given by

$$\mu_{\parallel} = \frac{m_e m_{\parallel h}}{m_e + m_{\parallel h}}, \tag{3a}$$

$$M_{\parallel} = m_e + m_{\parallel h}. \tag{3b}$$

Here, m_e is the isotropic mass of the electron. m_{\parallel} and $m_{\perp h}$ are the hole masses along the z -direction and in the xy plane, respectively, and they are determined by the Kohn-Luttinger parameters γ_1 and γ_2 as

$$\frac{1}{m_{\parallel h}} = \frac{1}{m_0} (\gamma_1 \pm \gamma_2), \tag{4a}$$

$$\frac{1}{m_{\perp h}} = \frac{1}{m_0} (\gamma_1 \mp 2\gamma_2), \tag{4b}$$

where the upper (lower) sign in Eqs. 4a and 4b refers to the heavy-hole (light-hole) branch.

$V_i(r)$ (where i stands for e or h) in Eq. 2 is the confining potential for the electron or hole:

$$V_i(r) = \begin{cases} 0 & r_i \leq R \\ \infty & r_i > R \end{cases} \tag{5}$$

H_F in Eq. 1 is the electric field energy of the electron-hole system in the presence of the external electric field, and it is given by

$$H_F = e\vec{F} \cdot (\vec{r}_e - \vec{r}_h), \tag{6}$$

where F stands for the strength of the electric field. The polar axis shall be considered to be along the direction of the applied field in the following calculations for convenience.

H_{ph} in Eq. 1 is the Hamiltonian of the free phonon field that includes both the LO and IO phonons:

$$H_{\text{ph}} = \sum_{mlk_z} \hbar\omega_{\text{LO}} a_{ml}^\dagger(k_z) a_{ml}(k_z) + \sum_{mq_z} \hbar\omega_{\text{IO}} b_m^\dagger(q_z) b_m(q_z), \quad (7)$$

where $\hbar\omega_{\text{LO}}$ and $\hbar\omega_{\text{IO}}$ are the dispersionless LO- and IO-phonon energies, respectively. $a_{ml}^\dagger(a_{ml})$ and $b_m^\dagger(b_m)$ are the creation (annihilation) operators for the LO and IO phonons with wave vectors k_z and q_z , respectively.

The last term in Eq. 1 describes the coupling of the phonon field with the exciton:

$$H_{\text{ex-ph}} = \sum_{mlk_z} \left(V_{\text{ex-LO}} e^{ik_z Z} a_{ml}^\dagger(k_z) + h.c. \right) + \sum_{mq_z} \left(V_{\text{ex-IO}} e^{iq_z Z} b_m^\dagger(q_z) + h.c. \right) \quad (8)$$

with

$$V_{\text{ex-LO}} = V_{\text{e-LO}}(r_e, k_z) e^{i\gamma_h k_z z} - V_{\text{e-LO}}(r_h, k_z) e^{-i\gamma_e k_z z}, \quad (9a)$$

$$V_{\text{ex-IO}} = V_{\text{e-IO}}(r_e, q_z) e^{i\gamma_h q_z z} - V_{\text{e-IO}}(r_h, q_z) e^{-i\gamma_e q_z z}, \quad (9b)$$

where $\gamma_e = m_e/M_{\parallel}$ and $\gamma_h = m_{\parallel h}/M_{\parallel}$; $V_{\text{e-LO}}$ and $V_{\text{e-IO}}$ are expressed as:

$$V_{\text{e-LO}}(r, k_z) = \Gamma_{\text{LO}}^{ml}(k_z) J_m \left(\frac{\chi_m^l}{R} r \right) e^{im\varphi}, \quad (10a)$$

$$V_{\text{e-IO}}(r, q_z) = \Gamma_{\text{IO}}^m(q_z) K_m(q_z R) I_m(q_z r) e^{im\varphi}, \quad (10b)$$

where

$$\Gamma_{\text{LO}}^{*ml} = \frac{i\sqrt{2}e(\hbar\omega_{\text{LO}})^{1/2}}{\sqrt{L} (\chi_m^l)^2 + k_z^2 R^2}^{1/2} J_{m+1}(\chi_m^l) \cdot \left(\frac{1}{\varepsilon_0} - \frac{1}{\varepsilon_\infty} \right)^{1/2}, \quad (11a)$$

$$\Gamma_{\text{IO}}^{*m} = \frac{i\sqrt{2}e(\hbar\omega_{\text{IO}})^{1/2}}{\sqrt{L} K_m(q_z R) \sqrt{I_m(q_z R) q_z R [I_{m-1}(q_z R) + I_{m+1}(q_z R)]}} \cdot \left(\frac{1}{\varepsilon - \varepsilon_0} - \frac{1}{\varepsilon - \varepsilon_\infty} \right)^{1/2}. \quad (11b)$$

J_m is the m -order Bessel function, and χ_m^l is the l th root of J_m . I_m and K_m are the first- and second-kind modified Bessel functions of m -order, respectively. L is the length of the quantum wire, and ε_0 and ε_∞ are the static and high frequency dielectric constants, respectively.

In order to calculate the energy of the exciton–phonon system in the presence of an external electric field, we first carry out two unitary transformations:

$$U_1 = \exp \left(-i \left[\sum_{mlk_z} k_z Z a_{ml}^\dagger(k_z) a_{ml}(k_z) + \sum_{mq_z} q_z Z b_m^\dagger(q_z) b_m(q_z) \right] \right) \quad (12)$$

and

$$U_2 = \exp \left(\sum_{mlk_z} [f_{ml}^*(k_z) a_{ml}(k_z) - h.c.] + \sum_{mq_z} [g_m^*(q_z) b_m(q_z) - h.c.] \right), \quad (13)$$

where the displacement amplitudes are set as

$$f_{ml}(k_z) = -\frac{V_{\text{ex-LO}}(r_{\text{e,h}}, k_z)}{\hbar\omega_{\text{LO}} + \frac{\hbar^2 k_z^2}{2M_{\parallel}}}, \quad (14)$$

and

$$g_m(q_z) = -\frac{V_{\text{ex-IO}}(r_{\text{e,h}}, q_z)}{\hbar\omega_{\text{IO}} + \frac{\hbar^2 q_z^2}{2M_{\parallel}}}. \quad (15)$$

The ground-state energy of the system is then calculated by using a variational method by choosing the tried wave function as

$$|\Phi\rangle = \Psi(\vec{r}_e, \vec{r}_h, \vec{z}) U_1 U_2 |0\rangle, \quad (16)$$

where $|0\rangle$ is the phonon vacuum state and $\Psi(r)$ is the exciton wave function, which is given by

$$\begin{aligned} \Psi(\vec{r}_e, \vec{r}_h, \vec{z}) = & N J_0 \left(\frac{\chi_0^1}{R} r_e \right) \exp(-\alpha r_e \cos(\varphi_e)/R) \\ & \cdot J_0 \left(\frac{\chi_0^1}{R} r_h \right) \exp(-\beta r_h \cos(\varphi_h + \pi)/R) \\ & \cdot \exp \left(-\lambda \sqrt{z^2 + |\vec{r}_e - \vec{r}_h|^2} \right), \end{aligned} \quad (17)$$

where α , β , and λ are the variational parameters and N is the normalization constant of Ψ .

The variational energy is given by

$$\begin{aligned}
\langle \Phi | H | \Phi \rangle &= \langle \Psi | H_{\text{ex}} | \Psi \rangle + \langle \Psi | H_{\text{F}} | \Psi \rangle \\
&- \sum_{mlk_z} \frac{|\langle \Psi | V_{\text{e-LO}}(r_e, k_z) | \Psi \rangle|^2}{\hbar\omega_{\text{LO}} + \frac{\hbar^2 k_z^2}{2M_{\parallel}}} - \sum_{mlk_z} \frac{|\langle \Psi | V_{\text{e-LO}}(r_h, k_z) | \Psi \rangle|^2}{\hbar\omega_{\text{LO}} + \frac{\hbar^2 k_z^2}{2M_{\parallel}}} \\
&- \sum_{mq_z} \frac{|\langle \Psi | V_{\text{e-IO}}(r_e, q_z) | \Psi \rangle|^2}{\hbar\omega_{\text{IO}} + \frac{\hbar^2 q_z^2}{2M_{\parallel}}} - \sum_{mq_z} \frac{|\langle \Psi | V_{\text{e-IO}}(r_h, q_z) | \Psi \rangle|^2}{\hbar\omega_{\text{IO}} + \frac{\hbar^2 q_z^2}{2M_{\parallel}}} \\
&- \sum_{mlk_z} \frac{\langle \Psi | 2 \cos(k_z z) V_{\text{e-LO}}(r_e, k_z) V_{\text{e-LO}}^*(r_h, k_z) | \Psi \rangle}{\hbar\omega_{\text{LO}} + \frac{\hbar^2 k_z^2}{2M_{\parallel}}} \\
&- \sum_{mq_z} \frac{\langle \Psi | 2 \cos(q_z z) V_{\text{e-IO}}(r_e, q_z) V_{\text{e-IO}}^*(r_h, q_z) | \Psi \rangle}{\hbar\omega_{\text{IO}} + \frac{\hbar^2 q_z^2}{2M_{\parallel}}}. \tag{18}
\end{aligned}$$

The ground-state energy of the exciton can then be calculated by

$$E_{\text{g}} = \min_{\alpha\beta\lambda} \langle \Psi | H | \Psi \rangle. \tag{19}$$

Finally, the binding energy of the exciton state is determined by subtracting the ground-state energy from the free electron-hole pair energy E_0 :

$$E_{\text{b}} = E_0 - E_{\text{g}}. \tag{20}$$

To calculate E_0 , we write down the Hamiltonian of the free electron-hole pair in the same system:

$$H_{\text{free}} = H_{\text{e}}^0 + H_{\text{h}}^0 + H_{\text{F}} + H_{\text{ph}} + H_{\text{e-ph}} + H_{\text{h-ph}}. \tag{21}$$

By carrying out the unitary transformations in a manner similar to the transformations for the exciton state and by choosing the tried wave function for the electron-hole pair without phonons as

$$\Psi_0 = \Psi_{\text{e}} \Psi_{\text{h}}, \tag{22}$$

$$\Psi_{\text{e}}(r) = N_0 J_0 \left(\frac{\chi_0^1}{R} r_{\text{e}} \right) \exp(-\alpha r_{\text{e}} \cos(\varphi_{\text{e}})/R), \tag{22a}$$

$$\Psi_{\text{h}}(r) = N_0 J_0 \left(\frac{\chi_0^1}{R} r_{\text{h}} \right) \exp(-\beta r_{\text{h}} \cos(\varphi_{\text{h}} + \pi)/R), \tag{22b}$$

the corresponding variational energy can be written as

$$\begin{aligned}
E_{\text{free}} = & \langle \Psi_0 | H_e^0 | \Psi_0 \rangle + \langle \Psi_0 | H_h^0 | \Psi_0 \rangle + \langle \Psi_0 | H_F^0 | \Psi_0 \rangle \\
& - \sum_{mlk_z} \frac{\left| \langle \Psi_0 | \Gamma_{\text{LO}}^{ml}(k_z) J_m \left(\frac{\chi_m^l}{R} r_e \right) | \Psi_0 \rangle \right|^2}{\hbar\omega_{\text{LO}} + \frac{\hbar^2 k_z^2}{2m_e}} \\
& - \sum_{mq_z} \frac{\left| \langle \Psi_0 | \Gamma_{\text{IO}}^m(q_z) I_m(q_z r_e) K_m(q_z R) | \Psi_0 \rangle \right|^2}{\hbar\omega_{\text{IO}} + \frac{\hbar^2 q_z^2}{2m_e}} \\
& - \sum_{mlk_z} \frac{\left| \langle \Psi_0 | \Gamma_{\text{LO}}^{ml}(k_z) J_m \left(\frac{\chi_m^l}{R} r_h \right) | \Psi_0 \rangle \right|^2}{\hbar\omega_{\text{LO}} + \frac{\hbar^2 k_z^2}{2m_{\parallel h}}} \\
& - \sum_{mq_z} \frac{\left| \langle \Psi_0 | \Gamma_{\text{IO}}^m(q_z) I_m(q_z r_h) K_m(q_z R) | \Psi_0 \rangle \right|^2}{\hbar\omega_{\text{IO}} + \frac{\hbar^2 q_z^2}{2m_{\parallel h}}} \tag{23}
\end{aligned}$$

The ground-state energy of the free electron-hole pair is then obtained by

$$E_0 = \min_{\alpha\beta} E_{\text{free}}, \tag{24}$$

and the Stark shift of the exciton binding energy is determined as

$$\Delta E_b = E_b(F) - E_b(F = 0). \tag{25}$$

III. RESULT AND DISCUSSION

The values of the binding energies of the excitons in several III-V and II-VI CQW systems are numerically calculated. As an example, the computed results for the heavy-hole excitons in the GaAs and CdTe CQWs are shown in Figs. 1–3. The results for the light-hole excitons are similar to those for the heavy-hole excitons; however, we have not plotted them here for short. The parameters of the wire material used in the calculations are shown in Table I.

TABLE I: Values of the physical parameters used in the calculations. Energy is measured in meV and mass in units of the mass of a free electron.

	ε_0	ε_∞	$\hbar\omega_{\text{LO}}$	$\hbar\omega_{\text{TO}}$	γ_1	γ_2	m^*
CdTe	9.6	7.13	20.84	17.96	4.67 ^a	1.31 ^a	0.091
GaAs	12.5	10.9	35.2	33.29	6.93	2.15	0.067

^aRef. [21].

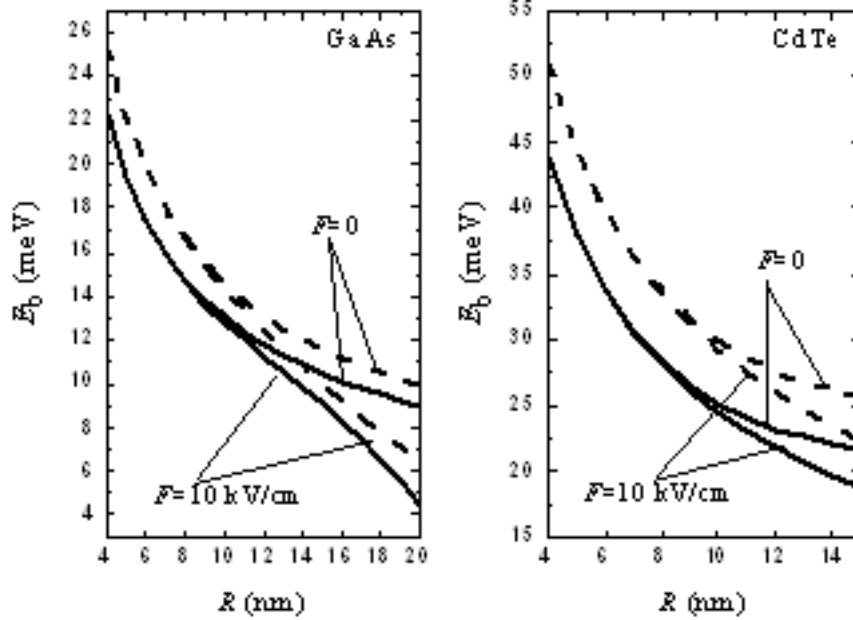


FIG. 1: Binding energies of the exciton as functions of the wire radius with (solid lines) and without (dashed lines) exciton-phonon interaction for the electric field of $F = 0$ and $F = 10$ kV/cm in the GaAs and CdTe CQWs.

The numerical results of the binding energies of the excitons in the GaAs and CdTe CQWs as functions of the wire radii are plotted in Fig. 1. It is seen that the exciton binding energies increase monotonically with a decrease in the wire radius for both the systems. The values of the exciton binding energies with the exciton-phonon interaction are lower than those without the phonon effect because of the screening of the Coulombic potential between the electron and hole by the phonon field. The decrease in the energy due to the phonon field is much larger in the CdTe quantum wire when compared to that in the GaAs quantum wire. This is because the polarity of the CdTe system is higher than that of the GaAs system. One can also find that the binding energies in the presence of the external electric field are lower than those without the electric field. This is because the electron is pushed in the direction opposite to the applied field while the hole is pushed in the direction of the applied field, which reduces the degree of overlap of their wave functions and results in a negative Stark shift.

Figure 2 shows the results of the binding energies of the excitons as functions of the electric field. In the calculations, the radii for the GaAs and CdTe CQWs are both chosen as $R = 7$ nm and $R = 15$ nm. From these figures, it is found that the binding energies of excitons decrease significantly with an increase in the electric field strength for the CQWs

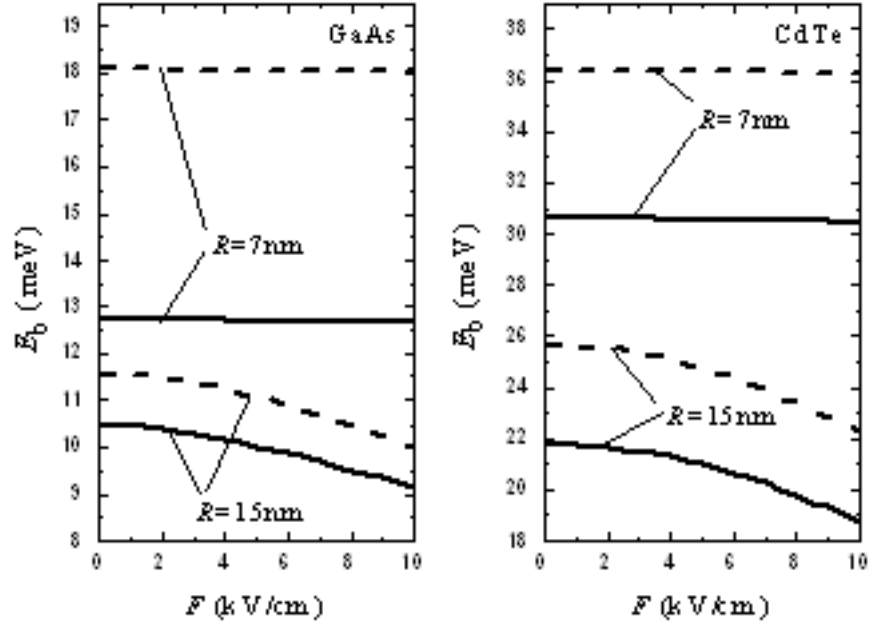


FIG. 2: Exciton binding energies as functions of the electric field for the GaAs and CdTe CQWs with $R = 7$ nm and $R = 15$ nm with (solid) and without (dashed) the influence of the phonon field.

with the larger radius, whereas the curves for the CQWs with the smaller radius are smooth because the wells of the CQWs strictly confine the electron as well as the hole to the wire, thereby preventing the external field from pulling them apart.

In order to illustrate the effect of the phonon field on the Stark effect, we have plotted the numerical results of the Stark shifts of the excitonic ground-state energies as functions of the electric field for the abovementioned systems with and without phonons in Fig. 3. It is clearly seen that the energy shifts increase rapidly with the electric field as well as with the wire radius. One can also find that the Stark shifts without phonon coupling are larger than those with phonon coupling. This is because the exciton-phonon interaction introduces a depolarized field that reduces the macroscopic electric field, and this, in turn, weakens the Stark shifts. Moreover, the phonon effect on the Stark shift in the CdTe (II-VI compounds) CQW is much stronger than that in the GaAs (III-V compounds) CQW; this is because the former has a higher polarity than the latter.

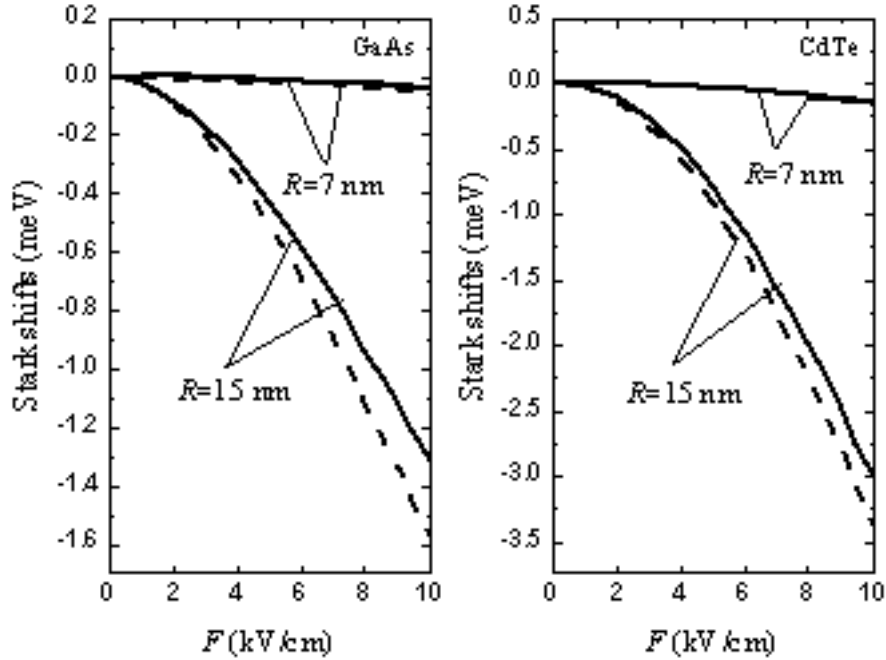


FIG. 3: Stark shifts of the exciton states as functions of the electric field for the GaAs and CdTe CQWs with $R = 7$ nm and $R = 15$ nm with (solid) and without (dashed) the influence of the phonon field.

IV. CONCLUSIONS

We have calculated the binding energies of the exciton in several III-V and II-VI cylindrical quantum wires in the presence of an external electric field by adopting a variational solution. The exciton-LO and exciton-IO phonon couplings are also taken into account in the calculations. The results show that the binding energies are highly dependent on the transverse dimension of the quantum wires. The electric field reduces the exciton binding energies, and the exciton-phonon coupling reduces the binding energies as well as the Stark shifts by screening both the Coulombic potential and the external field. Therefore, phonon effects on the binding energies and on the Stark effect cannot be neglected in quantum wires, particularly in II-VI compound quantum wires.

Acknowledgments

This study was supported by the National Natural Science Foundation of China (No. 10764003).

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