Polaronic effects on excitons in quantum wells

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A theory of exciton-phonon interaction in quantum wells is presented. Bound states of excitons in polar quantum wells are investigated by using an improved variation method. The interaction with both interface and confined longitudinal-optical phonons are included in consideration. A general expression of the bound-state energy of the exciton in a quantum well is obtained. The theoretical result is shown to be valid throughout the entire well-width range. Based on the theory, general properties of the exciton–optical-phonon coupling systems in quantum wells are discussed in detail. Some interesting futures of the system are concluded. [S0163-1829(98)04303-3]

I. INTRODUCTION

A semiconductor quantum well (QW) composed of a sandwich structure with two different materials has a quantum confinement effect both on charge carriers and phonons. The quantum-confinement effect makes the electronic and optical properties of QW's quite different from those of bulk materials. For an example, the enhancement effect of the exciton binding energy shows that the exciton states exhibit relatively high stability in QW's. In recent years the investigation of the exciton property in QW heterostructures has attracted much attention in condensed-matter physics.

In the past decade, quantum size effects on charge carriers were studied extensively by experimental and theoretical physicists,[1–10] and some second-order effects (such as the effects of excited subbands, the valence-band mixing, nonparabolicity of the dispersion relations, mass and dielectric constants mismatch, etc.) were also included in the works. From the view of elementary excitation in solid-state physics, the exciton-phonon interaction also has considerable effects and cannot be neglected in the study of transport and optical properties of most of the QW systems. Von Lehmen *et al.*[11] found that exciton–LO-phonon interaction plays an important role in determining the spectral characteristics and magnitude of the low-temperature absorption. A calculation of the absorption coefficient based on the two-dimensional Fröhlich interaction shows agreement with the experimental data.

As the simplest model, the bulk phonon approximation was used by many authors to study the exciton-phonon interaction in QW's.[12–21] The published results were very different due to different theoretical methods. Some authors reported that the polaronic effect on the exciton binding energy is rather noticeable, and increases with decreasing the well thickness,[12–14] but some authors found that the polaronic correction causes a decrease to the exciton binding energy in a $GaAs/Ga_{1-x}Al_xAs$ QW.[19] One of the present authors[15] pointed that the key point is that large polaron self-energy shifts of the electron and hole subbands were neglected in Refs. 12–14.

In recent years, the confined LO-phonon and the surface-optical (SO)-phonon models were introduced to study exciton-phonon interaction in QW's.[22–24] These approximations are better than the bulk phonon approximation, but are not entirely correct pictures of the QW cases. The optical-phonon modes and the interaction Hamiltonian of the electron (hole) with the phonons in QW structures have been investigated in detail by several study groups.[25–27] It was found that the phonon modes are very different from those of the bulk crystals because of the quantum confinement effect on the lattice vibration. In a double heterostructure made of two binary crystals, there are three types of optical phonons interacting with charge carriers: (i) symmetric and antisymmetric interface optical (IO) phonons, (ii) confined LO phonons in the well, and (iii) half-space LO phonons in the barrier. Works studying polaronic effects in polar QW's considered the effects of different types of the optical phonons in the QW's. Xie and Chen[28] studied the ground state of both heavy- and light-hole excitons in a $GaAs/Ga_{1-x}Al_xAs$ QW. Based on the work of Mori and Ando,[26] they took all the phonon modes into account. Unfortunately, some important terms which represent the features of the quantum confinement effects on the exciton-phonon interaction system were omitted in their algebraic calculations, which made the expressions and also the numerical results in their paper not entirely correct. The role of phonons, especially IO phonons, in the QW exciton state has not been very clear up to now.

Very recently we investigated polaronic effects on exciton states in GaAs/AlAs and CdSe/ZnSe QW's (Ref. 29) by including the different optical-phonon modes into consideration. By using a nonseparable trial wave function, the exciton binding energies and the interaction energies of the exciton with every phonon mode in two typical QW's have been calculated as functions of the well width. The features of the exciton–optical-phonon interaction have been discussed.

In the present paper we extend our work to general QW's

and study the general property of exciton–optical-phonon interaction systems in polar semiconductor QW's in detail. The subband effect and the anisotropy mass effect of the electron and hole are incorporated into our theory. The aim of the present paper is to introduce our theoretical treatment in detail, and give definite expressions of the bound-state energy and the average virtual phonon number of the QW exciton-phonon system. For theoretical completeness we show that our theory can be reduced to the published exciton theories in the three-dimensional (3D) and ideal 2D limits, and also to the free-polaron theory in the limiting case where the electron and hole are separated completely. Based on the theory, a series of numerical calculations is made for typical QW cases. The general properties of exciton-phonon interaction systems in polar QW's are discussed and concluded. The characteristic and relative importance of every phonon mode on the exciton state as a function of the well width are clarified from the theoretical results. Some very interesting features of the exciton-phonon system in polar semiconductor QW's are found and discussed in the paper. We believe that our works will be helpful to understand the optical and electronic properties of the QW structures.

II. HAMILTONIAN

For completeness, we give a short review of the Hamiltonian at first. A general QW made of two binary polar materials is considered. For academic purpose the infinite square-well model is used in this work. The z axis is taken as the growth direction. The system of an exciton in the well interacting with optical phonons is expressed within the framework of effective-mass and non-degenerate-band approximations as

$$H=\sum_j \left\{ \frac{P_{j\|}^2}{2m_{j\|}}+\frac{P_{jz}^2}{2m_{jz}}+V(z_j)+V_s(z_j)\right\} + V_{e\text{-}h}(\rho,z_e,z_h)+H_{\rm ph}+H_i, \tag{2.1}$$

with

$$V(z_j)=\begin{cases} 0, & |z_j|\leqslant d \\ \infty, & |z_j|>d \end{cases} \quad (j=e,h), \tag{2.2}$$

$$V_s(z_j)=\frac{e^2}{2\epsilon_{\infty 1}}\sum_{n\neq 0}\frac{\xi^{|n|}}{|z_j-(-1)^n z_j+nW|} \quad (j=e,h), \tag{2.3}$$

$$V_{e\text{-}h}(\rho,z_e,z_h) = -\frac{e^2}{\epsilon_{\infty 1} r}-\frac{e^2}{\epsilon_{\infty 1}}\sum_{n\neq 0}\frac{\xi^{|n|}}{\sqrt{\rho^2+[z_e-(-1)^n z_h+nW]^2}}, \tag{2.4}$$

$$\xi=\frac{\epsilon_{\infty 1}-\epsilon_{\infty 2}}{\epsilon_{\infty 1}+\epsilon_{\infty 2}}, \tag{2.5}$$

where $j=e,h$ refers to the electron and hole, respectively. $\mathbf{P}_j=(\mathbf{P}_{j\|},P_{jz})$, $\mathbf{r}_j=(\boldsymbol{\rho}_j,z_j)$, and $m=(m_{j\|},m_{jz})$ are the momentum, position, and effective band mass of the particles. $\mathbf{P}_{j\|}$ and $\boldsymbol{\rho}_j$ are two-dimensional vectors in the x-y plane. $V(z_j)$ for $j=e$ $(j=h)$ is the barrier potential experienced by the electron (hole). The width of the QW is W $(=2d)$. $V_s(z_j)$ for $j=e$ $(j=h)$ is the self-polarization potential from the interaction of the electron (hole) with its image charge distribution, where the summation index n runs from $-\infty$ to ∞. $V_{e\text{-}h}(\rho,z_e,z_h)$ is the Coulomb interaction potential of the electron-hole pair evaluated by the image charge method.[30] $\mathbf{r}=\mathbf{r}_e-\mathbf{r}_h=(\boldsymbol{\rho},z)$ is the relative position between the electron and the hole. ξ is a measure of the mismatch of dielectric constants at the interfaces. $\epsilon_{\infty 1}$ $(\epsilon_{\infty 2})$ is the optical dielectric constant of the well (barrier) material.

The free-phonon Hamiltonian $H_{\rm ph}$ is given by

$$H_{\rm ph}=\sum_\beta \sum_{\mathbf{k}} \hbar\omega_\beta(\mathbf{k}) a_{\mathbf{k}\beta}^\dagger a_{\mathbf{k}\beta}, \tag{2.6}$$

where $a_{\mathbf{k}\beta}^\dagger(a_{\mathbf{k}\beta})$ is the creation (annihilation) operator of an optical phonon with frequency $\omega_\beta(\mathbf{k})$ and wave vector $(\mathbf{k},k_\beta)$. $\beta=m$ refers to the confined LO phonon in the well material with frequency ω_{L1} and wave vector $k_m=m\pi/2d$. The positive integer m is limited by the Brillouin-zone boundary, that is, $m_{\max}=\text{int}(W/a)$. a is the lattice constant of the well material. $\beta=(\sigma,p)$ refers to the IO phonon. The index $p(=+,-)$ refers to the symmetric and antisymmetric IO-phonon modes, and $\sigma(=+,-)$ to the high- and low-frequency IO-phonon modes, respectively. The dispersion relation of the frequency $\omega_{\sigma p}$ is given by[25,27,31]

$$\omega_{\pm p}^2(kd)=\frac{1}{2(\epsilon_{p1}+\epsilon_{p2})}\{[\epsilon_{p1}(\omega_{L1}^2+\omega_{T2}^2)+\epsilon_{p2}(\omega_{L2}^2+\omega_{T1}^2)]\pm\{[\epsilon_{p1}(\omega_{L1}^2-\omega_{T2}^2)+\epsilon_{p2}(\omega_{L2}^2-\omega_{T1}^2)]^2+4\epsilon_{p1}\epsilon_{p2}(\omega_{L2}^2-\omega_{L1}^2)(\omega_{T2}^2-\omega_{T1}^2)\}^{1/2}\}, \tag{2.7}$$

with

$$\epsilon_{\pm 1}(kd)=(1\mp e^{-2kd})\epsilon_{\infty 1}, \tag{2.8}$$

$$\epsilon_{\pm 2}(kd)=(1\pm e^{-2kd})\epsilon_{\infty 2}, \tag{2.9}$$

where the subscript $i=1$ and 2 refers to the well and the barrier, respectively. ϵ_{0i} is the static dielectric constant, ω_{Li} (ω_{Ti}) is the longitudinal- (transverse-) optical-phonon frequency of the material indicated by i.

The exciton–optical-phonon interaction Hamiltonian takes the form of

$$H_i=\sum_\beta \sum_{\mathbf{k}} \sum_j [\theta_j V_{\mathbf{k}\beta} L_{\mathbf{k}\beta}(z_j)\exp(i\mathbf{k}\cdot\boldsymbol{\rho}_j)a_{\mathbf{k}\beta}+\text{H.c.}], \tag{2.10}$$

where

$$\theta_j=\begin{cases} -1, & j=e \\ 1, & j=h, \end{cases} \tag{2.11}$$

which shows that the electron– and hole–optical-phonon interactions have opposite effects. The coefficient $V_{\mathbf{k}\beta}$ and $L_{\mathbf{k}\beta}(z_j)$ are well understood. For confined LO phonons it takes the forms of

$$V_{km}=i\left(\frac{\hbar\omega_{L1}}{2dS\epsilon_1}\frac{4\pi e^2}{k^2+k_m^2}\right)^{1/2}, \tag{2.12}$$

$$L_{km}(z_j)=\sin[k_m(z_j+d)] \quad (j=e,h), \tag{2.13}$$

where $\epsilon_i^{-1}=\epsilon_{\infty i}^{-1}-\epsilon_{0i}^{-1}$, $(i=1,2)$. S stands for the area of the interface. The coefficient of IO phonons takes the forms of

$$V_{k,\sigma p}=i\left(\frac{\hbar\omega_{\sigma p}}{S\epsilon_{\sigma p}}\frac{\pi e^2}{k}\right)^{1/2}, \tag{2.14}$$

$$L_{k,\sigma+}(z_j)=\frac{\cosh(kz_j)}{\cosh(kd)}, \tag{2.15}$$

$$L_{k,\sigma-}(z_j)=\frac{\sinh(kz_j)}{\sinh(kd)}, \tag{2.16}$$

with

$$\epsilon_{\sigma p}=\frac{\epsilon_{p1}\xi_{1\sigma p}+\epsilon_{p2}\xi_{2\sigma p}}{1+pe^{-2kd}}, \tag{2.17}$$

$$\xi_{i\sigma p}(kd)=\left\{\frac{\omega_{Li}^2-\omega_{Ti}^2}{\omega_{Ti}^2-\omega_{\sigma p}^2}\right\}^2\frac{\omega_{\sigma p}^2\epsilon_i}{\omega_{Ti}^2\epsilon_{0i}} \quad (i=1,2). \tag{2.18}$$

The coefficient of $V_{k,\sigma p}$ is essentially the same as our previous papers,[31,32] but the physical meaning of the definitions of Eqs. (2.14), (2.17), and (2.18) is clearer than that used previously.

III. VARIATION TREATMENT

In this paper we use a reasonable variational method to study the exciton-phonon interaction problem. Based on the Lee-Low-Pines (LLP) variational theory,[33] the phonon state of an exciton-phonon coupling system is considered as a coherentlike state $U(F)|0\rangle$, where $|0\rangle$ is the zero-phonon state. $U(F)$ is a unitary transformation operator, which is defined as

$$U(F)=\exp\left(\sum_\beta\sum_{\mathbf{k}}\sum_j F_{\mathbf{k}\beta j}(\mathbf{r}_j)a_{\mathbf{k}\beta}^\dagger-\text{H.c.}\right), \tag{3.1}$$

$$F_{\mathbf{k}\beta j}(\mathbf{r}_j)=f_{\mathbf{k}\beta j}L_{\mathbf{k}\beta}(z_j)\exp(-i\mathbf{k}\cdot\boldsymbol{\rho}_j), \tag{3.2}$$

where $f_{\mathbf{k}\beta j}$ is a variational parameter, which will be subsequently determined by the minimization condition of the energy. It should be stressed that the phonon state $U(F)|0\rangle$ has a direct relation with the exciton wave function in the present theoretical method. $F_{\mathbf{k}\beta j}(\mathbf{r}_j)$ is a function of the coordinates of the electron and hole. The value of $f_{\mathbf{k}\beta j}$ depends on the average effect of the exciton state as well as the phonon states. The inclusion of $L_{\mathbf{k}\beta}(z_j)$ in $F_{\mathbf{k}\beta j}(\mathbf{r}_j)$ greatly enhances the mathematical difficulties, but it can give good theoretical results of the exciton-phonon interaction system in the whole range of the well width, as seen later.

The translation relations are given as the following:

$$U^\dagger a_{\mathbf{k}\beta}U=a_{\mathbf{k}\beta}+\sum_j F_{\mathbf{k}\beta j}(\mathbf{r}_j), \tag{3.3}$$

$$U^\dagger a_{\mathbf{k}\beta}^\dagger U=a_{\mathbf{k}\beta}^\dagger+\sum_j F_{\mathbf{k}\beta j}^*(\mathbf{r}_j), \tag{3.4}$$

$$\begin{aligned}U^\dagger\mathbf{P}_{j\parallel}U=\mathbf{P}_{j\parallel}-\tfrac{1}{2}\sum_\beta\sum_{\mathbf{k}}\hbar\mathbf{k}\Bigg\{F_{\mathbf{k}\beta j}^*\Bigg(\sum_{j'}F_{\mathbf{k}\beta j'}\Bigg)\\+F_{\mathbf{k}\beta j}\Bigg(\sum_{j'}F_{\mathbf{k}\beta j'}^*\Bigg)\Bigg\}-\sum_\beta\sum_{\mathbf{k}}\hbar\mathbf{k}\{F_{\mathbf{k}\beta j}a_{\mathbf{k}\beta}^\dagger\\+F_{\mathbf{k}\beta j}^*a_{\mathbf{k}\beta}\},\end{aligned} \tag{3.5}$$

$$\begin{aligned}U^\dagger P_{jz}U=P_{jz}+\frac{i}{2}\sum_\beta\sum_{\mathbf{k}}\hbar k_\beta\{f_{\mathbf{k}\beta j'}f_{\mathbf{k}\beta j}^*L_{\mathbf{k}\beta}(z_{j'})J_{\mathbf{k}\beta}(z_j)\\\times\exp[i\mathbf{k}\cdot(\boldsymbol{\rho}_j-\boldsymbol{\rho}_{j'})]-f^*{}_{\mathbf{k}\beta j'}f_{\mathbf{k}\beta j}L_{\mathbf{k}\beta}(z_{j'})J_{\mathbf{k}\beta}(z_j)\\\times\exp[-i\mathbf{k}\cdot(\boldsymbol{\rho}_j-\boldsymbol{\rho}_{j'})]\}\\+i\sum_\beta\sum_{\mathbf{k}}\hbar k_\beta\{f_{\mathbf{k}\beta j'}^*J_{\mathbf{k}\beta}(z_j)\exp(i\mathbf{k}\cdot\boldsymbol{\rho}_j)a_{\mathbf{k}\beta}\\-f_{\mathbf{k}\beta j'}J_{\mathbf{k}\beta}(z_j)\exp(-i\mathbf{k}\cdot\boldsymbol{\rho}_j)a_{\mathbf{k}\beta}^\dagger\} \quad (j'\neq j),\end{aligned} \tag{3.6}$$

where the notation $J_{\mathbf{k}\beta}(z_j)$ is defined as

$$J_{\mathbf{k}\beta}(z_j)=\mathbf{k}_\beta^{-1}\frac{\partial}{\partial z_j}L_{\mathbf{k}\beta}(z_j). \tag{3.7}$$

Since there is translational symmetry in the x-y direction, we can divide the x-y motion of the exciton into center of mass motion and relative motion. The position and momentum of the center-of-mass (relative) motion are denoted by $\mathbf{R}_\parallel(\boldsymbol{\rho})$ and $\mathbf{P}_\parallel(\mathbf{p}_\parallel)$, respectively. The corresponding center of-mass and reduced mass are noted as $M_\parallel$ and $\mu_\parallel$, respectively.

The transformed Hamiltonian $H^*=U^\dagger HU$ is very lengthy, but one can distinguish them clearly by zero-, one-, and two-phonon contributions. Since we are only interested in the state involved in the optical absorption, we set $\mathbf{P}_\parallel=0$ in the following. The correlation between the virtual phonons emitted and absorbed by the particles will be neglected in the following calculation, since it is very weak in the weak and intermediate coupling cases, as proved by LLP earlier. This approximation was used successfully in the exciton-phonon interaction systems by many authors.[34,35] Then the zero-phonon part of the transformed Hamiltonian is given as

$$H_0^*=\frac{p^2}{2\mu_\parallel}+V_{e\text{-}h}(\rho,z_e,z_h)+\sum_j\left\{\frac{P_{jz}^2}{2m_{jz}}+V(z_j)+V_s(z_j)\right\}$$
$$+\sum_\beta\sum_{\mathbf{k}}\sum_j\left\{\frac{\hbar^2k^2}{2m_{j\parallel}}L_{\mathbf{k}\beta}^2(z_j)+\frac{\hbar^2k_\beta^2}{2m_{jz}}J_{\mathbf{k}\beta}^2(z_j)\right\}|f_{\mathbf{k}\beta j}|^2$$
$$+\sum_\beta\sum_{\mathbf{k}}\hbar\omega_\beta(\mathbf{k})\Bigg\{\sum_j|f_{\mathbf{k}\beta j}|^2L_{\mathbf{k}\beta}^2(z_j)$$
$$+f_{\mathbf{k}\beta e}^*f_{\mathbf{k}\beta h}L_{\mathbf{k}\beta}(z_e)L_{\mathbf{k}\beta}(z_h)\exp(i\mathbf{k}\cdot\boldsymbol{\rho})$$
$$+f_{\mathbf{k}\beta e}f_{\mathbf{k}\beta h}^*L_{\mathbf{k}\beta}(z_e)L_{\mathbf{k}\beta}(z_h)\exp(-i\mathbf{k}\cdot\boldsymbol{\rho})\Bigg\}$$
$$+\sum_\beta\sum_{\mathbf{k}}\Bigg\{\sum_j\theta_jV_{\mathbf{k}\beta}f_{\mathbf{k}\beta j}L_{\mathbf{k}\beta}^2(z_j)$$
$$+V_{\mathbf{k}\beta}f_{\mathbf{k}\beta h}L_{\mathbf{k}\beta}(z_e)L_{\mathbf{k}\beta}(z_h)\exp(i\mathbf{k}\cdot\boldsymbol{\rho})$$
$$-V_{\mathbf{k}\beta}f_{\mathbf{k}\beta e}L_{\mathbf{k}\beta}(z_e)L_{\mathbf{k}\beta}(z_h)\exp(-i\mathbf{k}\cdot\boldsymbol{\rho})+\text{H.c.}\Bigg\}. \quad (3.8)$$

The trial wave function of the exciton can be physically chosen in many forms, and can also contain variational parameters. The subband effect of the electron and hole and also the ground or low-lying excited internal state of the exciton can be put into consideration in the function. It is convenient to use the variational wave function

$$\Psi_{n,l_e,l_h}(\rho,z_e,z_h,\lambda)=N_{n,l_e,l_h}\phi_n(\mathbf{r},\lambda)\psi_{l_e}(z_e)\psi_{l_h}(z_h), \quad (3.9)$$

where the constant N_{n,l_e,l_h} is determined by orthonormalization conditions, and λ is a set of variational parameters that will be determined by the procedure of minimizing the energy of the system. $\phi_n(\mathbf{r},\lambda)$, in which λ is placed, is the exciton wave function with the quantum number n. Usually, the hydrogenlike wave function is chosen as the candidate for the envelope function. $\psi_{l_e}(z_e)$ and $\psi_{l_h}(z_h)$ are the subband wave functions of the electron and hole moving in the QW in the subbands l_e and l_h, respectively. It has been shown[30,36,37] that the effect of the self-polarization potential $V_s(z_j)$ $(j=e,h)$ can be satisfactorily accounted for by a shift in the subband energy, without significant modification of the subband wave functions. So that the function $\psi_{l_e}(z_e)\psi_{l_h}(z_h)$ can be written by

$$\psi_{l_e}(z_e)\psi_{l_h}(z_h)=\sin\left(\frac{l_e\pi}{2d}(z_e+d)\right)\sin\left(\frac{l_h\pi}{2d}(z_h+d)\right). \quad (3.10)$$

The total trial wave function of the system is assumed to be a product of the exciton wave function and the phonon wave function; it take the form of

$$|\Psi\rangle=U(F)|0\rangle|\Psi_{n,l_e,l_h}\rangle. \quad (3.11)$$

Then the energy of exciton-optical phonon system is given by

$$E(\lambda)=\langle\Psi|H|\Psi\rangle=\langle\Psi_{n,l_e,l_h}|\langle 0|U^\dagger HU|0\rangle|\Psi_{n,l_e,l_h}\rangle$$
$$=\langle\Psi_{n,l_e,l_h}|H_0^*|\Psi_{n,l_e,l_h}\rangle=E_0(\lambda)+E_s$$
$$+\sum_\beta\sum_{\mathbf{k}}\sum_j\left\{\frac{\hbar^2k^2}{2m_{j\parallel}}A_{\mathbf{k}\beta j}+\frac{\hbar^2k_\beta^2}{2m_{jz}}B_{\mathbf{k}\beta j}\right\}|f_{\mathbf{k}\beta j}|^2$$
$$+\sum_\beta\sum_{\mathbf{k}}\hbar\omega_\beta(\mathbf{k})\Bigg\{\sum_j|f_{\mathbf{k}\beta j}|^2A_{\mathbf{k}\beta j}+f_{\mathbf{k}\beta e}^*f_{\mathbf{k}\beta h}C_{\mathbf{k}\beta}$$
$$+f_{\mathbf{k}\beta e}f_{\mathbf{k}\beta h}^*C_{\mathbf{k}\beta}^*\Bigg\}+\sum_\beta\sum_{\mathbf{k}}\Bigg\{\sum_j\theta_jV_{\mathbf{k}\beta}f_{\mathbf{k}\beta j}A_{\mathbf{k}\beta j}$$
$$+V_{\mathbf{k}\beta}f_{\mathbf{k}\beta h}C_{\mathbf{k}\beta}-V_{\mathbf{k}\beta}f_{\mathbf{k}\beta e}C_{\mathbf{k}\beta}^*+\text{H.c.}\Bigg\}, \quad (3.12)$$

with the following abbreviations:

$$E_0(\lambda)=\left\langle\Psi_{n,l_e,l_h}\left|\frac{p^2}{2\mu_\parallel}+V_{e\text{-}h}(\rho,z_e,z_h)\right|\Psi_{n,l_e,l_h}\right\rangle, \quad (3.13)$$

$$E_s=\left\langle\Psi_{n,l_e,l_h}\left|\sum_j\left\{\frac{P_{jz}^2}{2m_{jz}}+V(z_j)+V_s(z_j)\right\}\right|\Psi_{n,l_e,l_h}\right\rangle, \quad (3.14)$$

$$A_{\mathbf{k}\beta j}=\langle\Psi_{n,l_e,l_h}|L_{\mathbf{k}\beta}^2(z_j)|\Psi_{n,l_e,l_h}\rangle, \quad (3.15)$$

$$B_{\mathbf{k}\beta j}=\langle\Psi_{n,l_e,l_h}|J_{\mathbf{k}\beta}^2(z_j)|\Psi_{n,l_e,l_h}\rangle, \quad (3.16)$$

$$C_{\mathbf{k}\beta}=\langle\Psi_{n,l_e,l_h}|L_{\mathbf{k}\beta}(z_e)L_{\mathbf{k}\beta}(z_h)\exp(i\mathbf{k}\cdot\boldsymbol{\rho})|\Psi_{n,l_e,l_h}\rangle, \quad (3.17)$$

where $E_0(\lambda)$ is the binding energy of a bare exciton in the QW. E_s represents the subband energy of the electron and hole in the dielectric QW. Since this energy is a simple function of the well width and is canceled out in the results for the exciton binding energy,[2,30,36] it need not be considered further, and will not be mentioned again in the rest of this paper. By using the variational condition $\delta\langle\Psi|H|\Psi\rangle/\delta f_{\mathbf{k}\beta j}=0$, the parameter $f_{\mathbf{k}\beta j}$ is determined as

$$f_{\mathbf{k}\beta e}=\frac{Q_{\mathbf{k}\beta e}P_{\mathbf{k}\beta h}-Q_{\mathbf{k}\beta h}G_{\mathbf{k}\beta}}{P_{\mathbf{k}\beta e}P_{\mathbf{k}\beta h}-|G_{\mathbf{k}\beta}|^2}, \quad (3.18)$$

$$f_{\mathbf{k}\beta h}=\frac{Q_{\mathbf{k}\beta h}P_{\mathbf{k}\beta e}-Q_{\mathbf{k}\beta e}G_{\mathbf{k}\beta}^*}{P_{\mathbf{k}\beta e}P_{\mathbf{k}\beta h}-|G_{\mathbf{k}\beta}|^2}. \quad (3.19)$$

Here we have defined the following notations as

$$Q_{\mathbf{k}\beta e}=-V_{\mathbf{k}\beta}^*(A_{\mathbf{k}\beta e}-C_{\mathbf{k}\beta}), \quad (3.20)$$

$$Q_{\mathbf{k}\beta h}=V_{\mathbf{k}\beta}^*(A_{\mathbf{k}\beta h}-C_{\mathbf{k}\beta}^*), \quad (3.21)$$

$$P_{\mathbf{k}\beta j}=\left\{\hbar\omega_\beta(\mathbf{k})+\frac{\hbar^2k^2}{2m_{j\parallel}}\right\}A_{\mathbf{k}\beta j}+\frac{\hbar^2k_\beta^2}{2m_{jz}}B_{\mathbf{k}\beta j}\quad(j=e,h), \quad (3.22)$$

$$G_{\mathbf{k}\beta}=\hbar\omega_\beta(\mathbf{k})C_{\mathbf{k}\beta}. \quad (3.23)$$

Inserting Eqs. (3.18) and (3.19) into Eq. (3.12), then the general expression of the bound-state energy of the exciton-phonon interaction system is given in a very abbreviated form:

$$E=\min_{\lambda} E(\lambda)=\min_{\lambda}\Bigg\{E_0(\lambda)-\sum_{\beta}\sum_{\mathbf{k}}\,(P_{\mathbf{k}\beta e}P_{\mathbf{k}\beta h} -|G_{\mathbf{k}\beta}|^2)^{-1}(P_{\mathbf{k}\beta e}|Q_{\mathbf{k}\beta h}|^2+P_{\mathbf{k}\beta h}|Q_{\mathbf{k}\beta e}|^2 -Q_{\mathbf{k}\beta e}Q^*_{\mathbf{k}\beta h}G^*_{\mathbf{k}\beta}-Q^*_{\mathbf{k}\beta e}Q_{\mathbf{k}\beta h}G_{\mathbf{k}\beta})\Bigg\}. \tag{3.24}$$

The binding energy of the exciton-phonon coupling system is defined as the difference of the bound-state energy of the exciton and the sum of the polaron self-energies of a free electron-polaron and a free hole-polaron in the same QW. The polaron energy can be calculated by the same theoretical method as we used in Refs. 31 and 32.

If the form of the trial wave function $\phi_n(\mathbf{r},\lambda)$ has been chosen, then one can use the expression and relating abbreviations given above to calculate the bound-state energy and the binding energy of the exciton-phonon interaction system in a polar semiconductor QW by a standard numerical variational method. The quantum-confinement effect, polaronic effect, subband effect, and nonisotropic band mass effect on the exciton states can be studied based on our theory.

The average phonon number of the virtual phonons absorbed and emitted by the exciton is defined by

$$N_{\rm ph}=\left\langle \Psi\left|\sum_{\beta}\sum_{\mathbf{k}} a^{\dagger}_{\mathbf{k}\beta}a_{\mathbf{k}\beta}\right|\Psi\right\rangle. \tag{3.25}$$

Performing the unitary transformation, then the average virtual phonon number can be given in an abbreviated form,

$$N_{\rm ph}=\sum_{\beta}\sum_{\mathbf{k}}\Bigg\{\sum_{j}|f_{\mathbf{k}\beta j}|^2A_{\mathbf{k}\beta j}+f^*_{\mathbf{k}\beta e}f_{\mathbf{k}\beta 2}C_{\mathbf{k}\beta} +f_{\mathbf{k}\beta e}f^*_{\mathbf{k}\beta h}C^*_{\mathbf{k}\beta}\Bigg\}. \tag{3.26}$$

IV. GROUND STATE

Since the ground state is very important in experiments, we give more detailed expressions of the ground-state energy and the average virtual phonon number of the QW exciton-phonon system in this section.

In the ground state both the electron and the hole are in the lowest subbands, and the internal state of the exciton is the hydrogenlike $1s$ state, so that the trial wave function of the ground state is chosen as

$$\Psi_{1,1,1}=N_{1,1,1}\exp\left(-\frac{r}{\lambda}\right)\cos\left(\frac{\pi z_e}{2d}\right)\cos\left(\frac{\pi z_h}{2d}\right). \tag{4.1}$$

This type of trial wave function is simple, but it can give reasonable results throughout the entire well-width range, and has been used successfully by many authors.[2] In this case, since $l_{j1}=l_{j2}=1$, we thus find

$$A_{\mathbf{k}\beta e}=A_{\mathbf{k}\beta h}=A_{\mathbf{k}\beta}, \tag{4.2}$$

$$B_{\mathbf{k}\beta e}=B_{\mathbf{k}\beta h}=B_{\mathbf{k}\beta}, \tag{4.3}$$

$$C^*_{\mathbf{k}\beta}=C_{\mathbf{k}\beta}. \tag{4.4}$$

It is helpful to introduce dimensionless units, where energy is in units of $\hbar\omega_{L1}$ and lengths in units of the electron-polaron radius $R_p[=(\hbar/2m_e\omega_{L1})^{1/2}]$. Some dimensionless notations are defined as

$$q=k(\hbar/2m_e\omega_{L1})^{1/2}, \tag{4.5}$$

$$G_{\mathbf{q}\beta}=C_{\mathbf{q}\beta}\omega_\beta/\omega_{L1}, \tag{4.6}$$

$$K_{\mathbf{q}\beta j}=\left(\frac{\omega_\beta}{\omega_{L1}}+\frac{m_e}{m_{j\|}}q^2\right)A_{q\beta}+\frac{m_e}{m_{jz}}q_\beta^2B_{q\beta}\quad(j=e,h). \tag{4.7}$$

Inserting the above expressions into Eq. (3.24), and transforming the sum over $\mathbf{k}$ into an integral form

$$\sum_{\mathbf{k}}\Rightarrow\frac{S}{4\pi^2}\int 2\pi k\,dk\Rightarrow\frac{Sm_e\omega_{L1}}{\pi\hbar}\int q\;dq, \tag{4.8}$$

we then obtain the ground-state energy of a QW exciton-phonon system in unit of $\hbar\omega_{L1}$,

$$\mathcal{E}_g=\min_{\lambda}\left[\mathcal{E}_0(\lambda)+\mathcal{E}_{\text{ex-LO}}(\lambda)+\mathcal{E}_{\text{ex-IO}}(\lambda)\right], \tag{4.9}$$

where $\mathcal{E}_0(\lambda)$ is the ground-state energy of a bare exciton in the QW, $\mathcal{E}_{\text{ex-LO}}(\lambda)$ is the interaction energy of the exciton with the confined LO phonons, and $\mathcal{E}_{\text{ex-IO}}(\lambda)$ is that of the exciton with the IO phonons. They are defined by

$$\mathcal{E}_0(\lambda)=\left\langle\Psi_{1,1,1}\left|\left\{\frac{m_e}{\mu_\|}\frac{1}{\lambda}\left(\frac{2}{r}-\frac{\rho^2}{r^3}-\frac{\rho^2}{\lambda r^2}\right)+\frac{m_e}{\mu_z}\frac{1}{\lambda}\left(\frac{\rho^2}{r^3}-\frac{z^2}{\lambda r^2}\right) -\frac{\kappa}{r}-\kappa\sum_{n\neq0}\frac{\xi^{|n|}}{\sqrt{\rho^2+[z_e-(-1)^nz_h+nW]^2}} -\frac{\pi}{\lambda d}\frac{z}{r}\left[\frac{m_e}{m_{ez}}\tan\left(\frac{\pi z_e}{2d}\right)-\frac{m_e}{m_{hz}}\tan\left(\frac{\pi z_h}{2d}\right)\right]\right\}\right|\Psi_{1,1,1}\right\rangle, \tag{4.10}$$

$$\mathcal{E}_{\text{ex-LO}}(\lambda)=-\alpha_{e1}\frac{2}{d}\sum_m\int dq\frac{q}{q^2+q_m^2}\cdot \times\frac{(A_{qm}-C_{qm})^2(K_{qme}+K_{qmh}+2C_{qm})}{K_{qme}K_{qmh}-C_{qm}^2}, \tag{4.11}$$

$$\mathcal{E}_{\text{ex-IO}}(\lambda)=-\alpha_{e1}\sum_{\sigma p}\int dq\left(\frac{\omega_{\sigma p}}{\omega_{L1}}\frac{\epsilon_1}{\epsilon_{\sigma p}}\right) \times\frac{(A_{q\sigma p}-C_{q\sigma p})^2(K_{q\sigma pe}+K_{q\sigma ph}+2G_{q\sigma p})}{K_{q\sigma pe}K_{q\sigma ph}-G_{q\sigma p}^2}, \tag{4.12}$$

with

$$\kappa=\frac{2}{\epsilon_{\infty 1}}\left(\frac{m_e e^4}{2\hbar^3\omega_{L1}}\right)^{1/2}, \tag{4.13}$$

$$\alpha_{ji}=\frac{1}{\epsilon_i}\left(\frac{m_j e^4}{2\hbar^3\omega_{Li}}\right)^{1/2} \quad (j=e,h;\ \ i=1,2). \tag{4.14}$$

By the same process, the average virtual phonon number of the ground state can be calculated, and is given by

$$N_{\text{ph}}=N_{\text{ex-LO}}+N_{\text{ex-IO}}, \tag{4.15}$$

with

$$\begin{aligned}N_{\text{ex-LO}}=\alpha_{e1}\frac{2}{d}\sum_m \int dq\frac{q}{q^2+q_m^2}\frac{(A_{qm}-C_{qm})^2}{(K_{qme}K_{qmh}-C_{qm}^2)^2}\\ \times\{A_{qm}[(K_{qme}+C_{qm})^2+(K_{qmh}+C_{qm})^2]\\ -2C_{qm}(K_{qme}+C_{qm})(K_{qmh}+C_{qm})\},\end{aligned} \tag{4.16}$$

$$\begin{aligned}N_{\text{ex-IO}}=\alpha_{e1}\sum_{\sigma p}\int dq\left(\frac{\omega_{\sigma p}}{\omega_{L1}}\frac{\epsilon_1}{\epsilon_{\sigma p}}\right)\frac{(A_{q\sigma p}-C_{q\sigma p})^2}{(K_{q\sigma pe}K_{q\sigma ph}-G_{q\sigma p}^2)^2}\\ \times\{A_{q\sigma p}[(K_{q\sigma pe}+G_{q\sigma p})^2+(K_{q\sigma ph}+G_{q\sigma p})^2]\\ -2C_{q\sigma p}(K_{q\sigma pe}+G_{q\sigma p})(K_{q\sigma ph}+G_{q\sigma p})\}.\end{aligned} \tag{4.17}$$

V. ANALYSIS

It is important academically for theoretical works dealing with QW problems to give correct approaches in 2D and 3D limit cases, which are judgments of the justice to the theory. In this section we intend to analyze the validity of the present theory in the whole well-width range from the ideal 3D limit to the ideal 2D limit, and also to show the relationship of the present theory to the published polaron and exciton theories.

In order to compare with other authors' published theories, we also use the isotropic mass approximation, that is, $m_{j\|}=m_{jz}=m_j$, and study the limiting property of the exciton-phonon interaction system in the ground state.

A. $r\to\infty$ limit

From Eq. (3.17), it is seen that the parameter $C_{\mathbf{k}\beta}$ depends very much on the overlap probability of the electron and hole. When the electron and hole are separated enough, the value of $C_{\mathbf{k}\beta}$ goes to zero. With a very simple calculation, the displacement amplitudes $f_{\mathbf{k}\beta j}$ and the energy $E(\lambda)$ are reduced, respectively, to

$$f_{\mathbf{k}\beta j}\overset{r\to\infty}{\Rightarrow}\frac{-\theta_j V_{\mathbf{k}\beta}^* A_{\mathbf{k}\beta}}{P_{\mathbf{k}\beta j}}, \tag{5.1}$$

$$E(\lambda)\overset{r\to\infty}{\Rightarrow}E_p=-\sum_j\sum_\beta\sum_{\mathbf{k}}\frac{|V_{\mathbf{k}\beta}A_{\mathbf{k}\beta}|^2}{P_{\mathbf{k}\beta j}}. \tag{5.2}$$

The properties of polarons in infinite and finite QW's were investigated in our previous papers[31,32] with the same theoretical method; it is understood that E_p is just the sum of the self-energies of a free electron-polaron and a free hole-polaron in the QW. Based on this fact, the binding energy of the exciton-phonon system can be calculated self-consistently in this paper by

$$E_b=E_p-\min_\lambda E(\lambda). \tag{5.3}$$

B. $r\to 0$ limit

If the radius of the exciton is much smaller than the polaron radius, as it is the cases of $z_e=z_h$ and $\rho=0$ in the theoretical treatment, then from the definitions of Eqs. (3.15) and (3.17)–(3.21) we find that $C_{\mathbf{k}\beta}=A_{\mathbf{k}\beta}$ and $f_{\mathbf{k}\beta j}=0$. In this limit the polaronic effects are compensated for completely because of the opposite polarization effects of the electron and hole.

C. Ideal 3D limit

If the well width is much larger than the polaron radius and the exciton Bohr radius, the quantum-confinement effect and the IO-phonon effect will disappear and the present theory will reduce to bulk exciton–LO-phonon interaction theory. This is seen in the following by the limit analysis method:

(a) For the IO phonons: It is easy to confirm that $\omega_{\sigma p}$ and $\epsilon_{\sigma p}$ go to finite values, and

$$\lim_{d\to\infty}A_{\mathbf{k}\sigma p}=0, \tag{5.4}$$

$$\lim_{d\to\infty}B_{\mathbf{k}\sigma p}=0, \tag{5.5}$$

$$\lim_{d\to\infty}C_{\mathbf{k}\sigma p}=0, \tag{5.6}$$

which yield the effects of the exciton-IO-phonons interaction to be zero:

$$\lim_{d\to\infty}E_{\text{ex-IO}}=0. \tag{5.7}$$

(b) For the confined LO phonon,

$$\lim_{d\to\infty}A_{\mathbf{k}m}=\tfrac{1}{2}, \tag{5.8}$$

$$\lim_{d\to\infty}B_{\mathbf{k}m}=\tfrac{1}{2}, \tag{5.9}$$

$$\lim_{d\to\infty}C_{\mathbf{k}m}=\tfrac{1}{2}\langle\Psi_{1s}|\exp(i\mathbf{K}\cdot\mathbf{r})|\Psi_{1s}\rangle, \tag{5.10}$$

where $m\neq 1,2$ in the case of $l_e=l_h=1$, $\mathbf{K}=(\mathbf{k},k_m)$. Then the displacement amplitude f_{qmj} is reduced as

$$f_{qmj}=\frac{-\theta_j v_{qm}^*(1-G_{qm}^{1s})(K_{qmi}+G_{qm}^{1s})}{K_{qme}K_{qmh}-(G_{qm}^{1s})^2}\quad (i\neq j=e,h), \tag{5.11}$$

where

$$\mathbf{Q}=(\mathbf{q},q_m), \tag{5.12}$$

$$v_{qm}=V_{\mathbf{k}m}/(\hbar\omega_{L1}), \tag{5.13}$$

$$K_{qmj}^{1s}=\left(1+\frac{m_e}{m_j}Q^2\right) \quad (j=e,h), \tag{5.14}$$

$$G_{qm}^{1s}=\langle\Psi_{1s}|\exp(i\mathbf{Q}\cdot\mathbf{r})|\Psi_{1s}\rangle. \tag{5.15}$$

Inserting Eq. (5.11) into Eq. (3.24) and transforming the sum over m into an integral form by

$$\frac{1}{d}\sum_m \Rightarrow \frac{1}{\pi}\int dq_m, \tag{5.16}$$

then the ground-state energy $\mathcal{E}_g$ is given in dimensionless units

$$\mathcal{E}_g=\min_{\lambda}[\mathcal{E}_0(\lambda)+\mathcal{E}_{\text{ex-LO}}(\lambda)], \tag{5.17}$$

with

$$\mathcal{E}_0(\lambda)=\left\langle\Psi_{1s}\left|\left[\frac{m_e}{\mu}\frac{1}{\lambda}\left(\frac{2}{r}-\frac{1}{\lambda}\right)-\frac{\kappa}{r}\right]\right|\Psi_{1s}\right\rangle=\frac{m_e}{\mu}\frac{1}{\lambda^2}-\frac{\kappa}{\lambda}, \tag{5.18}$$

$$\mathcal{E}_{\text{ex-LO}}(\lambda)=-\frac{\alpha_{e1}}{\pi}\int\int q\ dq\ dq_m\ \frac{(1-G_{qm}^{1s})^2}{q^2+q_m^2} \times\frac{K_{qme}^{1s}+K_{qmh}^{1s}+2G_{qm}^{1s}}{K_{qme}^{1s}K_{qmh}^{1s}-(G_{qm}^{1s})^2}. \tag{5.19}$$

If we compare Eq. (5.11) with Eq. (4.4) in Ref. 34, in which the interaction of Wannier excitons with LO-phonon field in polar semiconductors was investigated in detail by a variation calculation, it is found that the two equations are really the same except for the differences of some definitions. Our theory gives correct result in the wide well-width limit.

(c) From Eqs. (5.17)–(5.19), one can easily obtain the following limit values.

When there are no phonon effects ($\alpha_{e1}=0$), then $\lambda=2(m_e/\mu)/\kappa$ for minimizing the energy, and the bare exciton energy is given as $\mathcal{E}_g=-(\mu/m_e)\kappa^2/4$ in the unit $\hbar\omega_{L1}$. This result is equal to $E_g=-R_y$, where R_y is the effective Rydberg energy defined by

$$R_y=\frac{\mu e^4}{2\epsilon_{\infty 1}^2\hbar^2}. \tag{5.20}$$

When phonon effects are considered and the electron and hole are separated enough from each other, then, by simple analytical calculation, we find

$$\lim_{d\to\infty}E_{\text{ex-LO}}=-(\alpha_{e1}+\alpha_{h1})\hbar\omega_{L1}. \tag{5.21}$$

This is the sum of the self-energies of a free electron-polaron and a free hole-polaron in weak- and middle-coupling cases. α_{e1} (α_{h1}) is just the Fröhlich electron (hole)–LO-phonon coupling constant in the well material.

D. The ideal 2D limit

(a) For the confined LO phonons, since $m_{\max}=\text{int}(W/a)$, if $W<a$ then $m=0$ and the confined LO phonon disappears, then we have

$$\lim_{d\to 0}E_{\text{ex-LO}}=0. \tag{5.22}$$

(b) For the IO phonons, from the expressions in Secs. II and IV, one can obtain the following limit values at the $d\to 0$ limit:

$$\omega_{++}=\omega_{L2},\quad \omega_{-+}=\omega_{T1},\quad \omega_{+-}=\omega_{T2},\quad \omega_{--}=\omega_{L1},$$

$$\epsilon_{++}=\epsilon_2,\quad \epsilon_{-+}=\infty,\quad \epsilon_{+-}=\infty,\quad \epsilon_{--}=\infty,$$

$$A_{\mathbf{k}\sigma+}=1,\quad B_{\mathbf{k}\sigma+}=0,$$

$$C_{\mathbf{k}\sigma+}=C_q^{1s}=\left(\frac{2}{\lambda}\right)^3\left[\left(\frac{2}{\lambda}\right)^2+q^2\right]^{-3/2}.$$

Keeping the above expressions in mind and doing standard limit analysis, then the ground-state energy of the QW exciton-phonon system at the 2D limit is given by

$$\mathcal{E}_g=\min_{\lambda}\left(\frac{m_e}{\mu}\frac{1}{\lambda^2}-\frac{2\kappa}{\lambda}-\frac{2\kappa}{\lambda}\sum_{n\neq 0}\xi^{|n|}+\mathcal{E}_{\text{ex-IO}}(\lambda)\right), \tag{5.23}$$

$$\mathcal{E}_{\text{ex-IO}}(\lambda)=-\alpha_{e2}\left(\frac{\omega_{L2}}{\omega_{L1}}\right)^{3/2} \times\int dq\frac{(1-C_q^{1s})^2\left(K_{qe}^{1s}+K_{qh}^{1s}+2\frac{\omega_{L2}}{\omega_{L1}}C_q^{1s}\right)}{K_{qe}^{1s}K_{qh}^{1s}-\left(\frac{\omega_{L2}}{\omega_{L1}}C_q^{1s}\right)^2}, \tag{5.24}$$

where

$$K_{qj}^{1s}=\left(\frac{\omega_{L2}}{\omega_{L1}}+\frac{m_e}{m_j}q^2\right) \quad (j=e,h). \tag{5.25}$$

(c) One can see clearly that the above expressions give correct theoretical results in the 2D limit case. Two special results are the following.

When the electron (hole)–IO-phonon interaction is absent, i.e., $\alpha_{e2}=0$, then the minimum value of the bare exciton energy is given as

$$\mathcal{E}_g=-\frac{\mu\kappa^2}{m_e}\left(1+\sum_{n\neq 0}\xi^{|n|}\right)^2=-\frac{\mu\kappa^2}{m_e}\left(\frac{1+\xi}{1-\xi}\right)^2 =-\frac{\mu\kappa^2}{m_e}\left(\frac{\epsilon_{\infty 1}}{\epsilon_{\infty 2}}\right)^2 \tag{5.26}$$

in the unit $\hbar\omega_{L1}$. Obviously, this result is equal to the exciton energy in a dielectric QW in the 2D limit, that is,

$$E_g=-4R_y\left(\frac{\epsilon_{\infty 1}}{\epsilon_{\infty 2}}\right)^2. \tag{5.27}$$

The factor $(\epsilon_{\infty 1}/\epsilon_{\infty 2})^2$ is contributed by the image charge distributions. If the effect of the image charge is not put into consideration, or the dielectric constant of the well is equal to that of the barrier, then E_g is reduced to the conventional 2D exciton binding energy $-4R_y$. Remembering the defini-

tion of R_y, it is found that $R_y(\epsilon_{\infty 1}/\epsilon_{\infty 2})^2$ is just the Rydberg energy of the barrier material. Since the contribution of the image charges increases with decreasing the well width, the factor $(\epsilon_{\infty 1}/\epsilon_{\infty 2})^2$ gives a maximum correction to the quasi-2D exciton binding energy. This factor can be used to estimate the importance of the image charge in narrow QW's.

When the electron (hole)–IO-phonon interaction is included and the electron and hole are separated from each other and move freely, $\lambda \to \infty$ and $G_q^{1s} \to 0$, then by simple analytical calculation we find

$$\lim_{d\to 0} E_{\text{ex-IO}} = -(\pi/2)(\alpha_{e2}+\alpha_{h2})\hbar\omega_{L2}. \tag{5.28}$$

This result is in agreement with the polaron theory in the infinite QW cases.[31,38] It should be noted that this result is not completely the same as the self-energy of a surface electron-polaron and a hole-polaron in the barrier material. The reason is that α_{e2} (α_{h2}) defined by Eq. (4.14) is not the Fröhlich coupling constant of the electron (hole) in the barrier material because the band mass used in the definition is not the mass of the electron (hole) in the barrier material.

From the above analysis it is shown that our theory can yield correct theoretical results in 2D and 3D limits analytically. It is very important academically to have a theory which is valid in the whole range of the well width from ideal 2D limit to 3D limit cases.

VI. NUMERICAL CALCULATION AND DISCUSSION

As an application of the present theory, properties of exciton-phonon systems are investigated numerically in this section. This quantitative investigation will give us a general knowledge of exciton-phonon interaction in QW's.

There are many physical parameters in the present problem. In order to discuss the essential property of the problem we use the isotropic mass approximation and study the ground state only. In this case the system is characterized by the following fundamental physical parameters:

$$W, m_e, m_h, \epsilon_{01}, \epsilon_{\infty 1}, \epsilon_{02}, \epsilon_{\infty 2}, \omega_{L1}, \omega_{T1}, \omega_{L2}, \omega_{T2}, a.$$

Since there is the well-known Lyddane-Sachs-Teller relationship

$$\left(\frac{\omega_{Li}}{\omega_{Ti}}\right)^2 = \frac{\epsilon_{0i}}{\epsilon_{\infty i}}, \quad i=1,2, \tag{6.1}$$

and the system is studied in dimensionless units, that is, the energy is in units of $\hbar\omega_{L1}$ and lengths in units of the polaron radius R_p, there are eight independent parameters. Based on the analysis of the feature of practical QW's we use the following characteristic parameters:

$$W,\ \frac{R_y}{\hbar\omega_{L1}},\ \alpha_{e1},\ \frac{m_e}{m_h},\ \frac{\omega_{L2}}{\omega_{L1}},\ \frac{\epsilon_{\infty 2}}{\epsilon_{\infty 1}},\ \frac{\epsilon_{02}}{\epsilon_{\infty 2}},\ a.$$

Here $R_y/\hbar\omega_{L1}$ represents the strength of the Coulomb binding energy of an electron-hole pair in unit of the LO-phonon energy, and α_{e1} is the Fröhlich electron–LO-phonon coupling constant of the well material. m_e/m_h is the ratio of the effective band mass of the electron to that of the hole. $\epsilon_{\infty 1}/\epsilon_{01}$ is not an independent parameter, which can be determined by

$$\frac{\epsilon_{\infty 1}}{\epsilon_{01}} = 1 - \alpha_{e1}\left[\frac{R_y}{\hbar\omega_{L1}}\left(1+\frac{m_e}{m_h}\right)\right]^{-1/2}. \tag{6.2}$$

Since $\epsilon_{\infty 1}/\epsilon_{01}$ must be positive and not larger than 1, the parameters involved in the right-hand side of Eq. (6.2) are restricted by this physical condition.

The lattice constant of the well material, a, is chosen as $0.1R_p$. Other choices will have very little influence on the interaction energy contributed by confined LO phonons in the narrow well range because the number of the LO phonon mode is determined by int(W/a), and will not affect the qualitative property of the exciton-phonon coupling system.

The influences of characteristic parameters on properties of exciton-phonon systems in QW's are calculated numerically, and are shown in Figs. 1–6. The average virtual phonon number N_{ph} reflects the coupling strength of the particle with the phonons. The numerical results of the present paper show that the variation of N_{ph} is similar to $E_{\text{ex-(LO+IO)}}$ in most of the cases except for the parameter ω_{L2}/ω_{L1}. The variation of N_{ph} with $R_y/\hbar\omega_{L1}$ is plotted in Fig. 7(a) as an example of the normal cases, and that of N_{ph} with ω_{L2}/ω_{L1} is plotted in Fig. 7(b) to show the special character of the studied system. Typical values of the parameters[35] are used in the numerical calculations, and listed in the figures and captions. The exciton binding energy, the exciton-phonon interaction energy, and the average virtual phonon number are plotted as functions of the well width. The quantum-confinement effects on the properties of the exciton-phonon system in every case can be seen clearly in the figures.

In order to give a clear picture of the polaronic effect, the bare exciton binding energy with optical dielectric constants $\epsilon_{\infty 1}$, the sum of the polaron energies of a free electron, and a free hole interacting with the phonons are also plotted in the figures with thin lines. The bare exciton binding energy is calculated independently by minimizing Eq. (4.10). The sum of the polaron energies contributed by the confined LO or/and IO phonons is calculated by Eqs. (4.11) and (4.12) with $C_{qm}=0$ and $C_{q\sigma p}=0$, as we discussed in Sec. V. The sum of average virtual phonon numbers of an electron-polaron and a hole-polaron are also plotted in Fig. 7 for comparison. For the convenience of the readers, the exciton binding energy is plotted in units of exciton Rydberg energy R_y, the length in units of the exciton Bohr radius a_B ($=\hbar^2\epsilon_{\infty 1}/\mu e^2$), the interaction energy of the exciton with phonons and the polaron energy in units of $\hbar\omega_{L1}$, and the corresponding length in units of the polaron radius R_p, respectively.

Figure 1 shows the influence of the Coulomb binding strength of the electron-hole pair on the property of the exciton-phonon coupling system in the whole range of the well width. According to Ref. 35 three typical values of $R_y/\hbar\omega_{L1}$ are used in the numerical calculations, which are $R_y/\hbar\omega_{L1}=0.2$, 1.0, and 10.0. It is clearly seen that the Coulomb binding strength has a significant effect on the property of the exciton-phonon system. The stronger the Coulomb binding, the weaker the exciton–optical-phonon interaction. The effects of the Coulomb binding strength is from two

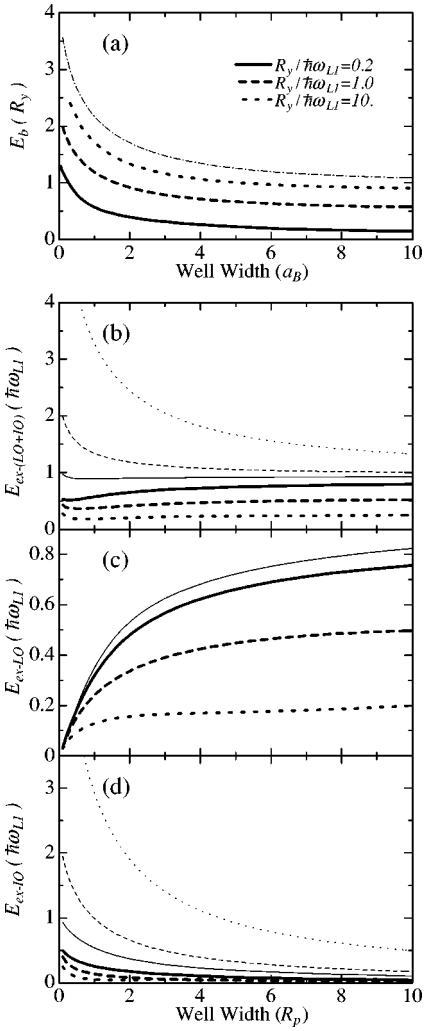

FIG. 1. Influence of the strength of the Coulomb binding, $R_y/\hbar\omega_{L1}$, on (a) the exciton binding energy, (b) the exciton–optical-phonon interaction energy, (c) the exciton–LO-phonon interaction energy, and (d) the exciton–IO-phonon interaction energy. The solid lines stand for $R_y/\hbar\omega_{L1}=0.2$, the dashed lines for $R_y/\hbar\omega_{L1}=1.0$, and the dotted lines for $R_y/\hbar\omega_{L1}=10$. The other physical parameters are set as $\alpha_{e1}=0.4$, $m_e/m_h=0.5$, $\omega_{L2}/\omega_{L1}=1.0$, $\epsilon_{\infty 2}/\epsilon_{\infty 1}=1.0$, and $\epsilon_{02}/\epsilon_{\infty 2}=2.0$. The thick lines stand for the exciton-phonon system. The thin dot-dashed line in (a) stands for the bare exciton binding energy. The thin lines in (b)–(d) stand for the sum of the polaron energies of a free electron-polaron and a free hole-polaron in the same cases as for excitons with the same line types.

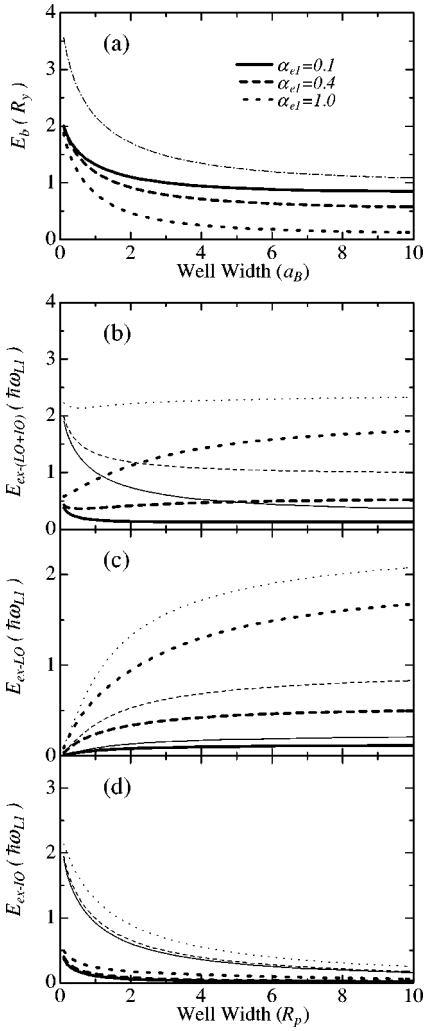

FIG. 2. Influence of the Fröhlich electron–LO-phonon coupling constant of the well material, α_{e1}, on (a) the exciton binding energy, (b) the exciton–optical-phonon interaction energy, (c) the exciton–LO-phonon interaction energy, and (d) the exciton–IO-phonon interaction energy. The solid lines stand for $\alpha_{e1}=0.1$, the dashed lines for $\alpha_{e1}=0.4$, and the dotted lines for $\alpha_{e1}=1.0$. The other physical parameters are set as $R_y/\hbar\omega_{L1}=1.0$, $m_e/m_h=0.5$, $\omega_{L2}/\omega_{L1}=1.0$, $\epsilon_{\infty 2}/\epsilon_{\infty 1}=1.0$, and $\epsilon_{02}/\epsilon_{\infty 2}=2.0$. The thick lines stand for the exciton-phonon system. The thin dot-dashed line in (a) stands for the bare exciton binding energy. The thin lines in (b)–(d) stand for the sum of the polaron energies of a free electron-polaron and a free hole-polaron in the same cases as for excitons with the same line types.

facts: (i) The electron and the hole which compose the exciton have opposite polaronic effects, as shown in Eqs. (2.10) and (2.11). If the two particles are forced close to each other, the interaction of the two particles with optical phonons will cancel each other. (ii) The strength of the Coulomb binding has a direct relation with the ratio of R_p/a_B,

$$R_p/a_B=(R_y/\hbar\omega_{L1})^{1/2}. \tag{6.3}$$

a_B/R_p is a criterion of the relative distance between the electron and hole. If the exciton Bohr radius a_B is smaller than the polaron radius R_p, the exciton–optical-phonon interaction will be canceled. Conversely, if a_B is larger than R_p, the exciton–optical-phonon interaction will be complete. This property can also be seen in Fig. 7(a). In the present paper, corresponding to $R_y/\hbar\omega_{L1}=0.2$, 1.0, and 10.0, the ratio of R_p/a_B are 0.447, 1.0, and 3.16, respectively.

It is seen from Fig. 1(c) that the strength of the Coulomb binding does not affect the polaron energy of a free electron and a free hole interacting with confined LO phonon, since this interaction energy in the dimensionless units is determined only by the Fröhlich coupling constant, but the Coulomb binding strength strongly affects the exciton–confined-LO-phonon interaction. On the other hand, as shown in Fig. 1(d), the Coulomb binding strength affects both the free-electron (hole)–IO-phonon interaction and the exciton–IO-phonon interaction obviously. The reason is that the IO pho-

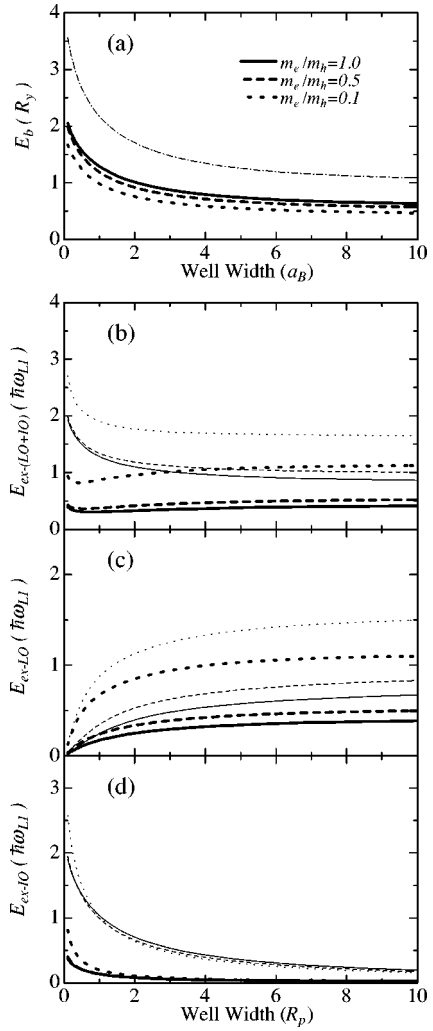

FIG. 3. Influence of the ratio of the electron band mass to the hole band mass, m_e/m_h, on (a) the exciton binding energy, (b) the exciton–optical-phonon interaction energy, (c) the exciton-LO–phonon interaction energy, and (d) the exciton–IO-phonon interaction energy. The solid lines stand for $m_e/m_h=1.0$, the dashed lines for $m_e/m_h=0.5$, and the dotted lines for $m_e/m_h=0.1$. The other physical parameters are set as $R_y/\hbar\omega_{L1}=1.0$, $\alpha_{e1}=0.4$, $\omega_{L2}/\omega_{L1}=1.0$, $\epsilon_{\infty 2}/\epsilon_{\infty 1}=1.0$, and $\epsilon_{02}/\epsilon_{\infty 2}=2.0$. The thick lines stand for the exciton-phonon system. The thin dot-dashed line in (a) stands for the bare exciton binding energy. The thin lines in (b)–(d) stand for the sum of the polaron energies of a free electron-polaron and a free hole-polaron in the same cases as for excitons with the same line types.

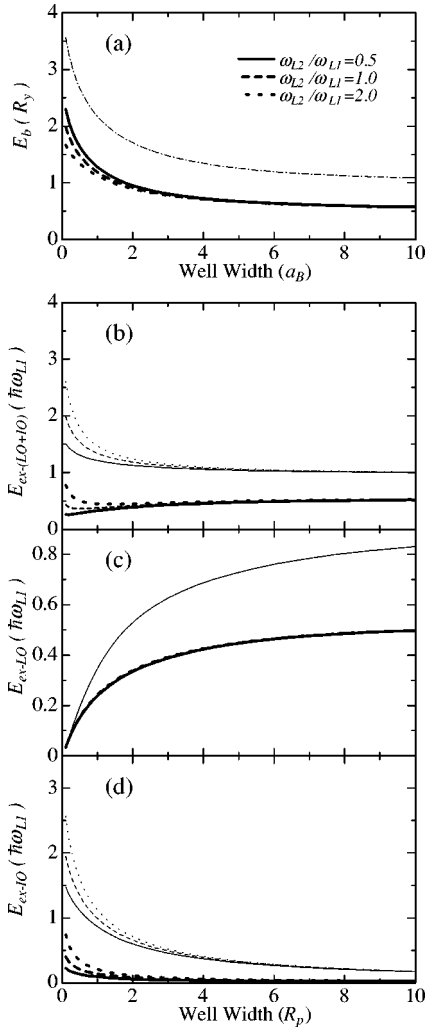

FIG. 4. Influence of the ratio of the LO-phonon frequency of well material to that of barrier material, ω_{L2}/ω_{L1}, on (a) the exciton binding energy, (b) the exciton–optical-phonon interaction energy, (c) the exciton–LO-phonon interaction energy, and (d) the exciton–IO-phonon interaction energy. The solid lines stand for $\omega_{L2}/\omega_{L1}=0.5$, the dashed lines for $\omega_{L2}/\omega_{L1}=1.0$, and the dotted lines for $\omega_{L2}/\omega_{L1}=2.0$. The other physical parameters are set as $R_y/\hbar\omega_{L1}=1.0$, $\alpha_{e1}=0.4$, $m_e/m_h=0.5$, $\epsilon_{\infty 2}/\epsilon_{\infty 1}=1.0$, and $\epsilon_{02}/\epsilon_{\infty 2}=2.0$. The thick lines stand for the exciton-phonon system. The thin dot-dashed line in (a) stands for the bare exciton binding energy. The thin lines in (b)–(d) stand for the sum of the polaron energies of a free electron-polaron and a free hole-polaron in the same cases as for excitons with the same line types.

non parameters of $\omega_{\sigma p}$ and $\epsilon_{\sigma p}$ relate with $\epsilon_{\infty 1}/\epsilon_{01}$, and $\epsilon_{\infty 1}/\epsilon_{01}$ is related with $R_y/\hbar\omega_{L1}$ by Eq. (6.2).

It should be noticed that Fig. 1(a) gives a relative relation of the exciton binding energies with the bare exciton binding energy because the energies are in units of R_y, and R_y is a variable parameter in this case.

The influence of the electron–LO-phonon coupling constant of the well material, α_{e1}, is shown in Fig. 2. Since there is the inequality

$$\alpha_{e1}<\left[\frac{R_y}{\hbar\omega_{L1}}\left(1+\frac{m_e}{m_h}\right)\right]^{1/2}, \tag{6.4}$$

three values of α_{e1} ($=0.1,0.4,1.0$) are chosen in the calculation corresponding to $R_y/\hbar\omega_{L1}=1$. The electron–LO-phonon coupling constant plays a determinate role in the interaction energies contributed by the confined LO phonon. The interaction energy increases in proportion to α_{e1}. On the other hand, the variation of α_{e1} has a small effect on the interaction energies contributed by the IO phonons. Since the modes of the confined LO phonons is determined by int(W/a), and decreases linearly with decreasing well width, and also since the IO phonon has no direct relation with α_{e1}, the change of α_{e1} does not affect the properties of the exciton-phonon systems and the free polarons in the QW's in the 2D limit.

Figure 3 shows the influence of the electron-hole mass

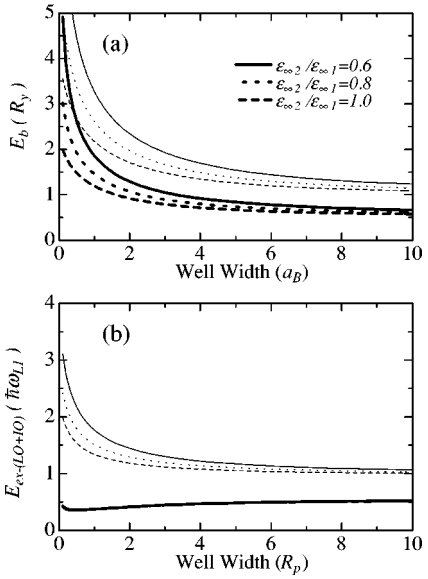

FIG. 5. Influence of the optical dielectric constant mismatch of well material with barrier material, $\epsilon_{\infty 2}/\epsilon_{\infty 1}$, on (a) the exciton binding energy, and (b) the exciton-optical phonons interaction energy. The solid lines stand for $\epsilon_{\infty 2}/\epsilon_{\infty 1}=0.6$, the dashed lines for $\epsilon_{\infty 2}/\epsilon_{\infty 1}=0.8$, and the dotted lines for $\omega_{L2}/\omega_{L1}=1.0$. The other physical parameters are set as $R_y/\hbar\omega_{L1}=1.0$, $\alpha_{e1}=0.4$, $m_e/m_h=0.5$, $\omega_{L2}/\omega_{L1}=1.0$, and $\epsilon_{02}/\epsilon_{\infty 2}=2.0$. The thick lines stand for the exciton-phonon system. The thin lines in (a) stand for the bare exciton binding energies, and the thin lines in (b) for the sum of the polaron energies of a free electron-polaron and a free hole-polaron in the same cases as for excitons with the same line types.

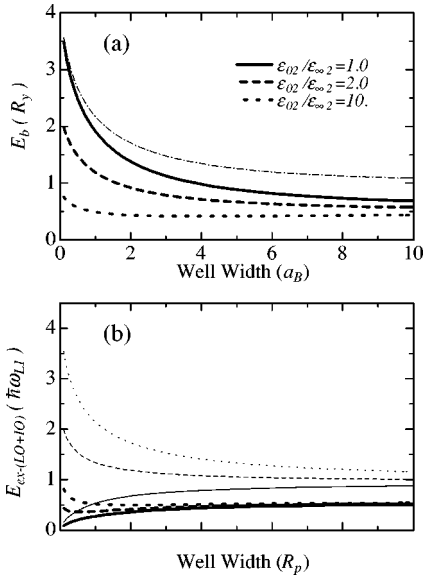

FIG. 6. Influence of the ratio of the static dielectric constant to the optical dielectric constant of barrier material, $\epsilon_{02}/\epsilon_{\infty 2}$ on (a) the exciton binding energy, and (b) the exciton-optical phonons interaction energy. The solid lines stand for $\epsilon_{02}/\epsilon_{\infty 2}=1.0$, the dashed lines for $\epsilon_{02}/\epsilon_{\infty 2}=2.0$, and the dotted lines for $\epsilon_{02}/\epsilon_{\infty 2}=10$. The other physical parameters are set as $R_y/\hbar\omega_{L1}=1.0$, $\alpha_{e1}=0.4$, $m_e/m_h=0.5$, $\omega_{L2}/\omega_{L1}=1.0$, and $\epsilon_{\infty 2}/\epsilon_{\infty 1}=1.0$. The thick lines stand for the exciton-phonon system. The thin dot-dashed line in (a) stands for the bare exciton binding energy. The thin lines in (b) stand for the sum of the polaron energies of a free electron-polaron and a free hole-polaron in the same cases as for excitons with the same line types.

ratio m_e/m_h on the properties of exciton-phonon coupling systems and polarons in QW's. It is seen that the exciton binding energy is affected obviously by the the mass ratio. For a fixed $R_y/\hbar\omega_{L1}$, the correction by the mass ratio originates from the different polaronic coupling strength of the electron- and hole-polarons with different mass ratios. It is somewhat beyond our expectation that the dependence of the polaronic effect of the IO phonons upon the mass ratio is completely different from that of the confined LO phonons. The mass ratio has obvious effects on the interaction energies of the exciton and the charged particles with the confined LO phonons, but has very little effect on that with the IO phonons except for very narrow well cases. The different characters of the confined LO and IO phonons are clearly shown in this case.

The roles of barrier parameters in exciton-phonon systems, and free polarons in QW's, are shown in Figs. 4–6. The common feature is that these parameters have no obvious influence on the contributions of the confined LO phonons because the confined LO phonons have no direct relation with the barrier parameters in the Hamiltonian and the expressions of the energies. The changes of the polaronic effects in Figs. 4–6 result completely from the IO phonons.

It is seen from Fig. 4 that, with increasing ω_{L2}/ω_{L1}, the exciton binding energy is decreased, and the exciton–IO-phonon interaction energy is increased in the narrow well range, but the changes go to zero rapidly outside the $W \leqslant 2R_p$ range. The reason for this is that the IO-phonon energy given by Eq. (2.7) is increased with increasing ω_{L2}/ω_{L1}, but, at the same time, the virtual IO-phonon numbers of the free polarons is decreased, as shown in Fig. 7(b); the two opposite effects make the influence of ω_{L2}/ω_{L1} on the exciton and free polaron states small, and it almost disappears in the $W>2R_p$ range.

In Fig. 5 three typical values of the parameter $\epsilon_{\infty 2}/\epsilon_{\infty 1}$ are chosen in the calculations. $\epsilon_{\infty 2}/\epsilon_{\infty 1}=1.0$ refers to a QW with no dielectric mismatch. It is shown that the dielectric mismatch greatly influences the properties of the exciton in the dielectric QW. Because of the image potential the exciton binding energy is enhanced by decreasing $\epsilon_{\infty 2}/\epsilon_{\infty 1}$. On the other hand, since the free-polaron energy increases with decreasing $\epsilon_{\infty 2}/\epsilon_{\infty 1}$, but the exciton-phonon interaction energy almost has no change at the same case, the polaronic effect reduces the exciton binding energy with decreasing $\epsilon_{\infty 2}/\epsilon_{\infty 1}$. The polaronic effect is opposite to the image charge effect for the exciton binding energy of dielectric QW's, but the increase caused by the image potential overcomes the decrease due to the polaronic effect. Both the image charge effect and the polaronic effect are important in this case, but the image potential effect is in dominant position.

The parameter $\epsilon_{02}/\epsilon_{\infty 2}$ represents the ratio of the polarizabilites of the barrier material in static and high-frequency cases. In Fig. 6 three typical values are used: $\epsilon_{02}/\epsilon_{\infty 2}=1$ is for the nonpolar material, $\epsilon_{02}/\epsilon_{\infty 2}=2$ for typical polar materials, and $\epsilon_{02}/\epsilon_{\infty 2}=10$ for some special polar material such as PbS, PbSe, and PbTe.[39] The most interesting fact is that, if the barrier is made of nonpolar material, the amplitude of the IO phonons and the interaction energy contributed by the IO phonons are considerably reduced, and go to zero in the 2D

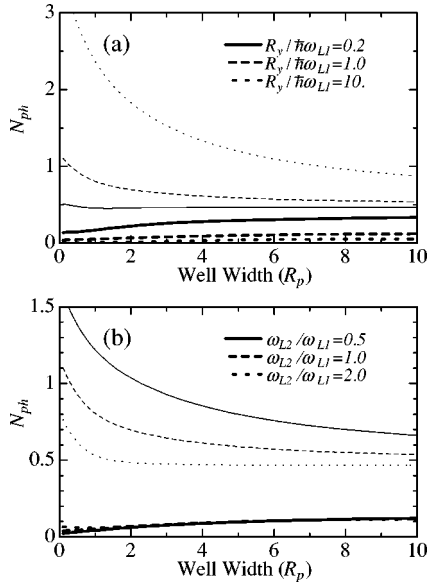

FIG. 7. (a) Influence of the strength of the Coulomb binding, $R_y/\hbar\omega_{L1}$, on the average virtual phonon numbers $N_{\rm ph}$. The parameters used in this case are the same as in Fig. 1. (b) Influence of the ratio of the LO-phonon frequency of well material to that of barrier material, ω_{L2}/ω_{L1}, on the average virtual phonon numbers $N_{\rm ph}$. The parameters used in the calculations are the same as in Fig. 4. The thick lines stand for the exciton-phonon system, and the thin lines for the sum of the average virtual phonon numbers of a free electron-polaron and a free hole-polaron in the same cases as for excitons with same line types.

limit. Consequently the exciton binding energy will go to the maximum theoretical value $4R_y$ in the 2D limit case. This fact may be important experimentally for the increase of the exciton binding energy of the manmade layered materials.

VII. CONCLUSION

From analytic and numerical results we can conclude some general properties of the exciton–optical-phonon interaction in polar semiconductor QW's.

(1) The exciton–optical-phonon interaction has an obvious effect on the exciton binding energy. When the lattice parameters related to the phonons are changed, the exciton binding energy receives a significant correction, especially in the narrow well cases.

(2) In spite of the free-electron- and hole-polaron energies increasing with decreasing well width in QW's, the exciton–optical-phonon interaction energy is reduced little by little decreasing the well width, except for the vary narrow well cases.

(3) If we compare the magnitudes of the exciton–IO-phonon interaction energies $E_{\text{ex-IO}}$ (thick lines) with the sum of the polaron energies of a free electron and a free hole interacting with IO phonons (thin lines) in the figures, it is clearly seen that, being very different from the confined LO phonons, the IO-phonon–exciton interaction energy is mostly canceled by the opposite polaronic effects of the electron and the hole. Only in narrow well cases, that is, $W \leqslant 2R_p$, do IO phonons have obvious effects on the exciton state. This feature shows the short-range nature of the IO phonons.

(4) The image charge effect due to the mismatch of the dielectric constants of the QW structures is important, and cannot be neglected in the study of the optical and electrical properties of dielectric QW's. Although the polaronic effect intends to reduce the exciton binding energy by increasing $\epsilon_{\infty 1}/\epsilon_{\infty 2}$, analytical and numerical calculations show that the image potential is dominant, and increases the exciton binding energy with increasing $\epsilon_{\infty 1}/\epsilon_{\infty 2}$.

(5) The weaker the polaronic effect of the barrier material, the larger the binding energy of the exciton in the QW. If the barrier material is of nonpolar material, then the exciton binding energy is close to the bare 2D exciton energy in the narrow QW limit. This fact shows that if we want to increase the exciton banding energy in manmade layered materials in experiments, we should select weakly polar or nonpolar materials as the barrier materials.

(6) The exciton–IO-phonon interaction energies are small, and go to zero rapidly as the well width is increased, and can be neglected in most of the cases, but, conversely, the free-polaron energies contributed by the IO phonon are very large and reduce slowly to zero with increasing width. Then we have a situation where the IO phonon has a small effect on the exciton state, but has a significant effect on the exciton binding energy because the exciton binding energy is defined as the difference between the exciton ground-state energy and the polaron energies of the electron and hole.

(7) The ratio of the effective exciton Bohr radius a_B to the polaron radius R_y plays an important role in determining the property of the exciton-phonon interaction system. In general, if $a_B/R_p > 3$, the polaronic effect will work completely, and the corresponding exciton binding energy will be close to the hydrogenic exciton binding energy with static dielectric constant ϵ_0. The GaAs-based QW structure is an example of this case. On the other hand, if $R_p/a_B > 3$ the exciton-phonon interaction will be canceled to some extent because of the opposite polaronic effect of the electron and hole; the corresponding exciton binding energy will be the hydrogenic exciton binding energy with effective dielectric constant $\epsilon_{\rm eff}$, whose value is between ϵ_0 and ϵ_∞.

In summary, we have presented a theory for investigating the exciton-phonon interaction in semiconductor QW's made of polar compounds. By using an improved variational method, expressions of the bound-state energy and the average virtual phonon numbers are obtained. It is proved that the present theory is valid in the entire well width range from the 2D limit to the 3D limit. Based on the isotropic approximation, the ground states of exciton-phonon interaction systems in QW's have been investigated numerically. Some interesting features of the system are found, and general properties of the exciton-phonon coupling system in QW's are discussed and concluded.

Our method is analytically simple, and also quite effective in discussing problems of two interacting fermions in boson fields in quantum-confinement structures. Furthermore, the procedure is easily extended to other systems, such as bipolarons, bound polarons, and bound excitons in QW's, These works will be under consideration.

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