Longitudinal-optical-phonon effects on the exciton binding energy in a semiconductor quantum well

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(Received 29 October 1993)

The longitudinal-optical-phonon effect on the exciton binding energies in a quantum well consisting of a single slab of GaAs sandwiched between two semi-infinite slabs of $Ga_{1-x}Al_xAs$ are studied. By using the Lee-Low-Pine unitary transformation, the Hamiltonian can be separated into two parts which contain the phonon variables and exciton variables, respectively, providing that the virtual phonon-electron and virtual phonon-hole interactions are neglected. A trial wave function, which is able to reproduce the correct exciton binding energy in a quantum well, is obtained by using a perturbative variational technique. The trial wave function consists of a product of the envelope function in the z direction (perpendicular to the layers) for electron and hole and a purely two-dimensional exciton wave function. The dependence of the ground-state binding energy, which includes the effect of electron-phonon interaction on the well width, is investigated. It is found that the correction due to polaron effects on the exciton binding energy is quite significant for a well width of several hundred angstroms and the effects of either surface phonons or bulk phonons on the binding energy of the heavy-hole exciton is always larger than that of the light-hole exciton. Our results are compared with some previous results, and satisfactory agreements are obtained.

I. INTRODUCTION

During the past decade it has become possible to grow systems consisting of alternate layers of two different semiconductors with controllable thickness and relatively sharp interfaces using epitaxial crystal growth techniques such as molecular beam epitaxy and metal-organic chemical vapor deposition. This situation allows the experimental studies of excitonic states to become possible. One of the most interesting features of photoexcited systems is that the electrons and the holes interact strongly at low temperature their kinetic energy is low enough for them to combine and form bound states (free exciton). This free exciton is analogous to a hydrogen atom or, more exactly, to positronium, since the mass of a hole is typically about the same as the mass of an electron. In some semiconductors an exciton can exist for a relatively long period of time—more than 10 μsec in silicon—before the electron-hole pair annihilates. The recombination involves a characteristic emission which can be detected to obtain information. The exciton in the quantum well behaves like a quasi-two-dimensional hydrogen atom; because that the exciton binding energy is observed to increase as the quantum well width decreases. The binding energy for an exciton is typically 100–1000 times smaller than that of a hydrogen atom.

The most extensively studied heterostructure is the one consisting of alternate layers of GaAs and $Ga_{1-x}Al_xAs$ with layer thicknesses varying from a few monolayers to more than 400 Å. The quantum states and band structure of a GaAs–$Ga_{1-x}Al_xAs$ quantum well has been observed by many authors.[1–4] Both of these two compounds have zinc blende lattices. For instance, the direct gap of GaAs is at $K = 0$ where the conduction band has a nondegenerate minimum and the valence band has a threefold-degenerate maximum if the spin is neglected. The inclusion of spin and spin-orbit interactions modifies the bands by splitting the sixfold-degenerate valence states into an upper fourfold ($J=3/2$) state and a lower twofold ($J=1/2$) state separated by spin-orbit splitting Δ. Several recent studies have shown that $Ga_{1-x}Al_xAs$ has a direct band gap at the Γ point for Al concentrations less than about 40% ($x = 0.4$).[5] The conduction and valence band discontinuities at the interface have been shown to be about 85% and 15%, respectively, of the band gap difference between the two semiconductors. Thus electrons and holes in the GaAs matrix find themselves in a potential well whose height depend on Al concentration in the surrounding $Ga_{1-x}Al_xAs$ layers. The transport and optical measurements of this heterostructure have been investigated.[3] The optical spectra are often dominated by excitonic transitions from hole subbands to elec-

0163-1829/94/49(20)/14554(10)/$06.00

tron subbands. The intersubband optical (or magneto-optical) transitions in GaAs–$Ga_{1-x}Al_xAs$ quantum wells have been observed.[6–15] The absorption, magnetoabsorption, and luminesence excitation spectra in high quality samples clearly display exciton features. Most of the attention has been focused on the excitons formed between the lower-lying electron and hole subbands, the latter being split into heavy-hole and light-hole subbands.

The binding energies of the exciton in a quantum well have been studied extensively by many authors.[6,16–25] The binding energies of the ground heavy-hole and light-hole excitons are still matters of experimental and theoretical controversy.[2,4,26–28] The magneto-optical observations give binding energies which are consistently larger than those deduced from the absorption or luminescence excitation experiments.[6,29] In previous works, the hole was usually treated as a particle with either the heavy-hole mass or the light-hole mass. Most previous calculations employed the variational approach.[6,16–21] Some works[23,25] included the nonparabolicity of the conduction band and the degeneracy of the valence band. It is well known that an electron staying in a low-lying level of the conduction band of a polar crystal will interact strongly with the longitudinal optical mode of lattice vibrations.[30–40] We may picture the electron as it moves through the crystal accompanied by a cloud of phonons. Since the III-V materials used in producing typical quantum well structures are polar crystals, an electron weakly bound in this system will interact with the phonons of the host semiconductor and so increase the donor binding energy. On the basis of the strong coupling scheme, Ercelebi and Özdincer[33] calculated the ground state binding energy of the exciton-phonon system in GaAs/GaAlAs quantum well structures and found that the corrections due to electron-phonon coupling are rather significant. Degani and Hipólito[34] also found the polaronic contribution to the exciton binding energies is quite significant and increases with decreasing well thickness. Rücker *et al.*[39] calculated the electron-LO-phonon scattering rate in quasi-two-dimensional systems, based on a fully microscopic description of the phonon spectra and concluded that interface phonons are of great importance.

As mentioned above, most previous theoretical studies employed the variation principle to construct the trial wave functions. However, the construction of variational trial wave functions relies heavily on physical intuition. And the errors involved in the construction are usually difficult to estimate. Since a good knowledge of the exciton binding energy is essential for an accurate interpretation of the experimental observations, therefore, it should be interesting to employ a more reliable method to study the binding energy of the exciton system more accurately. In this work we concentrate on the effect of electron-phonon coupling on the binding energy of Wannier excitons in quantum well structures. We will employ the perturbative variation technique[41] to construct a trial wave function which is separated into z and the $x-y$ coordinates. The interaction between the electron and surface phonon and the electron and bulk-longitudinal phonon will be taken into account. Lee-Low-Pines transformation will be applied to separate the electron and phonon variables. The reason that we take a separable form wave function is partly because of the numerical calculation involved using such a wave function is simpler. Another reason is because it has been shown[17] that the separable trial function is able to yield reasonably good results for thin layers.

II. THEORY

The Hamiltonian of an exciton associated with either the heavy-hole band or the light-hole band in a GaAs slab sandwiched between two semi-infinite slabs of $Ga_{1-x}Al_xAs$ interacting with the longitudinal optical phonon can be expressed within the framework of effective mass approximation as[49]

$$H = H_e + H_h + H_{e-h} + H_{\rm SP} + H_{{\rm SP}-e} + H_{{\rm SP}-h} + H_{\rm BP} + H_{{\rm BP}-e} + H_{{\rm BP}-h}, \tag{1}$$

where

$$H_e = -\frac{\hbar^2}{2m_e}\nabla_e^2 + V_{ew}, \tag{2}$$

$$H_h = -\frac{\hbar^2}{2m_h}\nabla_h^2 + V_{hw}, \tag{3}$$

$$H_{e\text{-}h} = \frac{-e^2}{\varepsilon_0\,|\vec{r}_e - \vec{r}_h|}, \tag{4}$$

$$H_{\rm SP} = \sum_q \hbar\omega_s\, a_q^\dagger a_q, \tag{5}$$

$$H_{{\rm SP}\text{-}e} = \sum_q \left(\Gamma_q \frac{2z_l}{L}\left[e^{q_z(z_e-\frac{L}{2})} - e^{-q_z(z_e+\frac{L}{2})}\right] e^{i\vec{q}_r\cdot\vec{r}_{e\parallel}}\, a_q + \text{H.c.}\right), \tag{6}$$

$$H_{{\rm SP}\text{-}h} = \sum_q \left(\Gamma_q \frac{2z_h}{L}\left[e^{q_z(z_h-\frac{L}{2})} - e^{-q_z(z_h+\frac{L}{2})}\right] e^{i\vec{q}_r\cdot\vec{r}_{h\parallel}}\, a_q + \text{H.c.}\right), \tag{7}$$

$$H_{\rm BP} = \sum_k \hbar\omega_b\, b_k^\dagger b_k, \tag{8}$$

$$H_{{\rm BP}\text{-}e} = \sum_k W_{ek}\,\theta(z_e)\,\cos k_z z_e\, e^{i\vec{k}_r\cdot\vec{r}_{e\parallel}}\, b_k + \text{ H.c.}, \tag{9}$$

$$H_{{\rm BP}\text{-}h} = \sum_k W_{hk}\,\theta(z_h)\,\cos k_z z_h\, e^{i\vec{k}_r\cdot\vec{r}_{h\parallel}}\, b_k + \text{ H.c.}, \tag{10}$$

where $V_{ew}(z_e)$ and $V_{hw}(z_h)$ are the well potentials seen by the electron and hole, a_q is the annihilation operator for optical surface (SO) phonons of wave vector $\mathbf{q} = (\vec{q}_r, \vec{q}_z)$ and frequency ω_s, b_k is the annihilation operator for the optical bulk (BO) phonons of vector $\mathbf{k} = (\vec{k}_r, \vec{k}_z)$ and frequency ω_b, $H_{\rm SP}$ is the surface phonon energy, and $H_{{\rm SP}\text{-}e}$ ($H_{{\rm SP}\text{-}h}$) is the interacting Hamiltonian between the sur-

face phonon and the electron (hole) in the well. $H_{\rm BP}$ is the bulk phonon energy and $H_{\text{BP-}e}$ ($H_{\text{BP-}h}$) is the interacting hamitonian between the bulk phonon and the electron (hole) in the well. And the interaction strengths are[42–44]

$$\Gamma_q = i\left(\frac{\pi\hbar\omega_s e^2}{\varepsilon^* Aq}\right)^{\frac{1}{2}}, \tag{11}$$

$$\varepsilon^* = \left(\frac{\varepsilon_0 - 1}{\varepsilon_0 + 1} - \frac{\varepsilon_\infty - 1}{\varepsilon_\infty + 1}\right)^{-1}, \tag{12}$$

$$\theta(z) = \begin{cases} 0, & z > \frac{L}{2} \text{ or } z < \frac{-L}{2} \\ 1, & \frac{-L}{2} < z < \frac{L}{2}, \end{cases} \tag{13}$$

$$W_{jk} = \frac{1}{k}\frac{U^j}{\sqrt{V}}, \tag{14}$$

$$U^j = \hbar\omega_b\sqrt{4\pi\eta_j\left(\frac{\hbar}{2m_j\omega_b}\right)^{1/2}}, \tag{15}$$

$$\eta_j = e^2\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right)\sqrt{\frac{m_j}{2\hbar^3\omega_b}}, \tag{16}$$

$$j = e, h \tag{17}$$

where V is the crystal volume, ε_0 and ε_∞ are the static and high frequency dielectric constants, and ω_s and ω_b are the dispersionless SO and BO phonon energies.

Now applying the first and second Lee-Low-Pines transformation[45] for the two-dimensional system

$$U_1 = \exp\left(-i\,\vec{r}_{e_\parallel}\cdot\sum_q \vec{q}\,a_q^\dagger\,a_q - i\vec{r}_{e_\parallel}\cdot\sum_k \vec{k}_r\,b_k^\dagger\,b_k\right), \tag{18}$$

$$U_2 = \exp\left(-i\,\vec{r}_{h_\parallel}\cdot\sum_q \vec{q}\,a_q^\dagger\,a_q - i\vec{r}_{h_\parallel}\cdot\sum_k \vec{k}_r\,b_k^\dagger\,b_k\right), \tag{19}$$

$$U_3 = \exp\left(\sum_q (a_q^\dagger\,f_g - a_q\,f_q^*)\right), \tag{20}$$

$$U_4 = \exp\left(\sum_k (b_k^\dagger\,g_k - b_k\,g_k^*)\right), \tag{21}$$

where $\vec{r}_{e_\parallel}$ and $\vec{r}_{h_\parallel}$ are the in-plane projection of the electron and hole positions and one obtains

$$H^0 = U_4^{-1}\,U_3^{-1}\,U_2^{-1}\,U_1^{-1}\,H\,U_1\,U_2\,U_3\,U_4, \tag{22}$$

$$\begin{aligned} H^0 = {} & H_e + H_h + H_{e\text{-}h} + \sum_q\left(\hbar\omega_s + \frac{\hbar^2q^2}{2m_e} + \frac{\hbar^2q^2}{2m_h}\right)(a_q^\dagger + f_q^*)(a_q + f_q) \\ & + \sum_q \Gamma_q\,e^{-q|z_e|}\,(a_q + f_q) + \text{H.c.} + \sum_q \Gamma_q\,e^{-q|z_h|}\,(a_q + f_q) + \text{H.c.} \\ & + \sum_k\left(\hbar\omega_b + \frac{\hbar^2k_r^2}{2m_e} + \frac{\hbar^2k_r^2}{2m_h}\right)(b_k^\dagger + g_k^*)(b_k + g_k) \\ & + \sum_k W_{ek}\,\theta(z_e)\,\cos k_z z_e\,(b_k + g_k) + \text{H.c.} + \sum_k W_{hk}\,\theta(z_h)\,\cos k_z z_h\,(b_k + g_k) + \text{H.c.} \end{aligned} \tag{23}$$

In the above derivation, we have neglected the terms involving the virtual phonon-electron and virtual phonon-hole interaction. The trial wave function for our system is assumed as a product of the exciton part and phonon part:

$$|\,\Psi\rangle = \phi(r)\,|\,\psi\rangle, \tag{24}$$

where $\phi(r)$ depends on the exciton coordinates and $|\,\psi\rangle$ depends on the phonon coordinates. Since the major contribution to the energies of the polaron system comes from the Coulomb interaction between the electron and hole, the realistic energies for the polaron states can be obtained only if the excitonic part can be solved more accurately. To achieve this goal we shall perform a perturbative variational approach to obtain more accurate eigenenergies for the excitonic part. Before we perform this, let us first manage the phonon part. The $|\,\psi\rangle$ can be expressed as $|\,\psi\rangle = \sum_n (\frac{1}{\sqrt{n!}}(a^+)^n\,|\,0\rangle$, and $|\,0\rangle$ is the phonon vacuum state. For the low-lying polaron states, $|\,\psi\rangle$ can be taken as $|\,0\rangle$. Then

$$\langle\,H^0\rangle = \langle 0\,|\,\phi^*(r)\,H^0\,\phi(r)\,|\,0\rangle \tag{25}$$

$$\begin{aligned} = {} & \langle\phi(r)\,|\,H_e + H_h + H_{e\text{-}h}\,|\,\phi(r)\rangle + \sum_q\left(\hbar\omega_s + \frac{\hbar^2q^2}{2m_e} + \frac{\hbar^2q^2}{2m_h}\right) f_q\,f_q^* \\ & + \sum_q \Gamma_q\,\beta_{eq}\,f_q + \text{H.c.} + \sum_q \Gamma_q\,\beta_{hq}\,f_q + \text{H.c.} + \sum_k\left(\hbar\omega_b + \frac{\hbar^2k_r^2}{2m_e} + \frac{\hbar^2k_r^2}{2m_h}\right) q_k\,q_k^* \\ & + \sum_k W_{ek}\,\alpha_{ek}\,g_k + \text{H.c.} + \sum_k W_{hk}\,\alpha_{hk}\,g_k + \text{H.c.}, \end{aligned} \tag{26}$$

where

$$\beta_{eq} = \int_{-L/2\le z_e,z_h\le L/2} \frac{2z_l}{L}\left[e^{q(z_e-\frac{L}{2})} - e^{-q(z_e+\frac{L}{2})}\right] \times|\phi(r)|^2 \times dx_e\,dy_e\,dz_e\,dx_h\,dy_h\,dz_h, \quad (27)$$

$$\beta_{hq} = \int_{-L/2\le z_e,z_h\le L/2} \frac{2z_h}{L}\left[e^{q(z_h-\frac{L}{2})} - e^{-q(z_h+\frac{L}{2})}\right] \times|\phi(r)|^2 \times dx_e\,dy_e\,dz_e\,dx_h\,dy_h\,dz_h, \quad (28)$$

$$\alpha_{ek} = \int_{-L/2\le z_e,z_h\le L/2} \theta(z_e)\cos k_z z_e\,|\phi(r)|^2 \times dx_e\,dy_e\,dz_e\,dx_h\,dy_h\,dz_h, \quad (29)$$

$$\alpha_{hk} = \int_{-L/2\le z_e,z_h\le L/2} \theta(z_h)\cos k_z z_h\,|\phi(r)|^2 \times dx_e\,dy_e\,dz_e\,dx_h\,dy_h\,dz_h. \quad (30)$$

The parameters f_q, f_q^*, g_k, and g_k^* can be obtained by minimizing the $\langle H^0\rangle$ with respect to the parameters f_q, f_q^*, g_k, and g_k^*, respectively,

$$f_q^* = -\frac{\Gamma_q\beta_{eq}+\Gamma_q\beta_{hq}}{\hbar\omega_s+\frac{\hbar^2q^2}{2m_e}+\frac{\hbar^2q^2}{2m_h}}, \quad (31)$$

$$g_k^* = -\frac{W_{ek}\alpha_{ek}+W_{hk}\alpha_{hk}}{\hbar\omega_b+\frac{\hbar^2k_r^2}{2m_e}+\frac{\hbar^2k_r^2}{2m_h}}, \quad (32)$$

$$f_q = (f_q^*)^*, \quad (33)$$

$$g_k = (g_k^*)^*, \quad (34)$$

Using these parameters, one obtains finally

$$\langle H^0\rangle = \langle\phi(r)\mid H_e+H_h+H_{e\text{-}h}\mid\phi(r)\rangle - \sum_q \frac{|\Gamma_q|^2\,|\beta_{eq}+\beta_{hq}|^2}{\hbar\omega_s+\frac{\hbar^2q^2}{2m_e}+\frac{\hbar^2q^2}{2m_h}} - \sum_k \frac{|W_{ek}\alpha_{ek}+W_{hk}\alpha_{hk}|^2}{\hbar\omega_b+\frac{\hbar^2k_r^2}{2m_e}+\frac{\hbar^2k_r^2}{2m_h}}. \quad (35)$$

Now let us turn to the excitonic part. The Hamiltonian of an exciton associated with either the heavy-hole band or the light-hole band in a GaAs slab sandwiched between the two semi-infinite slabs of GaAs–$Ga_{1-x}Al_xAs$ is modified by adding a term $\frac{\lambda e^2}{\varepsilon_0\sqrt{x^2+y^2}}$ to and then subtracting the same term from the Hamiltonian and rearranging as follows:

$$H = H_0(\lambda)+H'(\lambda) \quad (36)$$

$$= H_{z_e}+H_{z_h}+H_{xy}+H'(\lambda), \quad (37)$$

where

$$H_{z_e} = \frac{-\hbar^2}{2m_e}\frac{\partial^2}{\partial {z_e}^2}+V_{ew}(z_e), \quad (38)$$

$$H_{z_h} = \frac{-\hbar^2}{2m_h}\frac{\partial^2}{\partial {z_h}^2}+V_{hw}(z_h), \quad (39)$$

$$H_{xy} = \frac{-\hbar^2}{2\mu_\pm}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)-\frac{\lambda e^2}{\varepsilon_0\sqrt{x^2+y^2}}, \quad (40)$$

$$H'(\lambda) = \frac{\lambda e^2}{\varepsilon_0\sqrt{x^2+y^2}}-\frac{e^2}{\varepsilon_0\,|\,\vec{r}_e-\vec{r}_h\,|} \quad (41)$$

in the above equations and λ is treated as a parameter which can be varied to make the perturbation term $H'(\lambda)$ as small as possible. $\mu_\pm$ is the reduced mass corresponding to heavy (+) or light (−) hole bands in the plane perpendicular to the z direction. The potential wells seen by the electron $V_{ew}(z_e)$ and by the holes $V_{hw}(z_h)$ are assumed to be square wells with well width L:

$$V_{ew}(z_e) = \begin{cases} 0, & |\,z_e\,| < L/2 \\ V_e, & |\,z_e\,| > L/2, \end{cases} \quad (42)$$

$$V_{hw}(z_h) = \begin{cases} 0, & |\,z_h\,| < L/2 \\ V_h, & |\,z_h\,| > L/2, \end{cases} \quad (43)$$

Here we have chosen, without loss of generality, the origin of the coordinate system to be at the center of the GaAs well. The heights of the potential well V_e and V_h are determined from the Al concentration in $Ga_{1-x}Al_xAs$, using the following expression[5] for the total band gap discontinuity:

$$\Delta E_g = 1.155x+0.37x^2\ \text{eV}.$$

The value of V_e and V_h are 85% and 15% of ΔE_g, respectively. Now let us roughly estimate the magnitude of the term H' by the uncertainty relation for the ground state exciton:

$$\langle H'\rangle \sim \frac{e^2}{\varepsilon_0\rho}\frac{z^2}{\rho^2} \sim R\left(\frac{L}{a}\right)^2 \quad (44)$$

for small well width $L \ll a$ where L is the GaAs well width, $a = \varepsilon_0\hbar^2/\mu_\pm e^2$ is the transverse effective Bohr radius, and $R = \mu_\pm e^4/2\varepsilon_0^2\hbar^2$ is the three-dimensional effective Rydberg calculated with transverse reduced mass $\mu_\pm$. Hence as $(L/a)^2 \ll 1$, the term H' in H can be taken as a small perturbation. The introduction of the variational parameter λ ensures that the term H' can be made as small as possible. One can note that the eigenfunctions of H_0 can be solved exactly. The motions of the electron or hole along the z direction are just those of the one-dimensional square well potential. The solution to the transverse part H_{xy} is just the two-dimensional hydrogen problem. For illustration, we shall consider the ground state only; it is straightforward to obtain the excited states. Now the ground state eigenfunction and eigenvalue for $H_{z_e}(H_{z_h})$ and H_{xy} can be expressed as

$$f_e(z_e) = \begin{cases} \frac{1}{\sqrt{m_e}}A_e\cos k_e z_e, & |\,z_e\,| < L/2 \\ \frac{1}{\sqrt{M_e}}B_e\exp(-K_e\,|\,z_e\,|), & |\,z_e\,| > L/2 \end{cases} \quad (45)$$

where

$$k_e = \sqrt{\frac{2m_eE_e}{\hbar^2}}, \quad (46)$$

$$K_e = \sqrt{\frac{2M_e(V_e - E_e)}{\hbar^2}}, \tag{47}$$

$$K_e = k_e \tan\frac{k_e L}{2}, \tag{48}$$

and E_e is the ground state energy of electron in potential well of height V_e. M_e is interpolated effective mass of electron in the $Ga_{1-x}Al_xAs$ material and

$$\Phi_{00}(\rho,\phi) = \frac{1}{2\pi}\left(\frac{4\lambda}{a}\right) e^{\frac{-2\rho\lambda}{a}}, \tag{49}$$

$$E_0 = -4\lambda^2 R. \tag{50}$$

It was known that $Ga_{1-x}Al_xAs$ is direct for $x < 0.45$[46] the longitudinal effective masses in the GaAs region (denoted by m) and in the $GaAl_{1-x}As$ region (denoted by M) are

$$m_e = 0.067m_0, \tag{51}$$

$$m_+ = 0.45m_0, \tag{52}$$

$$m_- = 0.082m_0, \tag{53}$$

$$M_e = (0.067 + 0.083x)m_0, \tag{54}$$

$$M_+ = (0.45 + 0.2x)m_0, \tag{55}$$

$$M_- = (0.082 + 0.068x)m_0, \tag{56}$$

$$\varepsilon_0 = 12.5, \tag{57}$$

where m_0 is the free electron mass. Hence the wave function of the unperturbed part for the lowest subband exciton can be written as

$$\Psi(\rho,\phi,z) = f_e(z_e)\, f_h(z_h)\, \Phi_{00}(\rho,\phi) \tag{58}$$

and the first order perturbation to the ground state energy is

$$\Delta E_g^{(1)}(\lambda) = \int_{-\infty}^{\infty} dz_e\, |f_e(z_e)|^2 \int_{-\infty}^{\infty} dz_e\, |f_h(z_h)|^2 \int H'(\lambda)\, |\Phi_{00}(\rho,\phi)|^2 \rho\, d\rho\, d\phi$$

$$= \frac{16\lambda^2 e^2}{a^2\varepsilon_0^2} \int_{-\infty}^{\infty} dz_e\, |f_e(z_e)|^2 \int_{-\infty}^{\infty} dz_e\, |f_h(z_h)|^2 \left[\int_0^{\infty} \lambda\, e^{\frac{-4\lambda}{a}\rho}\, d\rho - \int_0^{\infty} \frac{\rho\, e^{\frac{-4\lambda}{a}\rho}}{\sqrt{\rho^2 + |z_e - z_h|^2}}\, d\rho\right] \tag{59}$$

$$= \frac{16\lambda^2 e^2}{a^2\varepsilon_0^2} \int_{-\infty}^{\infty} dz_e\, |f_e(z_e)|^2 \int_{-\infty}^{\infty} dz_e\, |f_h(z_h)|^2$$

$$\times \left\{\frac{a}{4} + |z_e - z_h| - \frac{\pi}{2}|z_e - z_h| \cdot \left[H_1\left(\frac{4\lambda\,|z_e - z_h|}{a}\right) - N_1\left(\frac{4\lambda\,|z_e - z_h|}{a}\right)\right]\right\}, \tag{60}$$

where $H_1(x)$ and $N_1(x)$ are the Struve and Neumann function of order 1.[47]

Based on the first order perturbation energy, the fast convergence condition requires $\Delta E_g^{(1)}(\lambda_0) = 0$, which yields the optimum value λ_0 for the variational parameter. Hence the binding energy of the ground state exciton without the polaron effect, which is defined as $-E_0$, is $4\lambda_0^2 R$.

III. RESULTS AND DISCUSSIONS

We have calculated the binding energy of the heavy hole (E_{BH}) and the light hole (E_{BL}) exciton of GaAs quantum wells for different Al concentrations $x = 0.15, 0.2, 0.25, 0.3, 0.4$ as a function of the well width L. The physical parameters are adopted from the previous works.[48,49] The reduced masses in the $x-y$ plane for the heavy-hole ($J = 3/2$) and the light-hole ($J = 1/2$) excitons are taken as $0.04m_0$ and $0.051m_0$, respectively. The reduced mass associated with $J = 3/2$ band is smaller than that of $J = 1/2$ band.

In Fig. 1 we display the variation of λ_0 as a function of the well width L for both heavy-hole exciton and light-hole exciton with $x = 0.15$. The range of widths considered is between 30 and 300 Å. One can see from Fig. 1 that for a given value of x, the value of λ_0 increases as L decreases. This result is similar to that obtained previously.[30] Furthermore, the value of λ_0 for the heavy-hole exciton is larger than that for light-hole exciton. The variation of binding energy with well width for $x = 0.15$ is displayed in Fig. 2. One can note that the binding energy decreases as the well width increases. This is because as L is reduced, the exciton wave function is

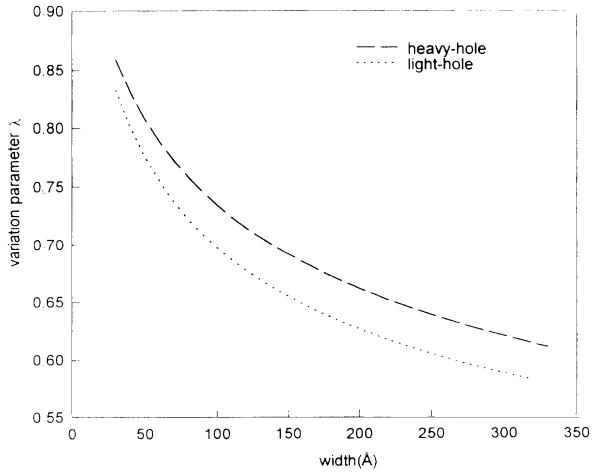

FIG. 1. The variation of λ_0 as a function of the well width L for both heavy-hole and light-hole excitons with concentration $x = 0.15$.

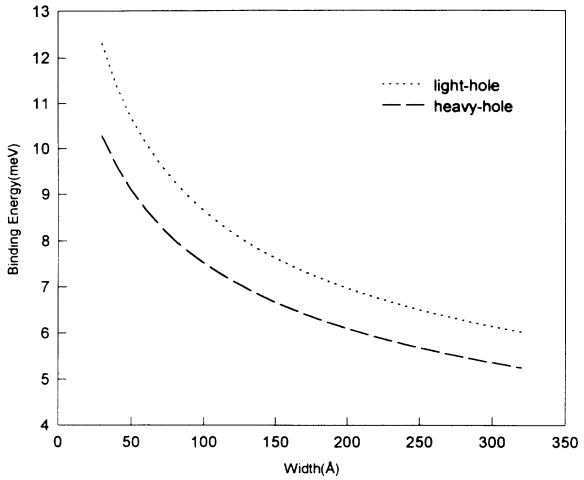

FIG. 2. The variation of heavy-hole and light-hole exciton binding energy (meV) as a function of the well L for concentration x=0.15.

compressed in the quantum well, thus leading to increase binding. When L is larger than a certain value of L, the spilling of the wave function becomes more important and this makes the binding energy get closer to the bulk value.[19] One can note from the figures that the binding energy of heavy-hole exciton is smaller than that of light-hole exciton. This is because the conduction-band nonparabolicity is enhanced by quantum confinement. According to the magneto-optics observation of Rogers *et al.*[15] the heavy-hole effective mass for motion in a layer plane is well thickness dependent and decreases considerably for decreasing well widths due to the decoupling of the light- and heavy-hole subbands, while the light hole exhibits electronlike dispersion relations with a large effective mass in the layer plane.[15] This makes the binding energy of heavy-hole exciton smaller than that of the light hole exciton. In Fig. 3 we plot the variations of binding energies with respect to the well width L for heavy- and light-hole excitons with $x = 0.15, 0.2, 0.25, 0.3$. We find that the binding energies decrease as L increases and the variation with L is almost independent of the concentration x.

The effects of the surface phonon and bulk phonon on the exciton binding energy for both heavy-hole and light-hole exciton in a quantum well for Al concentration $x = 0.15$ and 0.3 as a function of the well width L are presented in Figs. 4 and 5. One can see that the Al concentrations cannot significantly influence exciton binding energies. Table I presents our calculated exciton binding energies with and without the phonon effect for several well widths and concentration $x = 0.15$. We also list the percentage of the phonon effect in the last column of Table I. One can see from Table I that the polaron effect on the exciton binding energy is in general smaller for nar-

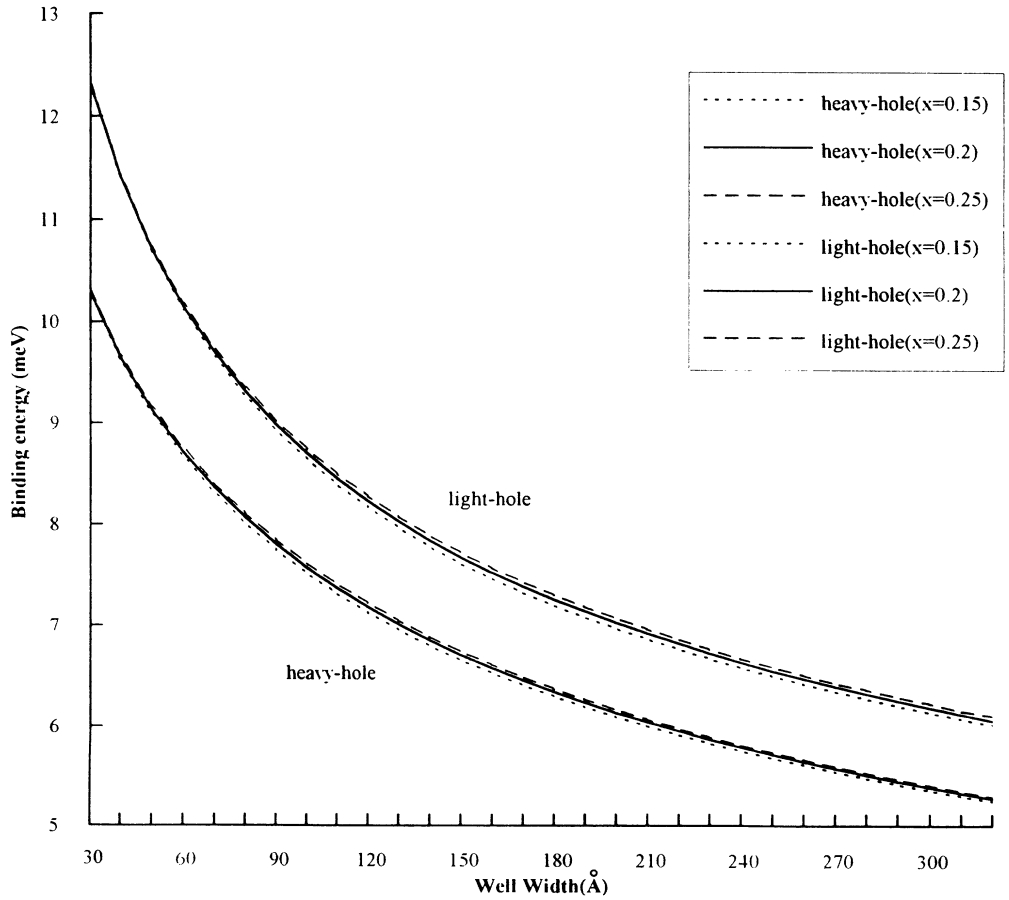

FIG. 3. The variation of heavy-hole and light-hole binding energies (meV) as a function of well width L for concentration x=0.15,0.2,0.25.

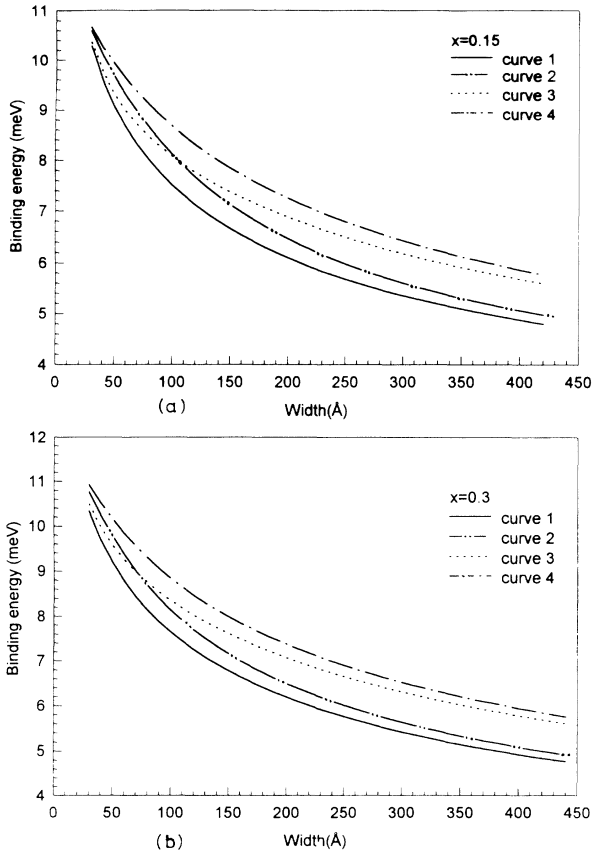

FIG. 4. The variation of heavy-hole exciton binding energy (meV) as a function of well width (Å) for E_0 (curve 1), E_0+SO (curve 2), E_0+BO (curve 3), and E_0+SO+BO (curve 4).

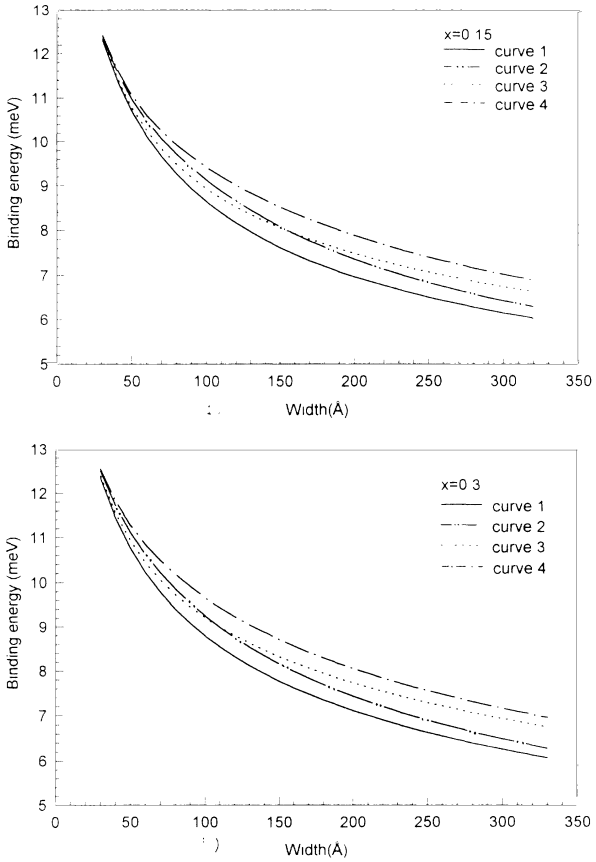

FIG. 5. The variation of light-hole exciton binding energy (meV) as a function of well width (Å) for E_0 (curve 1), E_0+SO (curve 2), E_0+BO (curve 3), E_0+SO+BO (curve 4).

row well width and becomes more pronounced as the well width becomes wider for either heavy-hole or light-hole exciton. Table II presents a comparison of our calculated results with recently observed data. In order to make a clear comparison, our results are calculated for some specific well widths and concentrations. One may note that the phonon effect on the heavy-hole exciton is larger than that on the light-hole exciton and the total binding energy of light-hole exciton is larger than that of heavy-hole exciton. This may be due to the effective mass difference as we mentioned above. One may also note from Table II that, although the observed data have some degree of uncertainty, our results agree satisfactorily with most recent observations,[8,15,25,50] except the experimental data of Maan *et al.*[14]

Figures 6 and 7 show the plot of the variation of percentage of effects of surface-phonon, bulk-phonon, and the total phonon effects on heavy-hole and light-hole exciton binding energies. Some interesting results can be noted in these two figures. The effect of the surface phonon decreases very fast for both cases of very large and very small well widths. For very large well width the reason for the decrease of the surface phonon effect on the total exciton binding energy is due to the large possibility of the exciton existing in the interior of the bulk semiconductor and thus reduce the interaction strength of the exciton and the surface phonon. On the contrary, the decrease of the surface phonon effect on the total exciton binding energy for very small well width is caused by the leakage of the exciton wave function out of the quantum well because the well potential height is finite. For the intermediate well width, the surface phonon effect on the total binding energy increases with well width for smaller well width, but after a maximum value the surface phonon effect decreases very fast for larger well width. This might be due to the smaller the well width, the more pronounced SO phonon modes, which in turn increases the importance of the exciton-surface phonon coupling. However, the wave function begins to leak out of the quantum well for well widths shrunk to a much smaller value so that the surface phonon effect reaches a maximum value for a well width of about 80 Å. It may be worthwhile to analyze here the competition between the surface phonon and the bulk phonon modes. One can see from the figures that the surface phonon effect grows larger than the bulk phonon effect when the width is reduced to a certain value. Therefore, the influence of the phonon effect on the exciton binding energy is dominated by the surface phonon as the well width becomes small while the polaron effect is dominated by the bulk phonon as the well width becomes large. This is because as the well width decreases, the exciton is close to the heterojunction and the confinement on the exciton becomes important which makes the interface phonon modes becomes more pronounced. This in turn makes the interaction between exciton and surface phonon stronger than

TABLE I. The binding energy (meV) of heavy hole and light hole exciton as a function of the well width (Å) with and without the phonon effect. E^* and E_0 are the binding energies with and without the phonon effect.

Width Å	Binding energy (meV) Exciton E_0	Exciton with phonon effect E^*	$(E^* - E_0)/E^*$ (%)
	Heavy-hole exciton $x = 0.15$		
30	10.28	10.66	3.63
40	9.61	10.25	6.27
50	9.09	9.92	8.44
60	8.66	9.63	10.07
70	8.31	9.36	11.28
80	8.01	9.12	12.19
90	7.74	8.89	12.90
100	7.51	8.68	13.45
150	6.67	7.85	15.12
200	6.10	7.26	15.94
250	5.68	6.80	16.41
290	5.42	6.50	16.64
300	5.35	6.43	16.68
	Light-hole exciton $x = 0.15$		
30	12.30	12.42	0.95
40	11.39	11.63	2.04
50	10.68	11.05	3.30
60	10.12	10.60	4.54
70	9.65	10.23	5.68
80	9.26	9.92	6.82
90	8.93	9.66	7.54
100	8.64	9.42	8.28
150	7.62	8.52	10.56
200	6.97	7.89	11.60
250	6.51	7.41	12.17
290	6.21	7.10	12.50
300	6.15	7.03	12.44

the interaction between exciton and bulk phonon. One can also note that the influence of the bulk phonon effect on the exciton binding energy increases with well width and thus the total phonon effect (including the surface and bulk phonon effects) increases with increasing well width. Our calculated percentage of phonon effects reach a saturation value of about 17.5% for heavy-hole exciton and 13.5% for light-hole exciton. One can see from Figs. 6 and 7 that the percentage of the effect of either surface phonon or bulk phonon on the heavy-hole exciton are always larger than that on the light-hole exciton. This is because the effective mass of the heavy hole

TABLE II. Comparison of our calculated results with some observed data.

Width (Å)	x	Hole level	Experimental data (meV)	Our results (meV)
75	0.4	H_1	10.5–11.5[a]	9.56
75	0.4	L_1	11.3–12.3[a]	10.45
75	0.35	H_1	10–12,[b] 9.3[c]	9.43
75	0.35	L_1	11,[b] 11[c]	10.31
92	0.35	H_1	9.5–10.5[a]	9.01
92	0.35	L_1	11.2–12.2[a]	9.80
100	0.35	H_1	13[d]	8.87
100	0.35	L_1	10[d]	9.63
110	0.35	H_1	8-9.5,[b] 8.4[c]	8.69
110	0.35	L_1	9,[b] 11[c]	9.42
112	0.3	H_1	12[e]	8.56
112	0.3	H_1		9.31

[a]Reference 8.
[b]Reference 15.
[c]Reference 25.
[d]Reference 14.
[e]Reference 50.

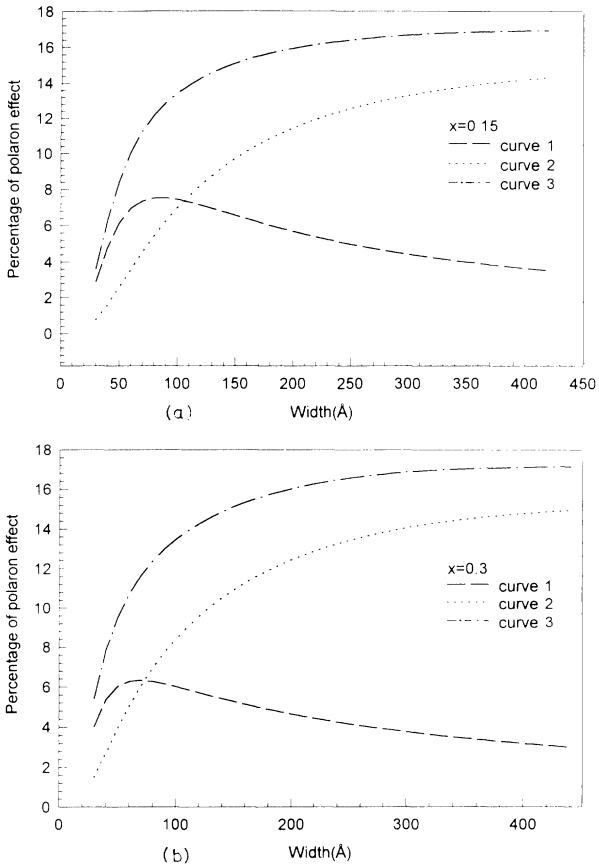

FIG. 6. The variation of percentage of phonon effect on the heavy-hole exciton as a function of well width (Å) for SO (curve 1), BO (curve 2), and SO+BO (curve 3).

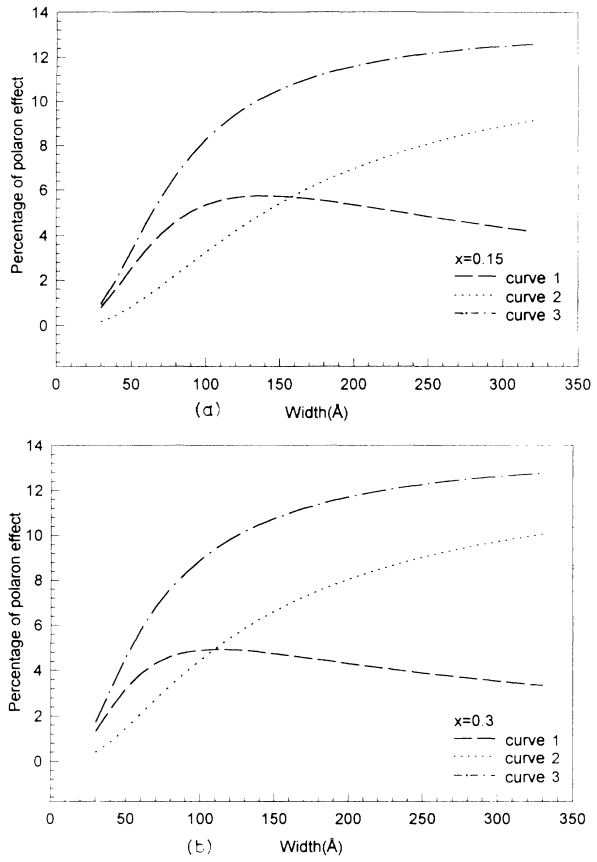

FIG. 7. The variation of percentage of phonon effect on the light-hole exciton as a function of well width (Å) for SO (curve 1), BO (curve 2), and SO+BO (curve 3).

along the z direction is heavier than that of the light hole; therefore the heavy hole is bound more tightly than light hole and yields a smaller interaction range. Therefore, a larger effect will be over a short distance for the surface phonon effect. The same reason can be applied to the bulk phonon case, so that the effect of BO phonon on the heavy-hole exciton is also larger than that on the light-hole exciton. Ercelebi and Özdincer[33] considered the electron (hole) lattice interaction and introduced a variational trial wave function in their calculation. They obtained an enhancement on the binding energy which increases as the well width becomes larger and larger. However, their results yield more than 30% phonon effect as the well width becomes larger than 150 Å. Their results seem to overestimate the phonon effect. Degani and Hipólito[34] studied the phonon effect on the binding energy of exciton and obtained a result of 26–20 % effect of phonons as the well width ranges from 10 to 150 Å. Comparing with the recent observations as listed in Table II, our calculated results seem to be more reliable.

IV. SUMMARY

In this work we studied the longitudinal optical surface and bulk phonon effects on the exciton binding energy. The results show that polaronic effects are important and cannot be neglected. Our results predict that the correction due to the polaron effect on the exciton binding energy ranges from several percent in the small well width to $\sim$ 17% in the bulk case. It has also been found that the energy correction due to the polaron effect is dominated by the SO phonon when the well width is sufficiently small while the electron and bulk phonon interaction becomes important when the well width becomes larger. The effects of either electon-surface-phonon interaction or electron-bulk-phonon on the binding energy are larger for the heavy-hole exciton. This may be ascribed to the effective mass difference for the heavy hole and the light hole. We also found that the total binding energy of the light-hole exciton is larger than that of heavy-hole exciton. This is consistent with recent observations and other theoretical calculations.

ACKNOWLEDGMENT

This work is partially supported by the National Science Council of the Republic of China.

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