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The influence of different phonon modes on the exciton energy in a quantum well

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Abstract. The ground-state energies of both heavy-hole and light-hole excitons in a GaAs/$Ga_{1-x}Al_xAs$ quantum well have been studied by taking into account the interaction of different optical phonon modes with the excitons. The exciton energies and the corrections to the effective masses are obtained as functions of the well width and the Al concentration. Numerical calculation shows the strong influences of different phonon modes on the exciton behaviour in a quantum well as well as their dependence on the well width and height.

1. Introduction

In recent years, the properties of a Wannier exciton in a quantum well (QW) have raised a great deal of interest [1–7]. This is because the quantum effect in such a localized semiconductor structure makes the properties of excitons different from those in a three-dimensional structure.

Many studies have been done on the properties of the electron–phonon system, i.e. the polaron, in a QW. However, when the exciton properties in a QW are considered, relatively fewer workers have taken the phonon affect into consideration. Of these, Gu and Shen [4] investigated the influence of the LO phonon and the SO phonon on the exciton ground-state energy in a polar crystal slab under the infinite-well-height model. Matsuura [5] took only the interaction of the LO phonon and exciton into consideration. However, the optical phonons in a quasi-two-dimensional system are also influenced by the presence of interfaces [9]. For a QW structure, it is essential to consider the finite-well model. Recently, Mori and Ando [8] established the optical-phonon modes in a single or double heterostructure and the theory of their interaction with electrons.

In this paper we shall investigate the influence of various phonon modes on the exciton ground-state property in a finite-height QW. The result shows a strong dependence of such an influence on the well width and height.

2. Theory

The Hamiltonian of a Wannier exciton–phonon system in a GaAs layer sandwiched between two semi-infinite layers of $Ga_{1-x}Al_xAs$ (figure 1) can be expressed under the effective-mass

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approximation as

$$H = H_{ez} + H_{hz} + (P_x^2 + P_y^2)/2M + (p_x^2 + p_y^2)/2\mu - e^2/\varepsilon_\infty\sqrt{\rho^2 + (z_e - z_h)^2} + H_{ph} + H_{int}. \tag{2.1}$$

The first two terms are the Hamiltonians of electrons and holes on the z axis, which is the growth axis of the QW:

$$H_{iz} = -(\hbar^2/2m_{iz})(d^2/dz_i^2) + V_i(z_i) \tag{2.2}$$

where $i \equiv e, h$. For a finite well, $V_i(z_i) = 0$ when $|z_i| < \frac{1}{2}W$ and $V_i(z_i) = V_{i0}$ when $|z_i| \geqslant \frac{1}{2}W$.

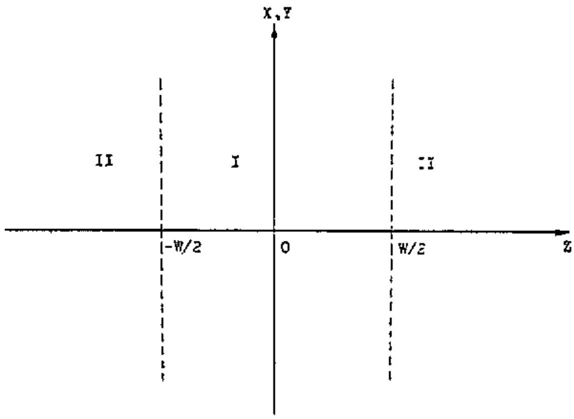

Figure 1. Geometry of a $GaAs/Ga_{1-x}Al_xAs$ QW: I, GaAs; II, $Ga_{1-x}Al_xAs$.

The third and fourth terms in (2.1) are the kinetic energies of the exciton centre of mass and relative motion perpendicular to the z direction. (P_x, P_y) and (p_x, p_y) are the in-x–y plane projections of the exciton centre-of-mass momentum and relative motion momentum, respectively. $M = m_e + m_h$ and $\mu = m_e m_h/(m_e + m_h)$ are the total and reduced effective masses, respectively, of the exciton related to the motion in the x–y plane. The fifth term is the Coulomb potential between electrons and holes. H_{ph} is the phonon Hamiltonian and H_{int} is the interaction Hamiltonian of excitons and phonons of various modes.

In our work (see figure 1), the phonon modes are modified because the materials no longer extend over all space in the z direction. Now there are four types of optical phonon mode which interact with the excitons:

(i) symmetric interface optical phonon modes S± with frequency $\omega_{S\pm}(Q)$;
(ii) antisymmetric interface optical phonon modes A± with frequency $\omega_{A\pm}(Q)$;
(iii) confined-slab LO-phonon modes SL in the well with frequency ω_{L_1};
(iv) half-space LO-phonon modes HS in the barrier layers with frequency ω_{L_2}.

So, we have

$$H_{ph} = \sum_{\sigma,Q} \hbar\omega_\sigma a_\sigma^+(Q) a_\sigma(Q) \tag{2.3}$$

$$H_{int} = \sum_{\sigma,Q} \{\exp(iQ \cdot R)[\Gamma_\sigma(Q, z_e)\exp(i\beta_h Q \cdot \rho) - \Gamma_\sigma(Q, z_h)\exp(-i\beta_e Q \cdot \rho)]a_\sigma^+(Q) + \mathrm{HC}\} \tag{2.4}$$

where σ denotes the phonon mode: $\sigma = \mathrm{SL, HS, S\pm, A\pm}$. $q = (Q, q_z)$; $\beta_e = m_e/M$; $\beta_h = m_h/M$.

The dispersion relation for the interface phonon is given by [11]

$$\omega_{l\pm}(Q) = [\![[1/2(\varepsilon_1^l + \varepsilon_2^l)](\varepsilon_1^l(\omega_{L_1}^2 + \omega_{T_2}^2) + \varepsilon_2^l(\omega_{L_2}^2 + \omega_{T_1}^2) \pm \{[\varepsilon_1^l(\omega_{L_1}^2 + \omega_{T_2}^2) + \varepsilon_2^l(\omega_{L_2}^2 + \omega_{T_1}^2)]^2 - 4(\varepsilon_1^l + \varepsilon_2^l)(\varepsilon_1^l \omega_{L_1}^2 \omega_{T_2}^2 + \varepsilon_2^l \omega_{L_2}^2 \omega_{T_1}^2)\}^{1/2})]\!]^{1/2} \tag{2.5}$$

where $\varepsilon_1^l = \varepsilon_{\infty 1}[1 - \gamma_l \exp(-QW)]$, $\varepsilon_2^l = \varepsilon_{\infty 2}[1 + \gamma_l \exp(-QW)]$, $\varepsilon_{\infty\nu}$ $(\nu = 1, 2)$ is the light frequency dielectric constant of material, and ω_{L_ν} and ω_{T_ν} are the frequencies of longitudinal optical vibration and transverse optical vibration, respectively. $l \equiv$ S and A refers to the symmetric and antisymmetric modes, respectively. $\gamma_S = 1$ and $\gamma_A = -1$. Also

$$\Gamma_{l,\pm}(Q, z) = -[2\pi e^2\hbar / A\omega_{l,\pm}(Q)]^{1/2}(C_{l,\pm}/Q) \begin{cases} \exp[-Q(z - \frac{1}{2}W)] & z > \frac{1}{2}W \\ f_l(Q, z) & |z| < \frac{1}{2}W \\ \gamma_l \exp[Q(z + \frac{1}{2}W)] & z < -\frac{1}{2}W \end{cases} \tag{2.6}$$

where A is the interface area and

$$C_{l,\pm} = \{\tfrac{1}{2}Q[1 + \gamma_l \exp(-QW)]\}^{1/2} [\![[\omega_{T_1}^2 - \omega_{l,\pm}^2(Q)]^2 [\omega_{T_2}^2 - \omega_{l,\pm}^2(Q)]^2 / \{\varepsilon_1^l(\omega_{L_1}^2 - \omega_{T_1}^2) \times [\omega_{T_2}^2 - \omega_{l,\pm}^2(Q)]^2 + \varepsilon_2^l(\omega_{L_2}^2 - \omega_{T_2}^2)[\omega_{T_1}^2 - \omega_{l,\pm}^2(Q)]^2\}]\!]^{1/2} \tag{2.7}$$

and

$$f_S(Q, z) = \cosh(Qz)/\cosh(\tfrac{1}{2}QW) \tag{2.8}$$

$$f_A(Q, z) = \sinh(Qz)/\sinh(\tfrac{1}{2}QW). \tag{2.9}$$

The coupling function of a single exciton with a confined-slab LO-phonon mode with frequency ω_{L_1} is given by

$$\Gamma_{L_1}^j(Q, z) = -[(4\pi\hbar^2\omega_{L_1}\alpha_1/AW)(2\hbar\omega_{L_1}/M_1)^{1/2}]^{1/2}\{\sin[q_1^j(z + \tfrac{1}{2}W)]\}/[Q^2 + (q_1^j)^2]^{1/2} \tag{2.10}$$

for $|z| < \frac{1}{2}W$ and is zero otherwise. The wavevector of the confined-slab LO phonon is $q = (Q, q_l^j)$, where $q_l^j = j\pi/W$, $j = 1, 2, \ldots$.

The coupling function of a single exciton with the half-space LO-phonon modes in the barrier material with frequency ω_{L_2} is given by

$$\Gamma_{L_2}(Q, q_z, z) = -\left[\frac{4\pi\hbar^2\omega_{L_2}\alpha_2}{V_G}(2\hbar\omega_{L_2}/M_2)^{1/2}\right]^{1/2} \times \begin{cases} \{\sin[q_z(z - \frac{1}{2}W)]\}/(Q^2 + q_z^2)^{1/2} & z > \frac{1}{2}W \\ 0 & |z| < \frac{1}{2}W \\ \{\sin[q_z(z + \frac{1}{2}W)]\}/(Q^2 + q_z^2)^{1/2} & z < -\frac{1}{2}W \end{cases} \tag{2.11}$$

where V_G is the volume of material II.

As is well known, the coupling constant characterizing the electron– or hole–LO-phonon potential strength is quite small for GaAs ($\alpha_1 \ll 1$) and $Ga_{1-x}Al_xAs$ ($\alpha_2 \ll 1$). The variational formalism proposed by Lee, Low and Pines (LLP) [12] to investigate the weak-coupling electron–phonon system will be employed in our present investigation [5, 13].

Since the total momentum

$$\hbar K = P + \sum_{\sigma,Q} \hbar Q a_\sigma^+(Q) a_\sigma(Q)$$

in the x–y plane commutes with the Hamiltonian of the system, therefore $\hbar K$ is the constant of motion. We perform a unitary transformation with the operator

$$S = \exp\left[\mathrm{i}\left(K - \sum_{\sigma,Q} Q a_\sigma^+(Q) a_\sigma(Q)\right) \cdot R\right]$$

in order to eliminate R, the coordinate of the exciton centre of mass in the x–y plane. We obtain a transformed Hamiltonian $\tilde{H} = S^{-1} H S$. Then we perform another unitary transformation with the operator

$$U = \exp\left(\sum_{\sigma,q} a_\sigma^+(Q) f_\sigma(Q,\rho) - a_\sigma(Q) f_\sigma^*(Q,\rho)\right) \tag{2.12}$$

where $f_\sigma(Q,\rho)$ and $f_\sigma^*(Q,\rho)$ are to be determined variationally.

After some direct algebraic calculation, we obtain the following transformed Hamiltonian (neglecting the interaction related to the emitting or absorbing of two or more virtual phonons):

$$\mathcal{H} = U^{-1} \tilde{H} U = \mathcal{H}_0 + \mathcal{H}_1 \tag{2.13}$$

$$\mathcal{H}_0 = H_{ez} + H_{hz} + \frac{\hbar^2 K^2}{2M} - \frac{e^2}{\varepsilon_\infty \sqrt{\rho^2 + (z_e - z_h)^2}} - \frac{\hbar^2}{2\mu} \nabla_\rho^2 + \frac{\hbar^2}{2M} \sum_{\sigma,Q} (Q^2 + u_\sigma^2) a_\sigma^+(Q) a_\sigma(Q)$$
$$- \frac{2M}{\hbar^2} \sum_{\sigma,Q} \frac{|V_\sigma(Q)|^2}{Q^2 + u_\sigma^2} + \frac{\hbar^2}{2M} \sum_{\sigma,Q} \frac{Q^2}{Q^2 + u_\sigma^2} |A_\sigma(Q)|^2 \tag{2.14}$$

$$\mathcal{H}_1 = \frac{\hbar^2}{2\mu} \sum_{\sigma,Q} \frac{\mathrm{i} Q \cdot \nabla_\rho}{Q^2 + u_\sigma^2} [a_\sigma^+(Q) A_\sigma^*(Q) + a_\sigma(Q) A_\sigma(Q)] - \frac{\hbar K}{M}$$
$$\times \sum_{\sigma,Q} \hbar Q [a_\sigma^+(Q) a_\sigma(Q) + f_\sigma(Q,\rho) a_\sigma^+(Q) + f_\sigma^*(Q,\rho) a_\sigma(Q) + |f_\sigma(Q,\rho)|^2] \tag{2.15}$$

where

$$f_\sigma(Q,\rho) = -(2M/\hbar^2)[V_\sigma^*(Q,\rho)/(Q^2 + u_\sigma^2)] \tag{2.16}$$

$$\hbar^2 u_\sigma^2 / 2M = \hbar \omega_\sigma \tag{2.17}$$

$$V_\sigma(Q,\rho) = \Gamma_\sigma(Q, z_e) \exp(\mathrm{i}\beta_h Q \cdot \rho) - \Gamma_\sigma(Q, z_h) \exp(-\mathrm{i}\beta_e Q \cdot \rho) \tag{2.18}$$

$$A_\sigma(Q) = (2M/\hbar^2)[\Gamma_\sigma(Q, z_e) \beta_h \exp(\mathrm{i}\beta_h Q \cdot \rho) + \Gamma_\sigma(Q, z_h) \beta_e \exp(-\mathrm{i}\beta_e Q \cdot \rho)]. \tag{2.19}$$

For the weak-coupling case, $\mathcal{H}_0$ in equation (2.13) can be considered as the unperturbed Hamiltonian and $\mathcal{H}_1$ as the perturbing Hamiltonian.

The wavefunction of unperturbed exciton–phonon system can be written as

$$\Psi = \psi(r)|0\rangle \tag{2.20}$$

where $\psi(r)$ is the normalized exciton wavefunction and $|0\rangle$ represents the normalized vacuum state (the state of no phonon); it satisfies

$$a_\sigma(Q)|0\rangle = 0.$$

For the low-temperature limit ($T \to 0$ K), the unperturbed effective Hamiltonian of the system will be

$$H^0_{\rm eff} = \langle 0|\mathcal{H}_0|0\rangle = H_{\rm ez} + H_{\rm hz} + \frac{\hbar^2 K^2}{2M} - \frac{e^2}{\varepsilon_\infty\sqrt{\rho^2 + (z_{\rm e} - z_{\rm h})^2}} - \frac{\hbar^2}{2\mu}\nabla^2_\rho + \frac{\hbar^2}{2\mu}\sum_{\sigma,Q}\frac{Q^2}{Q^2+u^2_\sigma}|A_\sigma(Q)|^2 - \frac{2M}{\hbar^2}\sum_{\sigma,Q}\frac{|V_\sigma(Q,\rho)|^2}{Q^2+u^2_\sigma}. \tag{2.21}$$

The perturbation effective Hamiltonian of the second order is

$$H'_{\rm eff} = -\sum_{\sigma,q}\frac{|\langle 1_{\sigma,q}|\mathcal{H}_1|0\rangle|^2}{E_{\sigma,q} - E_0} = \frac{8M}{\hbar^2}\sum_{\sigma,q}\frac{(K\cdot Q)^2}{(u^2_\sigma + Q^2)^3}|V_\sigma(Q,\rho)|^2 + \frac{\hbar^2 M}{2\mu^2}\sum_{\sigma,q}\frac{(Q\cdot\nabla_\rho)^2}{(u^2_\sigma + Q^2)^3}|A_\sigma(Q)|^2. \tag{2.22}$$

The effective Hamiltonian of the exciton–optical-phonon system is

$$H_{\rm eff} = H^0_{\rm eff} + H'_{\rm eff}. \tag{2.23}$$

Consider the finite-barrier QW model of the GaAs/$Ga_{1-x}Al_xAs$ material. The confining potentials are $V_{\rm e0} = 0.6(1.155x + 0.37x^2)$ eV for electrons and $V_{\rm h0} = 0.4(1.55x + 0.37x^2)$ eV for holes. The wavefunction in the z direction for an electron (hole) in the lowest subband is given by

$$\psi_1(z) = \begin{cases} B_0\cos(kz) & |z| \leqslant \frac{1}{2}W \\ B_0\cos(\frac{1}{2}kW)\exp[-k_1(|z| - \frac{1}{2}W)] & |z| > \frac{1}{2}W \end{cases} \tag{2.24}$$

where $k = \sqrt{2m_1E_1}/\hbar$, $k_1 = \sqrt{2m_1(V_0 - E_1)}/\hbar$; E_1 is determined by the following equation:

$$\tan(\tfrac{1}{2}W\sqrt{2m_1E_1}/\hbar) = [m_1(V_0 - E_1)/m_2E_1]^{1/2}. \tag{2.25}$$

The normalized constant B_0 is given by

$$B_0 = [\![2k/\{kW + \sin(kW) + [2k\cos^2(\tfrac{1}{2}kW)]/k_1\}]\!]^{1/2}. \tag{2.26}$$

The exciton wavefunction is

$$\psi(r) = \psi_{1e}(z_e)\psi_{1h}(z_h)\varphi_{1s}(\rho, \gamma) \tag{2.27}$$

where $\varphi_{1s}(\rho, \gamma)$ is the normalized wavefunction of the ground state of a two-dimensional hydrogen-like atom given by

$$\varphi_{1s}(\rho, \gamma) = \sqrt{2/\pi}\gamma \exp(-\gamma\rho) \tag{2.28}$$

where γ is the variational parameter.

The energy of an exciton is given by

$$E_{1s}(1e, 1h) = \min_{\gamma}\langle\psi(r)|H_{\rm eff}|\psi(r)\rangle \tag{2.29}$$

$$\begin{aligned}\langle\psi(r)|H_{\rm eff}|\psi(r)\rangle &= \langle\psi(r)|H_{\rm eff}^0 + H_{\rm eff}'|\psi(r)\rangle = E_{1e} + E_{1h} + \frac{\hbar^2K^2}{2M^*} + \frac{\hbar^2\gamma^2}{2\mu^*} - \frac{4e^2\gamma^2}{\varepsilon_\infty} \\ &\quad\times\int\int \psi_{1e}^2(z_e)\psi_{1h}^2(z_h)|z_e - z_h|\{\tfrac{1}{2}\pi[H_1(2\gamma|z_e - z_h|) \\ &\quad - N_1(2\gamma|z_e - z_h|)] - 1\}\,dz_e\,dz_h + \Delta E\end{aligned} \tag{2.30}$$

where $H_1(x)$ is the first-order Struve function, $N_1(x)$ is the Neumann function (the second-type Bessel function) of the first order,

$$\Delta E = \sum \Delta E_\sigma = \Delta E_{S+} + \Delta E_{S-} + \Delta E_{A+} + \Delta E_{A-} + \Delta E_{SL} + \Delta E_{HS} \tag{2.31}$$

is the exciton ground-state energy shift due to the interaction between excitons and various optical phonon modes, and

$$M^* = M\Big/\left(1 - \sum C_\sigma^M\right) \tag{2.32}$$

$$\mu^* = \mu\Big/\left(1 - \sum C_\sigma^\mu\right) \tag{2.33}$$

are the renormalized total and reduced effective masses of the exciton.

$$\begin{aligned}\Delta E_{l\pm} = \frac{2Me^2}{\hbar}\int_0^\infty \frac{C_{l\pm}^2}{Q(Q^2 + u_{l\pm}^2)}\left[\left(\frac{\beta_e}{\beta_h}\frac{Q^2}{Q^2 + u_{l\pm}^2} - 1\right)G_{l\pm,e}^2 + \left(\frac{\beta_h}{\beta_e}\frac{Q^2}{Q^2 + u_{l\pm}^2} - 1\right)\right. \\ \left.\times\, G_{l\pm,h}^2 + \frac{16\gamma^3}{(Q^2 + 4\gamma^2)^{3/2}}\left(\frac{Q^2}{Q^2 + u_{l\pm}^2} + 1\right)G_{l\pm,e}G_{l\pm,h}\right]\frac{dQ}{\omega_{l\pm}(Q)}\end{aligned} \tag{2.34}$$

where $l = S, A$

$$\begin{aligned}G_{S\pm}^2 = \{B_0^2/[4\cosh^2(\tfrac{1}{2}QW)]\}\{W + [\sin(kW)]/k + [\sin(QW)]/Q + [1/(k^2 + Q^2)] \\ \times[k\cosh(QW)\sin(kW) + Q\sinh(QW)\cos(kW)]\} + [B_0^2\cos^2(\tfrac{1}{2}kW)]/(Q + k_1)\end{aligned} \tag{2.35}$$

$$G_{S\pm} = \{B_0^2/[2\cosh(\tfrac{1}{2}QW)]\}\{[2\sinh(\tfrac{1}{2}QW)]/Q + [2/(4k^2+Q^2)][2k\cosh(\tfrac{1}{2}QW)\sin(kW) + Q\sinh(\tfrac{1}{2}QW)\cos(kW)]\} + [2B_0^2\cos^2(\tfrac{1}{2}kW)]/(2k_1+Q) \tag{2.36}$$

$$G_{A\pm}^2 = \{B_0^2/[4\sinh^2(\tfrac{1}{2}QW)]\}\{-[\sin(kW)]/k + [\sinh(QW)]/Q - W + [\tfrac{1}{2}/(k^2+Q^2)] \times [k\cosh(QW)\sin(kW) + Q\sinh(QW)\cos(kW)]\} + [B_0^2\cos^2(\tfrac{1}{2}kW)]/(k_1+Q) \tag{2.37}$$

$$G_{A\pm} = 0 \tag{2.38}$$

$$\Delta E_{SL} = \frac{4M\omega_{L_1}\alpha_1}{W}\left(\frac{2\hbar\omega_{L_1}}{M_1}\right)^{1/2}\sum_j\int_0^\infty \frac{Q}{Q^2+u_{SL}^2}\left[\left(\frac{\beta_e}{\beta_h}\frac{Q^2}{Q^2+u_{SL}^2}-1\right)G_{j,e}^2 + \left(\frac{\beta_h}{\beta_e}\frac{Q^2}{Q^2+u_{SL}^2}-1\right)G_{j,h}^2 + \frac{16\gamma^3}{(Q^2+4\gamma^2)^{3/2}}\left(\frac{Q^2}{Q^2+u_{SL}^2}\right)G_{j,e}G_{j,h}\right]dQ \tag{2.39}$$

$$G_j^2 = \{B_0^2/4[Q^2+(q_1^j)^2]\}[\![W + [\sin(kW)]/k - [\sin(2q_1^jW)]/2q_1^j + \{q_1^j/2[k^2-(q_1^j)^2]\} \times \cos(kW)\sin(2q_1^jW) - \{k/2[k^2-(q_1^j)^2]\}\sin(kW)[\cos(2q_1^jW)+1]]\!] \tag{2.40}$$

$$G_j = [B_0^2/2\sqrt{Q^2+(q_1^j)^2}][\![[1-\cos(q_1^jW)]/q_1^j + \{2k/[4k^2-(q_1^j)^2]\}\sin(kW)\sin(q_1^jW) + \{q_1^j/[4k^2-(q_1^j)^2]\}\cos(kW)[\cos(q_1^jW)-1]]\!] \tag{2.41}$$

$$\Delta E_{HS} = 2M\omega_{L_2}\alpha_2\left(\frac{2\hbar\omega_{L_2}}{M_2}\right)^{1/2}\int_0^\infty \frac{Q\,dQ}{Q^2+u_{HS}^2}\left[\left(\frac{\beta_e}{\beta_h}\frac{Q^2}{Q^2+u_{HS}^2}-1\right)G_{HS,e}^2 + \left(\frac{\beta_h}{\beta_e}\frac{Q^2}{Q^2+u_{HS}^2}-1\right)G_{HS,h}^2\right] \tag{2.42}$$

$$G_{HS}^2 = \tfrac{1}{2}B_0^2\cos^2(\tfrac{1}{2}kW)[1/k_1(k_1+Q)]. \tag{2.43}$$

Also

$$C_{l\pm}^M = \frac{8M^2e^2}{\hbar^3}\int_0^\infty \frac{Q\,dQ}{(u_l^2+Q^2)^3}\frac{C_{l\pm}^2}{\omega_{l\pm}(Q)} \times \left(G_{l\pm,e}^2 + G_{l\pm,h}^2 - 2G_{l\pm,e}G_{l\pm,h}\frac{8\gamma^3}{(Q^2+4\gamma^2)^{3/2}}\right) \tag{2.44}$$

$$C_{l\pm}^\mu = \frac{2M^2e^2}{\hbar^3}\int_0^\infty \frac{Q\,dQ}{(u_l^2+Q^2)^3}\frac{C_{l\pm}^2}{\omega_{l\pm}(Q)} \times \left(\frac{\beta_e}{\beta_h}G_{l\pm,e}^2 + \frac{\beta_h}{\beta_e}G_{l\pm,h}^2 + 2G_{l\pm,e}G_{l\pm,h}\frac{8\gamma^3}{(Q^2+4\gamma^2)^{3/2}}\right) \tag{2.45}$$

$$C_{\rm SL}^{M} = \frac{16M^2\omega_{\rm L_1}\alpha_1}{\hbar^2}\left(\frac{2\hbar\omega_{\rm L_1}}{M_1}\right)^{1/2}\int_0^\infty \frac{Q^3\,{\rm d}Q}{(u_{\rm SL}^2+Q^2)^3} \times\left(G_{\rm SL,e}^2+G_{\rm SL,h}^2-2G_{\rm SL,e}G_{\rm SL,h}\frac{8\gamma^3}{(Q^2+4\gamma^2)^{3/2}}\right) \tag{2.46}$$

$$C_{\rm SL}^{\mu} = \frac{4M^2\omega_{\rm L_1}\alpha_1}{\hbar^2}\left(\frac{2\hbar\omega_{\rm L_1}}{M_1}\right)^{1/2}\int_0^\infty \frac{Q^3\,{\rm d}Q}{(u_{\rm SL}^2+Q^2)^3} \times\left(\frac{\beta_{\rm e}}{\beta_{\rm h}}G_{\rm SL,e}^2+\frac{\beta_{\rm h}}{\beta_{\rm e}}G_{\rm SL,h}^2+2G_{\rm SL,e}G_{\rm SL,h}\frac{8\gamma^3}{(Q^2+4\gamma^2)^{3/2}}\right) \tag{2.47}$$

$$C_{\rm HS}^{M} = \frac{16M^2\omega_{\rm L_2}\alpha_2}{\hbar^2}\left(\frac{2\hbar\omega_{\rm L_2}}{M_2}\right)^{1/2}\int_0^\infty \frac{Q^3\,{\rm d}Q}{(u_{\rm HS}^2+Q^2)^3} \times\left(G_{\rm HS,e}^2+G_{\rm HS,h}^2-2G_{\rm HS,e}G_{\rm HS,h}\frac{8\gamma^3}{(Q^2+4\gamma^2)^{3/2}}\right) \tag{2.48}$$

$$G_{\rm HS}^{\mu} = \frac{4M^2\omega_{\rm L_2}\alpha_2}{\hbar^2}\left(\frac{2\hbar\omega_{\rm L_2}}{M_2}\right)^{1/2}\int_0^\infty \frac{Q^3\,{\rm d}Q}{(u_{\rm HS}^2+Q^2)^3} \times\left(\frac{\beta_{\rm e}}{\beta_{\rm h}}G_{\rm HS,e}^2+\frac{\beta_{\rm h}}{\beta_{\rm e}}G_{\rm HS,h}^2+2G_{\rm HS,e}G_{\rm HS,h}\frac{8\gamma^3}{(Q^2+4\gamma^2)^{3/2}}\right). \tag{2.49}$$

3. Results and discussion

We have now obtained the expression for the expectation value of the effective Hamiltonian of the exciton–phonon system for the ground state. A numerical calculation will be carried out for a GaAs/$Ga_{1-x}Al_xAs$ QW. We are going to calculate the ground-state energies of the heavy-hole exciton and the light-hole exciton in this material. The material parameters chosen are listed in table 1.

Table 1. Material parameters of GaAs and $Ga_{1-x}Al_xAs$ [9, 10].

	Value for the following materials		
	GaAs ($\nu = 1$)	$Ga_xAl_{1-x}As$ ($\nu = 2$)	AlAs
$m_{\nu,e}$ (units of m_0)	0.067	$0.067 + 0.083x$	0.15
$m_{\nu,hz}$ (units of m_0)	0.45	$0.45 + 0.31x$	0.76
$m_{\nu,lz}$ (units of m_0)	0.088	$0.088 + 0.049x$	0.137
$\hbar\omega_{L_\nu}$ (meV)	36.25	$36.25 + 3.83x + 17.12x^2 - 5.11x^3$	50.09
$\hbar\omega_{T_\nu}$ (meV)	33.29	$33.29 + 10.70x + 0.03x^2 + 0.86x^3$	44.88
$\varepsilon_{0\nu}$	13.18	$13.18 - 3.12x$	10.06
$\varepsilon_{\infty\nu}$	10.89	$10.89 - 2.73x$	8.16

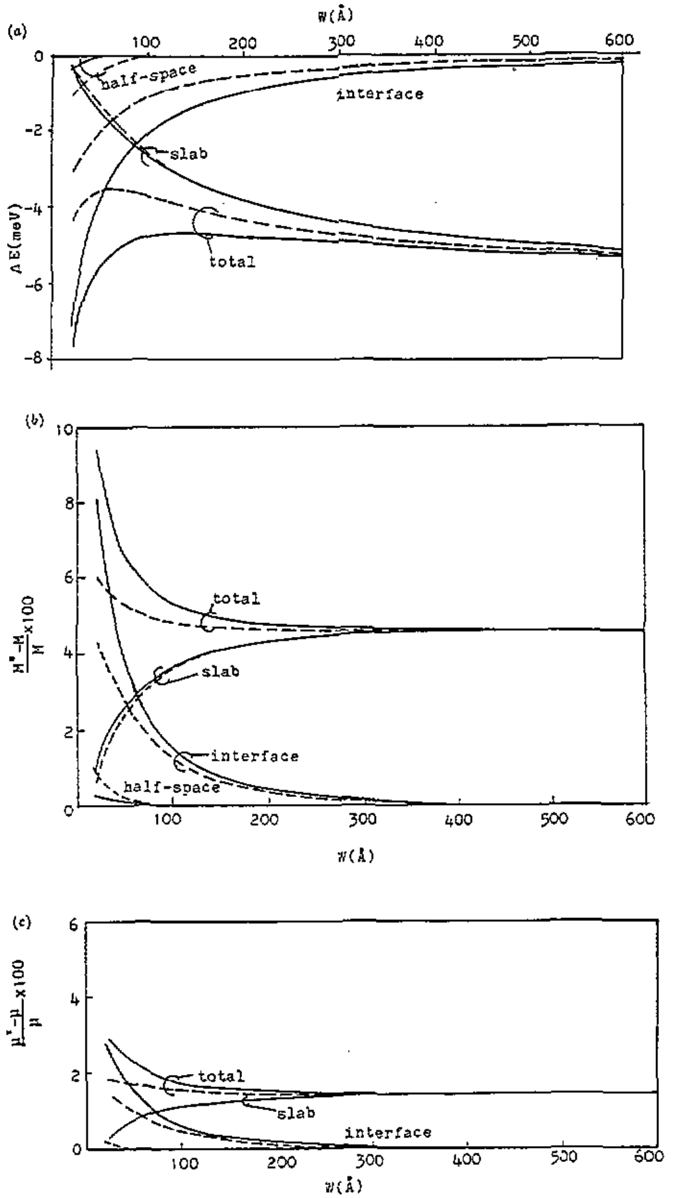

Figure 2. (*a*) The energy shift; (*b*) the correction to the total effective mass; (*c*) the correction to the reduced effective mass of the heavy-hole exciton in a QW with different Al concentrations (——, $x = 1$; - - -, $x = 0.3$).

The heavy-hole effective mass for motion in the x–y plane is [10] $m_{hxy} = (\frac{1}{4}m_{hz} + \frac{3}{4}m_{lz})^{-1}\, m_0$; the light-hole effective mass for motion in the x–y plane is $m_{lxy} = (\frac{1}{4}m_{lz} + \frac{3}{4}m_{hz})^{-1}\, m_0$. m_0 is the free-electron mass.

We have computed the ground-state energy of heavy-hole and light-hole excitons in a GaAs/$Ga_{1-x}Al_xAs$ QW for different Al concentrations x and different well widths. The contributions of different phonon modes to the exciton energy and the correction to the

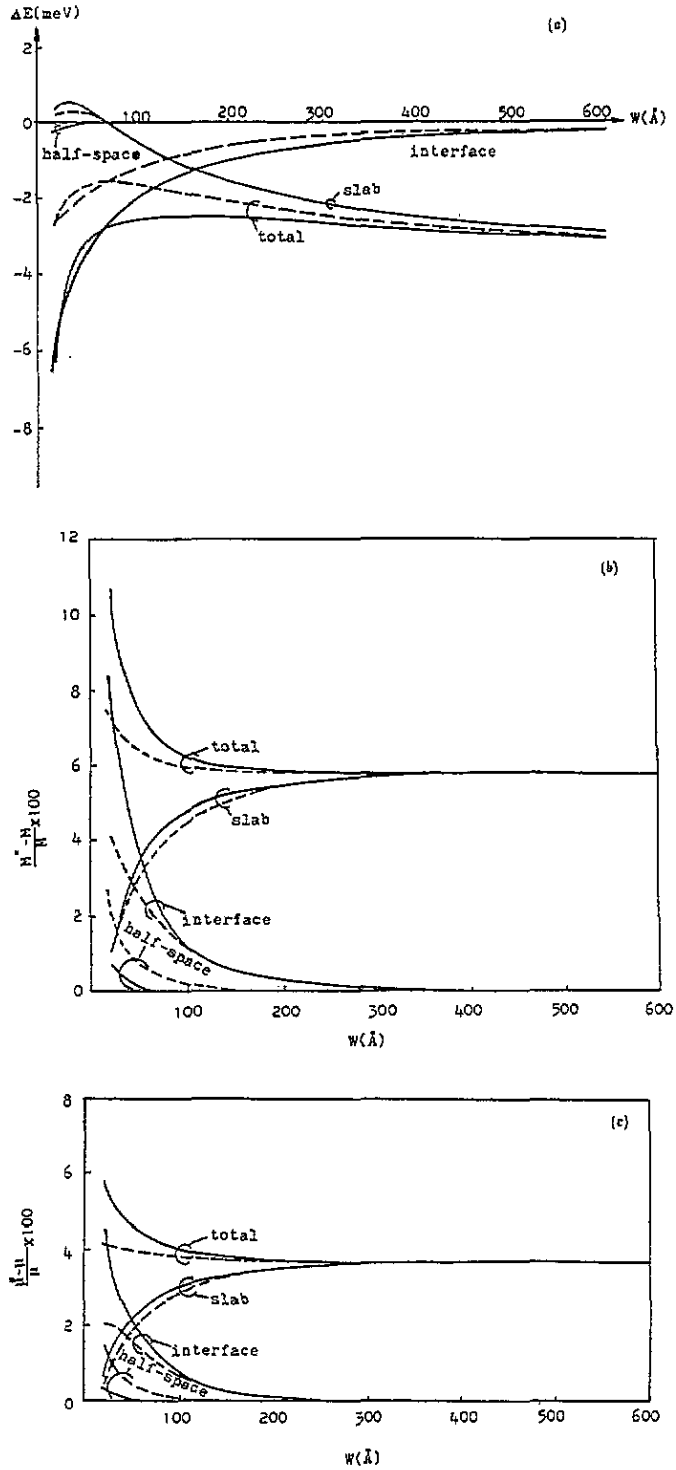

Figure 3. (*a*) The energy shift; (*b*) the correction to the total effective mass; (*c*) the correction to the reduced effective mass of the light-hole exciton in a QW with different Al concentrations (——, $x = 1$; – – –, $x = 0.3$).

exciton effective masses are separately plotted as functions of the well width.

First we plot the heavy-hole exciton ground-state energy shift due to the exciton–phonon interaction in figure 2(*a*) and the corrections to the total and reduced effective masses in figures 2(*b*) and 2(*c*), respectively. The corresponding values for the light-hole excitons are plotted in figure 3. From these figures we observe that the contribution of half-space LO-phonon mode to both the heavy-hole exciton energy and the exciton effective masses are very small. It reduces as the well becomes wider because the half-space phonons play a less important role in their interaction with the exciton inside the well as the well width increases. For $x = 0.3$, it becomes zero when the well width W is larger than 100 Å. The height of the well also acts on the influence of the half-space mode. The higher the well height, the weaker is the influence of the half-space mode. We could hardly see the curve of the half-space mode contribution when $x = 1$ in figure 2. However, for light-hole excitons, the correction to the effective masses due to the influence of the barrier layer phonon mode seems stronger, especially for the reduced effective mass (figure 3(*c*)). Such a difference between the heavy-hole exciton and the light-hole exciton obviously depends on the difference between the hole masses in equation (2.49). The result reveals that the motion of the light-hole exciton is much more easily influenced by the vibration of the crystal lattice.

The influences of the interface phonon mode on the exciton energy and effective masses change markedly as the well width changes. For wider wells the interface effect is weak because the interfaces are far away from the excitons inside the well. Of course a larger x will give a sharper interface and hence will cause a stronger interface effect (see figures 2 and 3.)

The influences of the confined-slab phonon mode on the exciton energy and effective masses increase as the well width increases. As the well becomes thicker, the changes ΔE_{SL} as well as $\Delta M/M = (M^* - M)/M$ and $\Delta\mu/\mu = (\mu^* - \mu)/\mu$ become less pronounced; they will approach those of the three-dimensional LO-phonon mode when the well is very wide [4]. We can also see that the curves change little from $x = 0.3$ to $x = 1$ (figures 2 and 3) because the change in Al concentration x does not change the material inside the well (material I in figure 1). However, when we compare ΔE_{SL} in figures 2(*a*) and 3(*a*), we can see that the curve in figure 3(*a*) (for light-hole excitons) is slightly unusual when the well is narrow ($W < 80$ Å). It has a positive value. This may be due to the difference between m_{exy}/m_{hxy} for heavy-hole excitons and for light-hole excitons. However, when the well is narrow, the contribution of the interface phonon modes prevails; so the total contribution to the exciton ground-state energy by phonons is negative.

In conclusion, we have investigated the phonon–exciton system in a QW structure using a generalized LLP formalism. For the first time, the interaction of excitons with the different phonon modes that can exist in such a structure are taken into consideration. The ground-state energy and the effective masses of the system are obtained as functions of the well width. Numerical calculations are carried out for a $GaAs/Ga_{1-x}Al_xAs$ QW with different Al concentrations for heavy-hole excitons and light-hole excitons. The results show that the interface phonons contribute greatly to both the exciton energy and the effective masses when the well is narrow and that the confined-slab phonons prevail when the well is sufficiently wide. So, in the problem of the exciton–phonon system in a QW, one should consider the performance of different phonon modes instead of treating them as a bulk phonon mode in the material.

Acknowledgments

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