Effects of interface and bulk optical phonons on polarons in a quantum well

Ruisheng Zheng and Shiliang Ban
Laboratory of Solid State Physics, Department of Physics, Inner Mongolia University, Hohhot, 010021, The People's Republic of China

Xi Xia Liang
Chinese Center of Advanced Science and Technology (World Laboratory), P.O. Box 8730, Beijing, 100080, The People's Republic of China
*and Laboratory of Solid State Physics, Department of Physics, Inner Mongolia University, Hohhot, 010021, The People's Republic of China**

(Received 24 June 1993; revised manuscript received 24 September 1993)

The properties of a confined electron interacting with both the confined longitudinal optical (LO) and interface optical (IO) phonons in a quantum well (QW) are investigated. By using a modified Lee-Low-Pines variational method, an analytical expression for the polaron ground-state energy is obtained. Numerical calculation is performed for a GaAs/AlAs QW as a typical case. The results show that only two symmetric IO-phonon modes as well as the confined LO-phonon mode contribute to the energies of the polaron. It is also found that one of the symmetric IO-phonon modes is more important, its contribution to the energies is much larger than the others when the QW width is smaller than the polaron radius.

I. INTRODUCTION

The properties of an electron confined in a quantum well (QW) have attracted much attention in recent years. Some usual QW structures, such as $GaAs/Ga_{1-x}Al_xAs$ structure, are composed of polar compounds, therefore the coupling of the electrons with polar-optical vibrations is in general important for determining the electron dynamics and has been studied a great deal.[1-7] The quasi-two-dimensional (Q2D) polaron problem has become a reference problem for testing various theoretical models and approximation methods because it presents a comparatively simple and physically realistic example for the interaction of a confined particle with quantized field.

By using the so-called bulk-phonon approximation, many authors have studied the properties of the Q2D polarons via the Fröhlich Hamiltonian,[8-10] and showed that the Q2D polaron effect becomes significant in the case of strong confinement. These works have qualitatively predicted the correct results for the self-energy and mass corrections of the polaron both in the three-dimensional (3D) and two-dimensional (2D) cases.[11,12] However they did not mention the contribution of the interface phonons, which have proved to be important in heterostructures.[2-6]

Recently, Lin, Chen, and Gorge,[13] using standard perturbation theory, calculated the ground-state energy and effective mass of a polaron confined in a GaAs/AlAs QW as functions of the QW width. In considering the electron-phonon interaction, they included the confined longitudinal-optical (LO)- as well as the interface-optical (IO)-phonon modes, and gave some qualitative results. Unfortunately, interband transitions were ignored in their calculation for simplicity, and as a result the correct limiting values could not be guaranteed. Hai, Peeters, and Devreese[14] reported a detailed investigation of the binding energy and effective mass of an electron in a QW by using second-order perturbation theory. IO- and LO-phonon modes were incorporated in the calculations, and a comparison of the results for different phonon modes was made. For the infinite-barrier QW, the transitions from the 2D to 3D limit were correctly obtained in their work. But for the finite-barrier QW, it is practically impossible to sum over all intermediate states, so that the so-called leading-term approximation had to be used in the calculations. As concluded by the authors, the finite-barrier QW model with the leading-term approximation is only adequate to study the polaron states in the wells that are neither too narrow nor too wide. Therefore it is not possible to obtain correct limits from this approximation. Based on intuitive arguments, they proposed an approximation that can lead to correct limits.

The purpose of the present paper is to investigate the properties of the Q2D polaron system by using a modified Lee-Low-Pines (LLP) variation method.[15] In order to provide insight into the problem, we perform an analytical calculation as far as possible. The analytical expression of the ground-state energy of the polaron is obtained. Numerical calculation is also performed for the GaAs/AlAs QW as a typical case to compare numerical results with other papers.

The paper is organized as following: in Sec. II the Hamiltonian of an electron in a QW interacting with the confined LO and IO phonons is given. In Sec. III, a modified LLP variational technique is presented, and the expressions for the ground-state and binding energies of the polaron are given. The numerical results are shown graphically in Sec. IV. Finally, the discussion and a brief conclusion are given in Sec. IV.

II. HAMILTONIAN

We consider a QW of polar dielectrics for which the well material is in the region 1, $-d \le z \le d$, and the barriers are in the region 2, $|z| > d$. Let us focus our attention on the interaction of a confined electron with the confined LO and IO phonons, and assume that the effective-mass approximation and the infinite-square-well approximation are valid. These approximations simplify the problems mathematically without losing the essential features of the Q2D polaron. Thus the total Hamiltonian of the electron-lattice system can be written as[4-6]

$$H = H_e + H_{\rm LO} + H_{e\text{-LO}} + H_{\rm IO} + H_{e\text{-IO}} \ . \tag{1}$$

Here the first term includes the electron kinetic energy and the well potential experienced by the electron, and is given by

$$H_e = \frac{\mathbf{p}_\parallel^2}{2m_\parallel} + \frac{p_z^2}{2m_z} + V(z) \ , \tag{2}$$

with

$$V(z) = \begin{cases} \infty \ , & |z| > d \\ 0 \ , & |z| \le d \ , \end{cases} \tag{3}$$

where $\mathbf{P} = (\mathbf{p}_\parallel, p_z)$ and $m^* = (m_\parallel, m_z)$ are the momentum and band mass of the electron, respectively. The second and third terms in (1) describe respectively the confined LO-phonon field and the interaction between the electron and the LO phonons, and are given by[1]

$$H_{\rm LO} = \sum_{\mathbf{k}mp} \hbar\omega_{L1} a^\dagger_{\mathbf{k}mp} a_{\mathbf{k}mp} \ , \tag{4}$$

$$H_{e\text{-LO}} = \sum_{\mathbf{k}mp} [V_{\mathbf{k}mp}(z) e^{i\mathbf{k}\cdot\boldsymbol{\rho}} a_{\mathbf{k}mp} + \text{H.c.}] \ , \tag{5}$$

with

$$V_{\mathbf{k}mp}(z) = \frac{iB}{(k^2 + k_m^2)^{1/2}} \text{csn}(k_m z) \ , \tag{6}$$

$$B = \sqrt{2} \left[\frac{4\pi\alpha_1}{\Omega} \right]^{1/2} \left[\frac{\hbar}{2m_0\omega_{L1}} \right]^{1/4} \hbar\omega_{L1} \ , \tag{7}$$

$$k_m = \frac{m\pi}{2d} \ , \tag{8}$$

$$\Omega = S2d \ , \tag{9}$$

$$\text{csn}(k_m z) = \begin{cases} \cos(k_m z), & m = 1,3,5,\ldots \\ \sin(k_m z), & m = 2,4,6,\ldots , \end{cases} \tag{10}$$

where $a^\dagger_{\mathbf{k}mp}$ ($a_{\mathbf{k}mp}$) is the creation (annihilation) operator for the confined LO phonon with frequency ω_{L1}, wave vector $(\mathbf{k}, k_m)$, and parity p. $\mathbf{r} = (\boldsymbol{\rho}, z)$ is the position vector of the electron. The parity p refers to the mirror symmetry with respect to the plane $z = 0$, and the positive integer m refers to the discrete values of the z component of the wave vector in units of $\pi/2d$. For even (odd) parity, p is positive (negative) and m odd (even). The wave vector k_m is limited by the Brillouin-zone boundary, that is, $m\pi/2d \le \pi/a$ (a is the lattice constant of the well material). $\alpha_1 = (\varepsilon_{\infty 1}^{-1} - \varepsilon_{01}^{-1})(m_0 e^4/2\hbar^3\omega_{L1})^{1/2}$ and $\varepsilon_{\infty 1}(\varepsilon_{01})$ are, respectively, the Fröhlich electron-phonon coupling constant and the high-frequency (static) dielectric constant for the well material labeled 1. Ω is the volume, S the interface area, and m_0 the effective mass of the electron.

The Hamiltonian of the IO-phonon modes (indexes $\sigma, p = +, -$ label the four branches of these modes) is represented by the fourth term in (1), which is given by

$$H_{\rm IO} = \sum_{\mathbf{k}\sigma p} \hbar\omega_{\sigma p} a^\dagger_{\mathbf{k}\sigma p} a_{\mathbf{k}\sigma p} \ , \tag{11}$$

where

$$\omega^2_{\pm p} = \frac{B_p(k) \pm \{B_p^2(k) - 4A_p(k)C_p(k)\}^{1/2}}{2A_p(k)} \ , \tag{12}$$

with

$$A_p(k) = a_1^p + a_2^p \ , \tag{13}$$

$$B_p(k) = a_1^p(\omega_{L1}^2 + \omega_{T2}^2) + a_2^p(\omega_{L2}^2 + \omega_{T1}^2) \ , \tag{14}$$

$$C_p(k) = a_1^p\omega_{L1}^2\omega_{T2}^2 + a_2^p\omega_{L2}^2\omega_{T1}^2 \ , \tag{15}$$

$$a_1^\pm = (1 \mp e^{-2kd})\varepsilon_{\infty 1} \ , \tag{16}$$

$$a_2^\pm = (1 \pm e^{-2kd})\varepsilon_{\infty 2} \ . \tag{17}$$

The last term in (1) is the Hamiltonian of the interaction between the electron and the IO phonons, and is given by[5]

$$H_{e\text{-IO}} = \sum_{\mathbf{k}\sigma p} [W_{\mathbf{k}\sigma p}(z) e^{i\mathbf{k}\cdot\boldsymbol{\rho}} a_{\mathbf{k}\sigma p} + \text{H.c.}] \ , \tag{18}$$

where

$$W_{k\sigma+}(z) = -iD_{\sigma+}(kd) \left[\frac{2\pi\hbar e^2}{Sk\omega_{\sigma+}} \right]^{1/2} \frac{\cosh(kz)}{\cosh(kd)} \ , \tag{19}$$

$$W_{k\sigma-}(z) = -iD_{\sigma-}(kd) \left[\frac{2\pi\hbar e^2}{Sk\omega_{\sigma-}} \right]^{1/2} \frac{\sinh(kz)}{\sinh(kd)} \ , \tag{20}$$

$$D_{\sigma+}(kd) = [2\xi_{1\sigma+}^2 \tanh(kd) + 2\xi_{2\sigma+}^2]^{-1/2} \ , \tag{21}$$

$$D_{\sigma-}(kd) = [2\xi_{1\sigma-}^2 \coth(kd) + 2\xi_{2\sigma-}^2]^{-1/2} \ , \tag{22}$$

$$\xi_{\lambda\sigma p} = \frac{(\varepsilon_{\lambda\sigma p} - \varepsilon_{\infty\lambda})}{\omega_{T\lambda}(\varepsilon_{0\lambda} - \varepsilon_{\infty\lambda})^{1/2}} \quad (\lambda = 1,2) \ , \tag{23}$$

$$\varepsilon_{\lambda\sigma p} = \varepsilon_{\infty\lambda} \frac{\omega_{L\lambda}^2 - \omega_{\sigma p}^2}{\omega_{T\lambda}^2 - \omega_{\sigma p}^2} \quad (\lambda = 1,2) \ , \tag{24}$$

where $a^\dagger_{\mathbf{k}\sigma p}$ ($a_{\mathbf{k}\sigma p}$) is the creation (annihilation) operator for the IO phonon with frequency $\omega_{\sigma p}$ and wave vector $\mathbf{k}$. ω_{L1} (ω_{L2}) and ω_{T1} (ω_{T2}) are the longitudinal and transverse optical phonon frequencies, respectively, for material 1 (2). $\varepsilon_{\infty 2}(\varepsilon_{02})$ is the high-frequency (static) dielectric constant for the barrier material labeled 2.

III. CALCULATION

Because the Hamiltonian in Sec. II appears exceedingly complicated, some methods of approximation must be used. In this paper we adopt a modified LLP variational method.[15] First, for the Hamiltonian (1) we perform a

unitary transformation with

$$U=\exp\left\{-\sum_{\mathbf{k}mp}[F_{\mathbf{k}mp}(\boldsymbol{\rho},z)a^{\dagger}_{\mathbf{k}mp}-F^{*}_{\mathbf{k}mp}(\boldsymbol{\rho},z)a_{\mathbf{k}mp}]+\sum_{\mathbf{k}\sigma p}[G_{\mathbf{k}\sigma p}(\boldsymbol{\rho})a^{\dagger}_{\mathbf{k}\sigma p}-G^{*}_{\mathbf{k}\sigma p}(\boldsymbol{\rho})a_{\mathbf{k}\sigma p}]\right\}, \tag{25}$$

in which

$$F_{\mathbf{k}mp}(\boldsymbol{\rho},z)=f_{\mathbf{k}mp}\mathrm{csn}(k_m z)\exp(-i\mathbf{k}\cdot\boldsymbol{\rho}) , \tag{26}$$

$$G_{\mathbf{k}\sigma p}(\rho)=g_{\mathbf{k}\sigma p}\exp(-i\mathbf{k}\cdot\rho) , \tag{27}$$

where $f_{\mathbf{k}mp}$ and $g_{\mathbf{k}\sigma p}$ are the variational parameters which will subsequently be determined by minimizing the energy of the system. The following relations holds for the transformation:

$$U^{\dagger}a_{\mathbf{k}mp}U=a_{\mathbf{k}mp}+F_{\mathbf{k}mp} , \tag{28}$$

$$U^{\dagger}a_{\mathbf{k}\sigma p}U=a_{\mathbf{k}\sigma p}+G_{\mathbf{k}\sigma p} , \tag{29}$$

$$U^{\dagger}P_z U=P_z-i\left\{\sum_{\mathbf{k}mp}\hbar k_m[f_{\mathbf{k}mp}\mathrm{scn}(k_m z)\times e^{-i\mathbf{k}\cdot\boldsymbol{\rho}}a^{\dagger}_{\mathbf{k}mp}-\mathrm{H.c.}]\right\}, \tag{30}$$

$$U^{\dagger}\mathbf{p}_{\parallel}U=\mathbf{p}_{\parallel}-\sum_{\mathbf{k}mp}\hbar\mathbf{k}(F_{\mathbf{k}mp}a^{\dagger}_{\mathbf{k}mp}+\mathrm{H.c.})-\sum_{\mathbf{k}mp}\hbar\mathbf{k}|F_{\mathbf{k}mp}|^2-\sum_{\mathbf{k}\sigma p}\hbar\mathbf{k}(G_{\mathbf{k}\sigma p}a^{\dagger}_{\mathbf{k}\sigma p}+\mathrm{H.c.})-\sum_{\mathbf{k}\sigma p}\hbar\mathbf{k}|G_{\mathbf{k}\sigma p}|^2 . \tag{31}$$

where, for convenience, the function $\mathrm{scn}(k_m z)$ is defined as

$$\mathrm{scn}(k_m z)=\begin{cases}-\sin(k_m z) & \text{for odd } m\\ \cos(k_m z) & \text{for even } m .\end{cases} \tag{32}$$

Then the transformed Hamiltonian $H^{*}=U^{\dagger}HU$ can be obtained, of which the part related to the zero-phonon state is given by

$$\begin{aligned}H^{*}_{0}=&\frac{p^2_{\parallel}}{2m_{\parallel}}-\frac{\mathbf{p}_{\parallel}}{m_{\parallel}}\left\{\sum_{\mathbf{k}mp}\hbar\mathbf{k}|f_{\mathbf{k}mp}|^2\mathrm{csn}^2(k_m z)+\sum_{\mathbf{k}\sigma p}\hbar\mathbf{k}|g_{\mathbf{k}\sigma p}|^2\right\}\\&+\frac{1}{2m_{\parallel}}\left\{\sum_{\mathbf{k}mp}\hbar\mathbf{k}|F_{\mathbf{k}mp}|^2+\sum_{\mathbf{k}\sigma p}\hbar\mathbf{k}|g_{\mathbf{k}\sigma p}|^2\right\}^2+\sum_{\mathbf{k}mp}\frac{\hbar^2k^2}{2m_{\parallel}}|F_{\mathbf{k}mp}|^2+\sum_{\mathbf{k}\sigma p}\frac{\hbar^2k^2}{2m_{\parallel}}|g_{\mathbf{k}\sigma p}|^2\\&+\frac{p_z^2}{2m_z}+V(z)+\sum_{\mathbf{k}mp}\frac{\hbar^2k_m^2}{2m_z}|f_{\mathbf{k}mp}|^2\mathrm{scn}^2(k_m z)+\sum_{\mathbf{k}mp}\hbar\omega_{L1}|f_{\mathbf{k}mp}|^2\mathrm{csn}^2(k_m z)+\sum_{\mathbf{k}\sigma p}\hbar\omega_{\sigma p}|g_{\mathbf{k}\sigma p}|^2\\&+\sum_{\mathbf{k}mp}\{V_{\mathbf{k}mp}(z)f_{\mathbf{k}mp}\mathrm{csn}(k_m z)+\mathrm{c.c.}\}+\sum_{\mathbf{k}\sigma p}\{W_{\mathbf{k}\sigma p}(z)g_{\mathbf{k}\sigma p}+\mathrm{c.c.}\} .\end{aligned} \tag{33}$$

Since we are interested only in the ground state of the confined polaron, and assume that the momentum of the electron in x-y plane is zero, the first two terms in (33) related to the kinetic energy of the confined polaron can be assumed to be zero. The third term describes the interaction between the virtual phonons emitted and reabsorbed by the recoiled electron, and is generally very small in the case of weak coupling.[15] It can be neglected in the following calculations since the electron-phonon coupling is rather weak for the real materials such as GaAs/AlAs etc.

The expectation value of the transformed Hamiltonian is evaluated by choosing the wave function $|\psi\rangle$ as a product of an electron wave function and a phonon vacuum state,

$$|\psi\rangle=\Phi_n(z)|0\rangle , \tag{34}$$

where $|0\rangle$ is the phonon vacuum state, and $\Phi_n(z)$ is the electron subband wave function for the motion along the z direction in an infinite square well potential, which is given by

$$\Phi_n(z)=\begin{cases}\left[\frac{1}{d}\right]^{1/2}\sin\{k_n(z+d)\}, & |z|\le d\\ 0 , & |z|>d ,\end{cases} \tag{35}$$

with

$$k_n=\frac{n\pi}{2d}\quad(n=1,2,3,\ldots) . \tag{36}$$

Then we obtain the expectation value of the transformed Hamiltonian of the confined polaron system:

$$E=\langle\psi|H^*|\psi\rangle=\langle\psi|U^\dagger HU|\psi\rangle$$
$$=\frac{\pi^2\hbar^2n^2}{8m_zd^2}+\sum_{\mathbf{k}\sigma p}\left[\hbar\omega_{\sigma p}+\frac{\hbar^2k^2}{2m_\parallel}\right]|g_{\mathbf{k}\sigma p}|^2+\sum_{\mathbf{k}\sigma p}[\langle\phi_n|W_{\mathbf{k}\sigma p}(z)|\phi_n\rangle g_{\mathbf{k}\sigma p}+\text{c.c.}]$$
$$+\sum_{\mathbf{k}mp}\left\{\left[\hbar\omega_{L1}+\frac{\hbar^2k^2}{2m_\parallel}\right]\langle\phi_n|\mathrm{csn}^2(k_mz)|\phi_n\rangle+\frac{\hbar^2k_m^2}{2m_z}\langle\phi_n|\mathrm{scn}^2(k_mz)|\phi_n\rangle\right\}|f_{\mathbf{k}mp}|^2$$
$$+\sum_{\mathbf{k}mp}\left\{\frac{iB}{(k^2+k_m^2)^{1/2}}\langle\phi_n|\mathrm{csn}^2(k_mz)|\phi_n\rangle f_{\mathbf{k}mp}+\text{c.c.}\right\}. \tag{37}$$

The variational conditions, $\delta E/\delta F_{\mathbf{k}mp}=0$ and $\delta E/\delta g_{\mathbf{k}\sigma p}=0$ can be used to determine the forms of $f_{\mathbf{k}mp}$ and $g_{\mathbf{k}\sigma p}$, which are

$$f_{\mathbf{k}mp}=\frac{\frac{iB}{(k^2+k_m^2)^{1/2}}\langle\phi_n|\mathrm{csn}^2(k_mz)|\phi_n\rangle}{\left[\hbar\omega_{L1}+\frac{\hbar^2k^2}{2m_\parallel}\right]\langle\phi_n|\mathrm{csn}^2(k_mz)|\phi_n\rangle+\frac{\hbar^2k_m^2}{2m_z}\langle\phi_n|\mathrm{scn}^2(k_mz)|\phi_n\rangle} \tag{38}$$

and

$$g_{\mathbf{k}\sigma p}=\frac{-\langle\phi_n|W^*_{\mathbf{k}\sigma p}(z)|\phi_n\rangle}{\left[\hbar\omega_{\sigma p}+\frac{\hbar^2k^2}{2m_\parallel}\right]}. \tag{39}$$

By substituting equations (38) and (39) into (37), we finally obtain

$$E=\frac{\pi^2\hbar^2n^2}{8m_zd^2}-E_{\mathrm{LO}}-E_{\mathrm{IO}}, \tag{40}$$

with

$$E_{\mathrm{IO}}=\sum_{\sigma p}E_{\mathrm{IO}}(\sigma,p), \tag{41}$$

where

$$E_{\mathrm{LO}}=\sum_{\mathbf{k}mp}\frac{\frac{B^2}{(k^2+k_m^2)}|\langle\phi_n|\mathrm{csn}^2(k_mz)|\phi_n\rangle|^2}{\left[\hbar\omega_{L1}+\frac{\hbar^2k^2}{2m_\parallel}\right]\langle\phi_n|\mathrm{csn}^2(k_mz)|\phi_n\rangle+\frac{\hbar^2k_m^2}{2m_z}\langle\phi_n|\mathrm{scn}^2(k_mz)|\phi_n\rangle} \tag{42}$$

and

$$E_{\mathrm{IO}}(\sigma,p)=\sum_{\mathbf{k}}\frac{|\langle\phi_n|W_{\mathbf{k}\sigma p}(z)|\phi_n\rangle|^2}{\left[\hbar\omega_{\sigma p}+\frac{\hbar^2k^2}{2m_\parallel}\right]}. \tag{43}$$

$E_{\mathrm{LO}}+E_{\mathrm{IO}}$ represents physically the self-energy of the polaron due to the electron-phonon interaction. E_{LO} comes from the interaction of the electron with the confined LO phonon, and E_{IO} from the electron–IO-phonon interaction.

Before giving further calculations, from equation (43) we note the interesting fact that two antisymmetric branches of the IO phonons labeled $p=-$ do not contribute to the electron-phonon interaction energy under the approximations used in this paper. That is to say, $E_{\mathrm{IO}}(+,-)$ and $E_{\mathrm{IO}}(-,-)$ are equal to zero. This fact can be proved as the following:

Since

$$W_{\mathbf{k}\sigma-}(-z)=-W_{\mathbf{k}\sigma-}(z)$$

and

$$|\phi_n(-z)|^2=|\phi_n(z)|^2,$$

thus

$$\langle\phi_n|W_{\mathbf{k}\sigma-}(z)|\phi_n\rangle=\int_{-d}^{d}W_{\mathbf{k}\sigma-}(z)|\phi_n(z)|^2dz=0.$$

To simplify the subsequent calculations, we set $m_0=m_\parallel=m_z$, and take $\hbar\omega_{L1}$ as the unit of the energy, and $(\hbar/2m_0\omega_{L1})^{1/2}$ as the unit of the length. In order to obtain the ground-state energy we evaluate expressions (40)–(43) for the lowest subband state ($n=1$). Now by using the relation

$$\sum_{\mathbf{k}}\Longrightarrow(S/4\pi^2)\int d\mathbf{k},$$

the sum over $\mathbf{k}$ becomes an integral which can be evaluated. We finally obtain

$$E=\frac{\pi^2}{4d^2}-E_{\mathrm{LO}}-E_{\mathrm{IO}}\ , \tag{44}$$

with

$$E_{\mathrm{LO}}=\frac{3\alpha_1}{4d}\frac{1}{1-\frac{2}{3}\left[\frac{\pi}{2d}\right]^2}\ln\left[\frac{1}{3}+\left[\frac{2d}{\pi}\right]^2\right]+\frac{\alpha_1}{2d}\sum_{m=2,3\ldots}\ln\left[1+\left[\frac{2d}{m\pi}\right]^2\right], \tag{45}$$

$$E_{\mathrm{IO}}(\sigma,+)=\frac{2\alpha_1\bar{\varepsilon}_1}{d}\int_0^\infty\frac{D^2_{\sigma+}(q)}{\omega_{\sigma+}\omega_{L1}}\frac{\tanh^2(q)dq}{q^2\left[1+\frac{q^2}{\pi^2}\right]^2\left[\frac{\omega_{\sigma+}}{\omega_{L1}}+k^2\right]}\ . \tag{46}$$

In Eq. (46), we have defined the variables $q=kd$, and $\bar{\varepsilon}_1=(\varepsilon_{\infty 1}^{-1}-\varepsilon_{01}^{-1})^{-1}$.

IV. RESULT AND DISCUSSION

In order to understand the change of the polaron properties with reducing dimensionality in graphical form, we evaluate the energies given by equations (44)–(46) over the entire range of the well width. For the sake of comparison we choose the GaAs/AlAs QW as a typical example and adopt the same parameters used in Ref. 13, which are listed in Table I. The results we obtain as functions of the QW width d are plotted in Fig. 1.

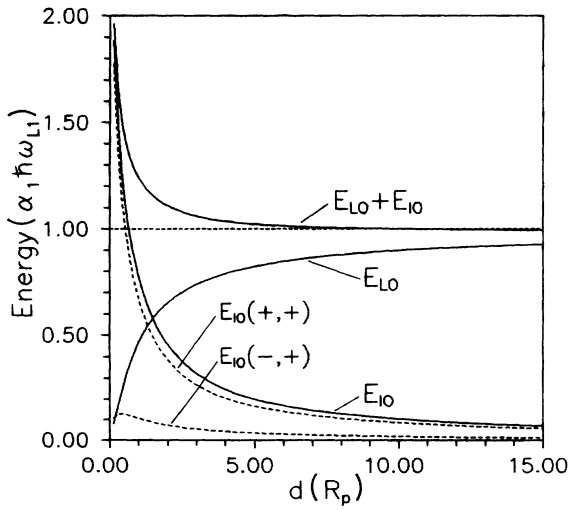

FIG. 1. Calculated polaron energies (in units of $\alpha_1\hbar\omega_{L1}$) as functions of the well width d (in units of the polaron radius R_p). $E_{\mathrm{LO}}+E_{\mathrm{IO}}$ represents the self-energy of the Q2D polaron confined in a GaAs/AlAs QW, and E_{LO} and E_{IO} are the contributions from confined LO and IO phonons, respectively. $E_{\mathrm{IO}}(+,+)$ and $E_{\mathrm{IO}}(-,+)$ correspond to the contributions from the two IO-phonon modes labeled $(+,+)$ and $(-,+)$, respectively.

TABLE I. Parameters used for the present calculation (m_e is the rest mass of a free electron). The electron-phonon coupling constant α is taken from Ref. 16, the other parameters from Ref. 13.

	m_0/m_e	ε_0	ε_∞	ω_L (cm^{-1})	ω_T (cm^{-1})	α
GaAs	0.067	12.5	10.06	297	273	0.068
AlAs		10.6	8.16	403.7	361.7	0.126

From Fig. 1 we can see that our result is almost the same as one of the results obtained by Hai, Peeters, and Devreese[14] with the infinite-barrier square well, although we use a different theoretical method. We also find that only two symmetric modes in the four IO-phonon modes contribute to the binding energy of the polaron. The energy $E_{\mathrm{IO}}(+,+)$ is always much larger than $E_{\mathrm{IO}}(-,+)$. Furthermore, it is dominant in all phonon modes when the QW width is smaller than the polaron radius R_p [for GaAs, $R_p=39.5$ Å (Ref. 13)]. This interesting result indicates that the IO-phonon mode labeled $(+,+)$ is more important, and should be paid more attention.

In Fig. 1, it is very clear that E_{LO}, the energy of the electron interacting with the confined LO phonons, increases monotonically with increasing QW width d, until it reaches the limiting value of the bulk case. As noted by Licari,[6] it is somewhat surprising that the energy E_{LO} rises to $\alpha_1\hbar\omega_{L1}$ very slowly when the well width is much greater than the polaron radius R_p, however, this is due simply to the neglect of the contribution of the interface/surface phonons. Our result here strongly supports this opinion, and gives a clear picture of the way in which the energies change with the QW width d. There are two effects when d becomes large: (1) the energy E_{LO} rises slowly to that of the bulk Fröhlich polaron, and (2) the energy E_{IO} reduces slowly to zero. These two effects combat each other, and make the self-energy $E_{\mathrm{LO}}+E_{\mathrm{IO}}$ close very fast to the value expected for the bulk polaron. When d is larger than $8R_p$, our result indicates that the self-energy of the Q2D polaron is almost exactly equal to $\alpha_1\hbar\omega_{L1}$.

We note that the self-energy of the Q2D polaron is qualitatively similar to that obtained by the bulk-phonon approximation.[8,14] This fact indicates that the bulk-phonon approximation can give some reasonable results for a Q2D polaron system with a not too narrow well width in spite of its simplicity. But, as Hai, Peeters, and Devreese have noted,[14] we also point out that there is an obvious quantitative deference between the self-energy given by the present paper and the result obtained by the bulk-phonon approximation in the narrow QW case. In the 2D limiting case, our result approaches $(\pi/2)\alpha_2\hbar\omega_{L2}$, which is the self-energy of a polaron on the surface of half-space barrier material. In contrast, the bulk-phonon approximation gives a limiting result of $(\pi/2)\alpha_1\hbar\omega_{L1}$, which is the self-energy of a 2D polaron in the well material layer. Our result is in keeping with the physical analysis on the problem. The quantitative difference indicates that the property of confined phonons in the QW is not the same as that of the ideal 2D or 3D phonons. The effects of the confined phonons, especially the interface

phonons, should not be neglected.

In this paper we also wish to discuss the range of validity of the infinite-barrier QW approximation. From quantum-mechanical theory, one can obtain the probability of finding a particle with energy eigenvalue E_n in the barrier region of a finite-barrier square well (the barrier height is V_0); that is,

$$P_{\text{out}}=\frac{E_n}{V_0}\left[\left[\frac{2m(V_0-E_n)}{\hbar^2}\right]^{1/2}d+1\right]^{-1}. \quad (47)$$

If the probability P_{out} is much smaller than 1, one can say that the perfect carrier confinement approximation is valid. We believe that this is a reasonable quantitative criterion. In the case of a GaAs/AlAs QW with $V_0=0.57$ eV,[16] when the QW width is $d=R_p$, one can obtain $P_{\text{out}}=0.02$ for an electron at the bottom of the lowest subband energy level. Thus we can say that the infinite-square-well approximation is valid at least in the range of $d>R_p$.

In conclusion, we have investigated the properties of a Q2D polaron confined in a QW by including the effects of LO and IO phonons, and given a clear picture of the way in which the energies of the Q2D polaron change with the QW width. Based on the approaches used in this paper, we have found that the following: (1) Only two symmetric IO-phonon modes and the confined LO-phonon mode contribute to the energies of the polaron in a symmetric QW. (2) The symmetric IO-phonon mode labeled $(+,+)$ is more important in the four branches of the IO phonons. Its contribution to the energies is always much larger than the others. Furthermore, it will be in the dominant position in all phonon modes when the QW width is smaller than the polaron radius. (3) By incorporating the contributions of the IO and LO phonons, the behavior of the Q2D polaron is qualitatively similar to that of the so-called bulk-phonon approximation, but there obviously is a quantitative difference between them.

ACKNOWLEDGMENT

This work is supported by the National Nature Science Foundation of the People's Republic of China.

*Mailing address.

[1]J. J. Licari and R. Evrard, Phys. Rev. B **4**, 2254 (1977).
[2]F. Comas, C. Trallero-Giner, and R. Riera, Phys. Rev. B **39**, 5907 (1989).
[3]T. Tsuchiya, H. Akera, and T. Ando, Phys. Rev. B **39**, 6025 (1989).
[4]L. Wendler and R. Pechstedt, Phys. Status Solidi B **141**, 129 (1987).
[5]X. X. Liang and X. Wang, Phys. Rev. B **43**, 5155 (1991).
[6]X. X. Liang, J. Phys. Condens. Matter **4**, 9769 (1992).
[7]J. J. Licari, Solid State Commun. **29**, 625 (1979).
[8]M. H. Degani and O. Hipólito, Solid State Commun. **65**, 1185 (1988).
[9]T. Yildirim and A. Erçelebi, J. Phys. Condens. Matter **3**, 1271 (1991).
[10]T. Yildirim and A. Erçelebi, J. Phys. Condens. Matter **3**, 4357 (1991).
[11]F. M. Peeters and J. T. Devreese, Phys. Rev. B **36**, 4442 (1987).
[12]Xiaoguang Wu, F. M. Peeters, and J. T. Devreese, Phys. Rev. B **31**, 3420 (1985).
[13]D. L. Lin, R. Chen, and T. F. George, J. Phys. Condens. Matter **3**, 4645 (1991).
[14]G. Q. Hai, F. M. Peeters, and J. T. Devreese, Phys. Rev. B **42**, 11 063 (1990).
[15]T. D. Lee, F. E. Low, and D. Pines, Phys. Rev. **90**, 297 (1953).
[16]S. Adachi, J. Appl. Phys. **58**, R1 (1985).