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Influence of the spatially dependent effective mass on bound polarons in finite parabolic quantum wells

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Abstract. The effect of the electron-phonon interaction including the longitudinal optical phonons, the four branches of interface optical phonons and the effect of spatial dependence effective mass have been considered to investigate the bound polaron energy levels in finite parabolic quantum wells. A modified variational method is adopted to obtain the dependence of the ground state and the binding energies of bound polarons on the alloy composition x in finite GaAs/$Al_xGa_{1-x}As$ quantum wells. It is found from the numerical result that there is an obvious contribution of the interaction between the electron and the longitudinal optical phonons as well as interface phonons on the polaron energy levels. The electron-phonon interaction should not be neglected to study the electron state problem in parabolic quantum wells.

PACS. 73.20.-r Electron states at surfaces and interfaces – 71.38.-k Polarons and electron-phonon interactions – 63.20.Kr Phonon-electron and phonon-phonon interactions

1 Introduction

For a compositional parabolic quantum well (PQW), the well material can be generated by alternate deposition of thin undoped layers of GaAs and $Al_xGa_{1-x}As$ with fixed composition x and varying layer thickness [1–5]. The relative thickness of the GaAs layers decrease quadratically with distance from the well centers while that of the $Al_xGa_{1-x}As$ layers increase. It can be, for this kind of PQWs, approximated in theory by continuously changing the alloy composition x from the well center ($x = 0$) to the well edge ($x = 0.32$).

In recent years, the properties of the electron (or hole) state in the PQW were studied in experimental and theoretical works. Some authors [6–9] studied the electronic state in the PQW by using different methods to derive the energy levels. Other authors [10–16] adopted the one- and two-parameter variational methods, respectively, to calculate the binding energy and the transition energy of hydrogenic impurity states in the PQW. The exciton energy levels in PQW structures have also been investigated in some works [17]. Unfortunately, the effect of electron-phonon (e-p) interaction on the energy level has not been included in the above theoretical works. It is well known that the e-p interaction has a considerable effect and can not be neglected in the study of electron states in a square quantum well (SQW). Similarly, the effects of e-p interaction on the electronic states in a PQW should be important.

The polaron effect of electrons coupled with longitudinal optical (LO) phonon modes in infinite PQWs in the presence or absence of a magnetic field has been investigated by several groups [18–30]. The approximation of three dimensional (3D) bulk LO-phonon modes and of infinite PQW used in their calculations needs to be improved. More recently, Gerlach *et al.* [31] presented a variational study of the ground-state energy of an exciton-(LO) phonon system in an infinite PQW. They also used a simple Hamiltonian of the 3D bulk LO e-p interaction to obtain the energy levels. The results with consideration of phonon modes in all above theoretical works surely are better than the results without consideration of phonon modes. However, they did not consider the effects of interface optical (IO) phonons and the spatially dependent effective masses (SDEM) in the PQW. Therefore a more detailed theoretical investigation of electron states in the PQW is needed.

In this paper we study the effect of the e-p interaction on the bound polaron energy levels in finite compositional PQWs. The influences of LO-phonons and the four branches of IO phonons between the material of well edge and the barrier materials, and the effect of the SDEM are all included. We have also considered the relation between the frequency of LO-phonons and alloy composition x. The impurity-phonon coupling as well as the

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e-p coupling have been taken into account in the calculation. A modified Lee-Low-Pines (LLP)-like variational method is adopted to deal with e-p interaction and to obtain the ground state and the binding energies of the bound polaron in a PQW. The numerical results for a finite GaAs/$Al_xGa_{1-x}As$ PQW are given and discussed.

2 Theory

We consider a PQW structure with the well width of $L = 2d$, where the well material is in region $\lambda = 1$, $|z| \leq d$, and the barrier materials in region $\lambda = 2$, $|z| > d$. The well material is generated by continuously changing the alloy composition x from the well center ($x = 0$) to the well edge ($x = 0.32$), and the barrier materials are AlAs. An electron in the system is coupled to a Coulomb impurity center (with a charge e) located at position Z_0 interacting with both LO and IO phonons. The Hamiltonian of the system can be written as [32–34]

$$H = p_z\left(\frac{p_z}{2m_\lambda(z)}\right) + \frac{p_x^2+p_y^2}{2m_\lambda(z)} + V(z) - \frac{e^2}{4\pi\varepsilon_\lambda(z)r} + \sum_{\mathbf{w}\lambda}\hbar\omega_{L\lambda}a^+_{\mathbf{w}\lambda}a_{\mathbf{w}\lambda} + \sum_{\mathbf{q}\sigma p}\hbar\omega_{\sigma p}b^+_{\mathbf{q}\sigma p}b_{\mathbf{q}\sigma p} + H_I, \quad (1)$$

where

$$V(z) = \begin{cases} V_0 z^2/d^2 & |z| \leq d \\ V_1 & |z| > d, \end{cases} \quad (2)$$

with

$$V_0 = 0.6 \times 1250\ x \qquad (x = 0.32), \quad (3)$$

$$m_\lambda(z) = \begin{cases} m_1(z) & |z| \leq d \\ m_2 & |z| > d, \end{cases} \quad (4)$$

and

$$\mathbf{W} = \begin{cases} (\mathbf{k}, m\pi/2d) & |z| \leq d \\ (\mathbf{k}, k_z) & |z| > d. \end{cases} \quad (5)$$

Here $\varepsilon_\lambda(z)$ is the high frequency dielectric constant in region λ, $a^+_{\mathbf{w}\lambda}$ and $a_{\mathbf{w}\lambda}$ are respectively the creation and annihilation operators of the LO phonons with frequency $\omega_{L\lambda}$, wave vector $\mathbf{W}$. $b^+_{\mathbf{q}\sigma p}(b_{\mathbf{q}\sigma p})$ is the corresponding creation (annihilation) operator of the IO-phonons with a 2D wave-vector $\mathbf{q}$. $\mathbf{k}$ is a 2D-vector in the x-y plane. The corresponding frequency $\omega_{\sigma p}$ labeled by $\sigma(= +, -)$ and parity $p(= +, -)$ is dispersionless and is given by references [33,34]. $V_1(= 750$ meV) is the depth of the PQW, m_2 the effective-band mass of the electron in barrier materials AlAs, $r = \sqrt{\rho^2 + (z - z_0)^2}$ is the distance between the electron and the hydrogenic impurity center. Considering the effect of the SDEM, the effective band mass of the electron in region 1 can be written [35] as

$$m_1(z) = 0.0665 + 0.0835\ x. \quad (6)$$

The relation between the alloy composition x and the coordinate z satisfies $x = 0.32z^2/d^2$. The last term in (1) is the e-p interaction Hamiltonian and is given by

$$H_I = \sum_{\mathbf{w}\lambda}\left\{\left[g^*_{w\lambda}(z)\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\boldsymbol{\rho}} - g^*_{w\lambda}(z_0)\right]a^+_{\mathbf{w}\lambda} + \mathrm{h.c.}\right\} + \sum_{\mathbf{q}\sigma p}\left\{\left[g^*_{q\sigma p}(z)\mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\boldsymbol{\rho}} - g^*_{q\sigma p}(z_0)\right]b^+_{\mathbf{q}\sigma p} + \mathrm{h.c.}\right\}. \quad (7)$$

Here factor $g^*(z_0)$ is related to the impurity coordinate Z_0 in the growing direction of the well, and the Hamiltonian does not have translational invariance in the Z-direction. A simpler Hamiltonian has been used to discuss the bound polarons in bulk materials [32]. Where a 3D plane-wave factor $\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}}$ instead of $\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\boldsymbol{\rho}}$ was used and the term related to the impurity center reduces to 1, since the 3D translational symmetry is hold and the impurity center can always treated to be at the coordinate origin, *i.e.* put $Z_0 = 0$. A Hamiltonian similar to equation (7) was also used for the heterojunction problem [36].

The coupling function in equation (7) is determined by following equation

$$g^*_{w\lambda}(z) = -\mathrm{i}\begin{cases} \hbar\omega_{L1}\left(\dfrac{\hbar}{2m_1(z)\omega_{L1}}\right)^{1/4} \times \dfrac{(4\pi\alpha_1/Sd)^{1/2}\sin[m\pi(z+d)/2d]}{\left[k^2+(m\pi/2d)^2\right]^{1/2}}, & |z| \leq d \\ \hbar\omega_{L2}\left(\dfrac{\hbar}{2m_2\omega_{L2}}\right)^{1/4} \times \dfrac{(4\pi\alpha_2/SD)^{1/2}\sin[k_z(|z|-d)]}{(k^2+k_z^2)^{1/2}} & |z| > d. \end{cases} \quad (8)$$

Here $m = 1, 3, 5...$ corresponds the even parity, $m = 2, 4, 6...$ the odd parity, and m is limited by $m\pi/L \leq \pi/a$, in which a is the lattice constant. α_λ is the electron-LO-phonon coupling parameter in region λ and

$$g^*_{q\sigma p}(z) = \mathrm{i}\left(\frac{\hbar e^2}{4qs\varepsilon_0\omega_{\sigma p}}\right)^{1/2} \times \begin{cases} \left[\xi_1^2\tanh(qd) + \xi_2^2\right]^{-1/2}\dfrac{\cosh(qz)}{\cosh(qd)}, & (p = +) \\ \left[\xi_1^2\coth(qd) + \xi_2^2\right]^{-1/2}\dfrac{\sinh(qz)}{\sinh(qd)}, & (p = -) \end{cases} \quad (9)$$

for $|z| \leq d$ and

$$g^*_{q\sigma p}(z) = \mathrm{i}\left(\frac{\hbar e^2}{4qs\varepsilon_0\omega_{\sigma p}}\right)^{1/2} \times \begin{cases} \left[\xi_1^2\tanh(qd) + \xi_2^2\right]^{-1/2}\mathrm{e}^{-q(|z|-d)}, & (p = +) \\ \left[\xi_1^2\coth(qd) + \xi_2^2\right]^{-1/2}\mathrm{e}^{-q(|z|-d)}\theta(|z|-d) & (p = -), \end{cases} \quad (10)$$

for $|z| > d$. D is the thickness of the barrier, S stands for the interface area, ε_0 is the vacuum dielectric constant.

In equation (10),

$$\xi_1 = \frac{\varepsilon_\lambda - \varepsilon_{\infty\lambda}}{\omega_{T\lambda(\varepsilon_{s\lambda}-\varepsilon_{\infty\lambda})}}, \quad \varepsilon_\lambda = \varepsilon_{\infty\lambda}\frac{\omega_{L\lambda}^2 - \omega_{\sigma p}^2}{\omega_{T\lambda}^2 - \omega_{\sigma p}^2},$$

$$\theta(|z| - d) = \begin{cases} +1, & z > d \\ -1, & z < d. \end{cases} \quad (11)$$

In equation (11), $\varepsilon_{s\lambda}$ and $\varepsilon_{\infty\lambda}$ are, respectively, the static and the high-frequency dielectric constants and $\omega_{T\lambda}$ is the transverse optical phonon frequency in region λ.

To solve the Hamiltonian H in equation (1), we first perform two unitary transformations with [37,38]

$$U_1 = \exp\left[-\mathrm{i}\left(\sum_{\mathbf{w}\lambda}\mathbf{k}\cdot\boldsymbol{\rho}a^+_{\mathbf{w}\lambda}a_{\mathbf{w}\lambda} + \sum_{\mathbf{q}\sigma p}\mathbf{q}\cdot\boldsymbol{\rho}b^+_{\mathbf{q}\sigma p}b_{\mathbf{q}\sigma p}\right)\right] \quad (12)$$

and

$$U_2 = \exp\left\{\sum_{\mathbf{w}\lambda}\left[f_{w\lambda}a^+_{\mathbf{w}\lambda} - f^*_{w\lambda}a_{\mathbf{w}\lambda}\right] + \sum_{\mathbf{q}\sigma p}\left[h_{q\sigma p}b^+_{\mathbf{q}\sigma p} - h^*_{q\sigma p}b_{\mathbf{q}\sigma\mathbf{p}}\right]\right\}, \quad (13)$$

with $f_{w\lambda}, h_{q\sigma p}$ and their complex conjugate as variational parameters, the transformed Hamiltonian is written as

$$H^* = U_2^{-1}U_1^{-1}H\,U_1U_2. \quad (14)$$

It is to be pointed out that in the bulk material case, a preceding canonical transformation U_0 [32] was employed to simplify the impurity-ion phonon interaction. As a result, the e-p contribution changed the high-frequency dielectric constant into the static one in the Coulomb potential, as well infinite self-energy of a static point charge was added to the Hamiltonian and dropped. Since the symmetry in the Z-direction is broken, the preceding transformation in reference [32] is invaluable to simplify the Hamiltonian and has not been used here. Therefore the dielectric constant in the Coulomb potential is kept unchanged and the added infinite self-energy does not appear in H^*.

For the ground state of the bound polaron, the trial wave function is chosen as the following form

$$\psi = N\varphi(z)\phi(\rho)|0\rangle, \quad (15)$$

with

$$\phi(\rho) = \left(\frac{1}{2\pi}\right)^{1/2}\beta\mathrm{e}^{-\beta\rho/2}, \quad (16)$$

where $|0\rangle$ is the zero-phonon state of the phonon field, β is a variational parameter, N is the normalization constant. The coordinate part of the wave function $\varphi(z)$, can be obtained by numerically solving the Schrodinger equation with the following boundary condition at $|z| = d$

$$\psi_- = \psi_+, \quad \frac{1}{m_\lambda(z)_-}\frac{\mathrm{d}\psi}{\mathrm{d}z}\bigg|_- = \frac{1}{m_\lambda(z)_+}\frac{\mathrm{d}\psi}{\mathrm{d}z}\bigg|_+, \quad (17)$$

here $\pm$ indicates $|z| \to d \pm 0_\pm$. Then the polaron energy can be written as

$$E(L,\beta) = \langle\psi\,|H^*|\,\psi\rangle\cdot \quad (18)$$

The ground state energy E_{1s} can be obtained by numerically solving equation (18) subject to the boundary condition (17). The binding energy is given as

$$E_b = E_f - E_{1s}, \quad (19)$$

where E_f is the ground state energy of the free-polaron in the system.

For comparison, we also calculated the energy levels of the bound polaron in the SQW. The Hamiltonian of the bound polaron in the SQW is taken from references [33,34] and the calculation to obtain energy is similar to reference [39].

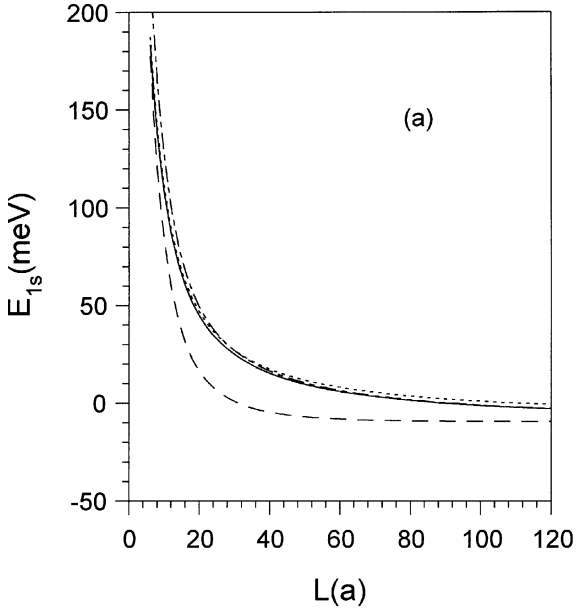
3 Numerical results and discussion

We have numerically calculated the energy levels of the ground state of the bound polaron in GaAs/$Al_xGa_{1-x}As$ PQWs by using equations (14–19). The parameters used in the calculation are listed in Table 1, and the numerical results are shown in Figures 1–3. The effective phonon-mode approximation has been used to obtain the LO and TO phonon modes of the ternary mixed crystal $Al_xGa_{1-x}As$ [40,41]. The reference energy levels for the electron are chosen at the bottom of the conductor-band.

Table 1. Parameters [40] used in the calculation.

Quantities	GaAs	$Al_xGa_{1-x}As$	AlAs
ε_s	13.18	$10.06x + 13.18(1-x)$	10.06
ε_∞	10.89	$8.16x + 10.89(1-x)$	8.16
$m_b(m_e)$	0.0665	$0.15x + 0.0665(1-x)$	0.15
a(nm)	0.5644	$0.566x + 0.5644(1-x)$	0.566
$\hbar\omega_L$ (meV)	36.25	$36.25 + 1.83x + 17.12x^2 - 5.11x^3$	50.09
$\hbar\omega_T$ (meV)	33.29	$33.29 + 10.7x + 0.03x^2 + 0.86x^3$	44.88

Figure 1a shows the ground state energy E_{1s} of the bound polaron with and without the effect of the SDEM in the PQW, and the results in the SQW, respectively, as a function of the well width L. One sees that E_{1s} decreases with increasing L rapidly at less L but slowly at larger L, the results are qualitatively similar to the results of the SQW, but the values in the PQW are larger than that in the SQW. On the other hand, the curve with the effect of the SDEM is lower than the curve without the effect of the SDEM since the effective band mass with the effect of the SDEM is larger than that without the effect of the SDEM. In the infinite harmonic oscillator limit for a spatially constant effective mass, the energy is proportional to $m_\lambda(z)^{-1/2}$ [8]. In order to understand the effects of e-p interaction clearly, the contribution of the difference branches of phonons and the summation of them to the



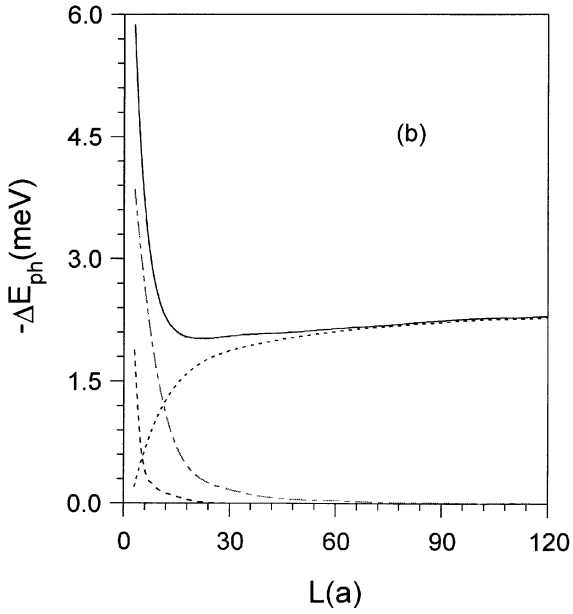
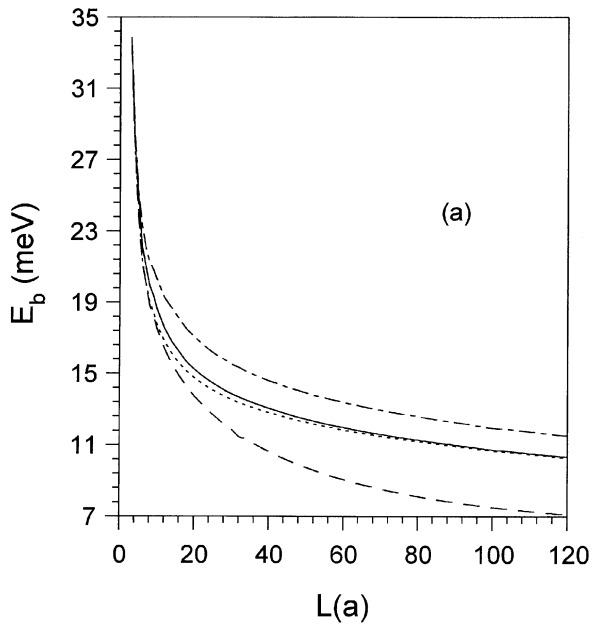


Fig. 1. (a) The ground state energies of the bound polaron as a function of well width L, in units of a. The solid line is the result with the influence of phonons and the effects of the SDEM, the dashed dotted line is the result with the influence of phonons and without the effects of the SDEM, the dotted line is the result without the influence of phonons and with the effects of the SDEM in the finite PQW, the dashed line is the result with the influence of phonons in the SQW; (b) the contributions of phonons to the bound polaron energy-levels in the finite PQW as a function of well width L, in units of a. Dashed line is the curve of the barrier LO-phonons contribution, dashed dot line is the IO-phonons contributions, dotted line is the confined LO-phonons contributions and the solid line is the total contributions.



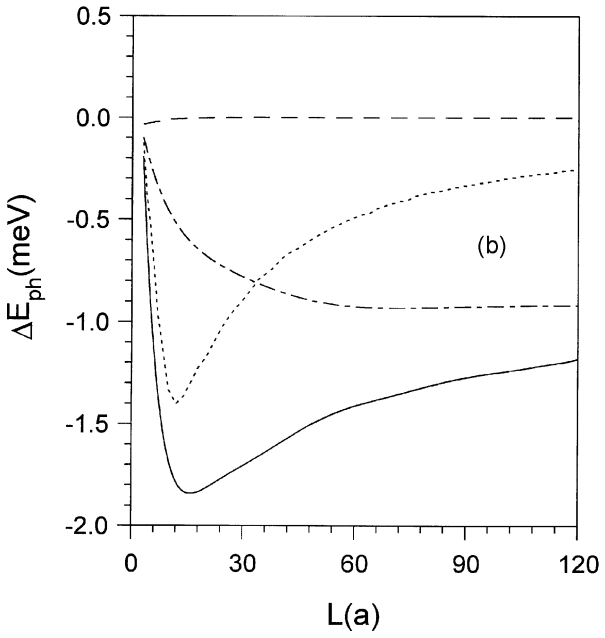


Fig. 2. (a) The ground state binding energies of the bound polaron as a functions of the well width L, in units of a, with the influence of phonons and the effect of the SDEM (solid line), without the influence of phonons and with the effect of the SDEM (dashed dot line), with the influence of phonons and without the effect of the SDEM (dotted line) in the PQW, with the influence of phonons (dashed line) in the SQW; (b) the contributions of phonons to the binding energies in the PQW as a functions of the well width L, in units of a. Dashed line is the curve of the barrier LO-phonon contribution, dashed dot line is the confined LO-phonon contribution, dotted line is the IO-phonon contribution and the solid line is the total contribution.

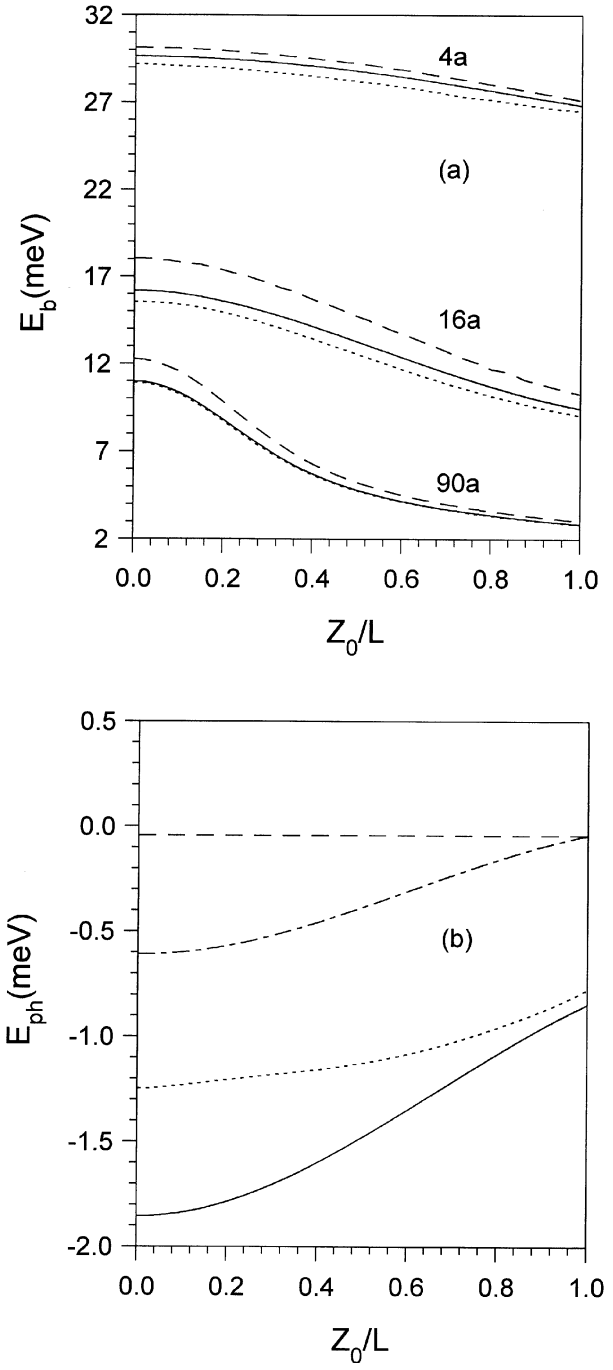


Fig. 3. (a) The ground state binding energies of the bound polaron as a functions of the impurity position z_0, in units of L, with the influence of phonons and the effect of the SDEM (solid line), without the influence of phonons and with the effect of the SDEM (dashed line), with the influence of phonons and without the effect of the SDEM (dotted line) in the PQW for the three given well widths (L are, respectively, $4a$, $16a$, and $90a$); (b) the contributions of phonons to the binding energies as a functions of the impurity position z_0, in units of L, in the PQW for given well width 16a. Dashed line is the barrier LO-phonon contribution, dashed dot line is the confined LO-phonon contribution, dotted line is the IO-phonon contribution and the solid line is the total contribution.

ground state energy of the bound polaron in the PQW as functions of L are shown in Figure 1b. It is found that the contribution of the confined LO-phonon to the ground state energy increases as increasing L, and finally closes to the total contribution. But the contribution of the barrier LO-phonon and the IO phonons decreases rapidly as increasing L at first, and approaches zero at large L. As a result of superposition the total contribution decreases with increasing L at first, and gets a minimum around $18a$, then increases slowly and at last approaches to the 3D-values of bulk GaAs. There is a minimum in the total contribution curve because we considered the impurity – IO and LO phonon interaction as well as the electron – IO and LO phonon interaction.

The binding energy E_b of the bound polaron as a function of the well width L is depicted in Figure 2a. It is seen that E_b decreases rapidly with increasing L at first, then decreases slowly, finally approaches the bulk values in GaAs. For comparison, the results without the e-p influences and with the SDEM effect, without the SDEM effect and with the e-p influences are respectively plotted in Figure 2a. E_b with the influence of phonons is smaller than that without the influence of phonons. It also shows that the phonon contributions to the binding energies are negative [36]. That the binding energies without the SDEM effect is lower than that with the SDEM effect is qualitatively similar to the results of reference [16]. The contributions of the difference branches of phonons to the binding energies are plotted in Figure 2b. It can be seen that the IO phonons contribution is larger than that of the confined LO phonons for less L, but the confined LO phonons contribution is larger than that of IO phonons for larger L, and the contribution of the barrier LO-phonons is very small. The total negative contribution increases rapidly with increasing L at first, then gets a maximum around $16a$, finally decreases slowly. The total contribution of the e-p interaction to the binding energies of the ground state is obvious. The typical value is given about 9% at $16a$. Therefore, the e-p effects should be considered in discussion the electronic states in a PQW. It can be found in Figure 1a and Figure 2a that the energy shifts with and without the SDEM effect decrease with increasing L (except for $L < 4a$), finally decrease to zero. The reason is that the probability of the electron locating the center of the PQW increases with increasing L and then the effective band mass in the PQW tends to the value in GaAs. Our result is qualitatively similar to the previous results without influence of phonons [12,14,16], but there is a quantitative difference.

E_b with the e-p interaction and without the e-p interaction as a function of the impurity position z_0 in the three given well widths ($4a$, $16a$, $90a$) is given in Figure 3a, along with that without the effects of the SDEM and with the influences of phonons. One can see that the E_b decreases with increasing z_0 in the all three cases, but the variation of the binding energies with increasing the impurity position is of a little difference. For example, in a narrower well ($L = 4a$), E_b decreases slowly with increasing z_0, whereas it decreases rather quickly with increasing z_0 in a larger

well width ($L = 90a$). Figure 3b shows the contributions of the difference branches of phonons to E_b as a function of z_0 in the given well width ($16a$). One can see that the contributions of the e-p interaction to the binding energies decrease with increasing z_0 and the IO phonon contribution is largest while the barrier LO-phonon contribution is least.

In conclusion, we have considered the effect of the electron – IO and LO phonon interaction and the SDEM effect the on the bound polaron energy levels in a finite PQW. A modified Lee-Low-Pines (LLP)-like method is adopted to deal with the e-p interaction as well as the impurity. The numerical results for finite GaAs/Al_xGa_{1-x}As PQWs are obtained and discussed. The result shows that there is an obvious contribution from the IO-phonons as well as LO-phonons on the energy levels. Thus, the electron-phonon interaction should not be neglected in the study of the electron state problem. One can also find that the effect of the SDEM on the energy levels in a finite PQW is obvious except for large ($L \to \infty$). In addition, the LO and IO phonons contributions to the binding energies are negative and obvious.

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