Bound polaron in a polar semiconductor heterojunction

S. L. Ban* and J. E. Hasbun
Department of Physics, State University of West Georgia, Carrollton, Georgia 30118
(Received 23 February 1998; revised manuscript received 10 June 1998)

The behavior of an optical polaron bound to a donor impurity near the interface of a polar semiconductor heterojunction is investigated with a variational method by considering the influence of a realistic heterojunction potential, the electron-phonon and impurity-phonon interactions, including the effect of half-space bulk longitudinal and interface-optical phonon modes. The bound-polaron binding energy is computed for $GaAs/Al_xGa_{1-x}As$ ($0.2<x<0.4$) heterojunction system. The result shows that the impurity-phonon interaction is important and that the phonon contribution to the binding energy is negative. Both of the bulk longitudinal and interface-phonon modes give important contributions to the binding energy when the impurity is located in GaAs. The interface modes are more important than the bulk-phonon modes when the impurity is located in $Al_xGa_{1-x}As$. [S0163-1829(99)06103-2]

I. INTRODUCTION

The properties of polarons bound to impurities near the interfaces or surfaces of layered semiconductors are considerably different from that in bulk materials.[1] This may bring about transport and optical properties, which have an important significance both in fundamental science and device development. A polaron bound to a donor in a polar-crystal slab[2] was discussed, including both the electron longitudinal-optical (LO) phonon interaction and the electron surface-optical (SO) phonon interaction. In a quantum well (QW), the polaron bound to a donor[3–6] has been a subject of interest during the past decade. Some authors adopted the approximation of considering only three-dimensional (3D) bulk LO phonon modes[3] or purely 2D phonon modes.[4] Some authors[5] neglected the effect of bulk LO phonons and only took the electron SO phonon interaction into account. For a GaAs slab or a $GaAs/Al_xGa_{1-x}As$ QW, the weak electron-phonon coupling gives a small contribution to the impurity binding energy even though it lowers the impurity energy levels. The influence of the electron-phonon coupling becomes significant for a thin QW when considering the screening effects of the impurity potential and the electron-phonon interaction.[6]

The impurity states of a donor on a semiconductor surface were initially studied three decades ago.[7] Later, the SO phonon effects were investigated for the bound-polaron ground state[8,9] and the excited states.[9] An electron bound to an impurity near the interface of a semiconductor heterojunction was discussed under the influence of a magnetic field.[10] For an impurity located at the interface, the polaronic effect was investigated while including the electron half-space bulk LO phonon and electron interface-optical (IO) phonon interactions.[11] Here the SO-like phonon modes were used as an approximation of the IO phonon modes. In an external electric field, the polaron bound to an impurity near the heterojunction interface[12] was investigated by considering not only the electron IO phonon coupling and electron half-space bulk LO phonon coupling, but also the impurity IO phonon coupling. Unfortunately, for an impurity placed 30 Å from the interface inside AlAs and the electron confined in GaAs, a very small binding energy was obtained; i.e., 1.2 and 0.2 meV corresponding, respectively, to the exclusion and inclusion of the phonon influence, in the zero-field limit. Thus, the phonon influence is found much too strong. This result does not reflect a realistic property of the heterojunction.

For $GaAs/Al_xGa_{1-x}As$ heterojunctions with low Al concentration, the ratio of the potential barrier to the impurity-state binding energy is on the order of a factor of 10. The effect of the finite barrier as well as the energy-band bending is to make the conduction electrons within the channel side (GaAs) penetrate the barrier side ($Al_xGa_{1-x}As$) of the heterojunction. The strong confinement of the electrons causes a shift in the average distance between the electron and the interface,[13] and will, therefore, affect the binding energy of a donor impurity near the interface. The infinite-barrier approximation[10–12] to the interface potential needs to be improved by treating it more realistically. More recently, the ground-state energy of a donor impurity, located on the heterointerface, was investigated without considering the contribution due to phonons.[14] The interface potential used did not include band-bending effects.

In the present paper the ground state of a polaron bound to a hydrogenlike donor impurity near the interface of a heterojunction is investigated by considering the effects of both half-space bulk LO phonons and IO phonons. Both the electron-phonon coupling and the impurity-phonon coupling have been taken into account. The influence of a realistic interface potential, including the electron-image potential and the conduction-band bending, is considered through a self-consistent computation. A one-subband model is used. A modified Lee, Low, and Pines (LLP) intermediate-coupling method[15] is adopted to deal with the interaction between the phonons and the electron as well as the impurity. The energy level, the binding energy, and the effective mass of the bound polaron in the ground state are obtained variationally. The numerical computation is performed for a $GaAs/Al_xGa_{1-x}As$ heterojunction. An effective phonon-mode[16] approximation (EPMA) has been used to obtain the LO and the transverse-optical (TO) phonon modes of the ternary-mixed crystal $Al_xGa_{1-x}As$. This approximation seems to work well[17] in such a weak polar semiconductor. The other parameters of $Al_xGa_{1-x}As$ used in this paper have

been calculated using the virtual-crystal approximation[18] (VCA). The phonons, at the most, may give a 7% contribution to reduce the binding energy when the impurity-phonon coupling is included. On the other hand, we also found that the phonon effect on the binding energy is negligibly small if the impurity-phonon coupling is neglected.

II. THEORY

We consider a heterojunction consisting of two semiconductors denoted by material 1 (channel side) for $z>0$ and material 2 (barrier side) for $z<0$, respectively. The interface of the heterojunction is chosen as the x-y plane. Without losing generality, the interface can be assumed infinite. In this coordinate system an external donor impurity bearing a charge e is located at $(0,0,z_0)$. A conduction electron with charge $-e$, located at (x,y,z) in the heterojunction potential, interacts with the impurity through the Coulomb potential. The Hamiltonian of the electron-impurity system including the LO and IO phonons and both the electron- and impurity-phonon coupling can be written as

$$H=H_{x\text{-}y}+H_z+H_c+H_{\rm ph}+H_{e,i\text{-ph}}, \tag{1}$$

with

$$H_{x\text{-}y}=\frac{p_x^2+p_y^2}{2m_{\|1}}\,\theta(z)+\frac{p_x^2+p_y^2}{2m_{\|2}}\,\theta(-z), \tag{2}$$

$$H_z=\frac{p_z^2}{2m_{\perp 1}}\,\theta(z)+\frac{p_z^2}{2m_{\perp 2}}\,\theta(-z)+V(z)+\frac{e^2(\epsilon_{\infty 1}-\epsilon_{\infty 2})}{4\epsilon_{\rm eff}(\epsilon_{\infty 1}+\epsilon_{\infty 2})z}, \tag{3}$$

$$H_c=-\frac{e^2}{\epsilon(z,z_0)[x^2+y^2+(z-z_0)^2]^{1/2}}, \tag{4}$$

$$H_{\rm ph}=\sum_{\mathbf{k}}\hbar\omega_{L1}a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}\theta(z)+\sum_{\mathbf{k}}\hbar\omega_{L2}a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}\theta(-z)+\sum_{\mathbf{q},\sigma}\hbar\omega_{\sigma}b_{\mathbf{q}\sigma}^{\dagger}b_{\mathbf{q}\sigma}, \tag{5}$$

and

$$H_{e,i\text{-ph}}=\sum_{\mathbf{k}}\left\{\frac{1}{k}\left[\sum_{\lambda}B_{\lambda}(z)\sin(k_z|z|)e^{-i\mathbf{k}_{\|}\cdot\boldsymbol{\rho}}-B_{\lambda'}(z_0)\sin(k_z|z_0|)\right]a_{\mathbf{k}}^{\dagger}+\text{H.c.}\right\}+\sum_{\mathbf{q},\sigma}\left[\frac{G_{\sigma}}{\sqrt{q}}\,(e^{-i\mathbf{q}\cdot\boldsymbol{\rho}}e^{-q|z|}-e^{-q|z_0|})b_{\mathbf{q}\sigma}^{\dagger}+\text{H.c.}\right], \tag{6}$$

where $m_{\|\lambda}$ and $m_{\perp\lambda}$ are the band mass of the conduction electron being in material λ ($\lambda=1,2$) in the x-y plane and in the z direction, respectively. $\theta(\pm z)$ is the step function. $\epsilon_{\infty\lambda}$ is the optical-dielectric constant of the λth material. The last term in Eq. (3) is the electron-image potential. The effective-dielectric constant $\epsilon_{\rm eff}$ is defined as $\epsilon_{\rm eff}=(\epsilon_{\infty 1}+\epsilon_{\infty 2})/2$, which removes the mismatch of the electron-image potential at $z=0$. The heterojunction potential $V(z)$ in Eq. (3) satisfies[19]

$$V(z)=V_0\theta(-z)+V_s(z)+V_d(z), \tag{7}$$

in which V_0 is the potential-barrier height. $V_s(z)$ and $V_d(z)$ are the electron contribution and the depletion-charge contribution to the potential, respectively. The depletion-charge contribution is obtained by solving

$$\frac{\partial}{\partial z}\,\epsilon_0(z)\,\frac{\partial}{\partial z}\,V_d(z)=-4\pi e^2[N_A(z)-N_D(z)], \tag{8}$$

where the static-dielectric constant is given by

$$\epsilon_0(z)=\begin{cases}\epsilon_{01} & \text{for } z>0\\ \epsilon_{02} & \text{for } z<0.\end{cases} \tag{9}$$

In Eq. (8), $N_A(z)$ and $N_D(z)$ are, respectively, the position-dependent acceptor and donor concentrations. In the Coulomb interaction term Eq. (4), the position-dependent dielectric constant is defined by

$$\epsilon(z,z_0)=\begin{cases}\epsilon_{\infty 1} & \text{for } z>0 \text{ and } z_0>0\\ (\epsilon_{\infty 1}+\epsilon_{\infty 2})/2 & \text{for } z>0,z_0<0 \text{ or } z<0,z_0>0\\ \epsilon_{\infty 2} & \text{for } z<0 \text{ and } z_0<0.\end{cases} \tag{10}$$

In Eq. (5), $\omega_{L\lambda}$ is the LO phonon frequency of the λth material. The ω_{σ}'s ($\sigma=\pm$) are, respectively, the higher and lower frequencies of the two IO phonon modes and can be obtained by solving[20] $\omega_{\pm}^2=(b\pm\sqrt{b^2-4ac})/2a$, in which $a=\epsilon_{\infty 1}+\epsilon_{\infty 2}$, $b=\epsilon_{\infty 1}(\omega_{L1}^2+\omega_{T2}^2)+\epsilon_{\infty 2}(\omega_{L2}^2+\omega_{T1}^2)$, and $c=\epsilon_{\infty 1}\omega_{L1}^2\omega_{T2}^2+\epsilon_{\infty 2}\omega_{L2}^2\omega_{T1}^2$; $\omega_{T\lambda}$ is the TO phonon frequency of the λth material. In Eq. (6), $\lambda'=1$ ($=2$) refers to the impurity being in the channel side (barrier side). The electron (impurity) LO phonon and electron (impurity) IO phonon interaction factors are given by

$$B_{\lambda}(z)=-i\left[\frac{4\pi e^2}{V}\,\hbar\omega_{L\lambda}\left(\frac{1}{\epsilon_{\infty\lambda}}-\frac{1}{\epsilon_{0\lambda}}\right)\right]^{1/2}\theta(\lambda,z), \tag{11}$$

in which

$$\theta(\lambda,z)=\begin{cases}\theta(z) & \text{for } \lambda=1\\ \theta(-z) & \text{for } \lambda=2,\end{cases} \tag{12}$$

and

$$G_{\sigma}=i\left(\frac{1}{\delta_1^2+\delta_2^2}\,\frac{2\pi\hbar e^2}{S\omega_{\sigma}}\right)^{1/2}, \tag{13}$$

where $\delta_{\lambda}=(\epsilon_{0\lambda}-\epsilon_{\infty\lambda})^{1/2}\omega_{T\lambda}/(\omega_{T\lambda}^2-\omega_{\sigma}^2)$.

For the ground state of the system, we choose the following variational trial-wave function:

$$|\psi\rangle=|\phi(x,y)\rangle|\zeta(z)\rangle|0\rangle=|\phi(\rho)\rangle|\zeta(z)\rangle\prod_{\mathbf{k},\mathbf{q},\sigma}|0_{\mathbf{k}}\rangle|0_{\mathbf{q}\sigma}\rangle, \tag{14}$$

with

$$\phi(\rho)=\left[\frac{1}{2\pi}\right]^{1/2}\gamma e^{i\mathbf{K}_\parallel\cdot\boldsymbol{\rho}}e^{-\gamma\rho/2}, \tag{15}$$

and

$$\zeta(z)=\begin{cases}\zeta_A(z)=Bb^{1/2}(bz+\beta)e^{-bz/2} & \text{for } z>0\\ \zeta_B(z)=B'b'^{1/2}e^{b'z/2} & \text{for } z<0,\end{cases} \tag{16}$$

where $\rho=\sqrt{x^2+y^2}$ is the radial component of the electron coordinate in the x-y plane and $\mathbf{K}_\parallel=(K_x,K_y,0)$. Also γ, b and b' are independent-variational parameters. In Eq. (15), we introduce the factor $e^{i\mathbf{K}_\parallel\cdot\boldsymbol{\rho}}$ in order to recover the free-polaron case when γ approaches 0. This free-polaron-limit case is fully discussed near the end of Sec. II A. According to the continuity condition of the wave function $\zeta(z)$ and its first-order differential at $z=0$, the normalization constants in Eq. (16) satisfy[18] $\beta=2b/(b'+b)$, $B=[\beta(1+b/b')+2\beta+2]^{-1/2}$, and $B'=B\beta(b/b')^{1/2}$. In Eq. (14), $|0\rangle$ is the phonon-vacuum state.

The electronic contribution to the potential in Eq. (7) can be obtained by solving

$$\frac{\partial}{\partial z}\,\epsilon_0(z)\,\frac{\partial}{\partial z}\,V_s(z)=-4\pi e^2N_s|\zeta(z)|^2, \tag{17}$$

where N_s is the areal electron density.

A. Displacement oscillator transformation with the coupling in the z direction (DOTC)

We use

$$U_1=\exp\left[-i\left(\sum_{\mathbf{k}}\mathbf{k}_\parallel a^\dagger_{\mathbf{k}}a_{\mathbf{k}}+\sum_{\mathbf{q},\sigma}\mathbf{q}b^\dagger_{\mathbf{q}\sigma}b_{\mathbf{q}\sigma}\right)\cdot\boldsymbol{\rho}\right], \tag{18}$$

and[21]

$$U_2=\exp\left[\sum_{\mathbf{k}}\left(f_k e^{-ik_z z}a^\dagger_{\mathbf{k}}-f^*_k e^{ik_z z}a_{\mathbf{k}}\right)+\sum_{\mathbf{q},\sigma}\left(g_{q\sigma}b^\dagger_{\mathbf{q}\sigma}-g^*_{q\sigma}b_{\mathbf{q}\sigma}\right)\right], \tag{19}$$

with f_k, $g_{q\sigma}$ and their complex conjugate as variational parameters, to perform two unitary transformations on Hamiltonian (1) and obtain the expectation energy for the bound polaron at ground state:

$$\begin{aligned}E(b,b',\gamma)&=\langle\psi|U_2^{-1}U_1^{-1}HU_1U_2|\psi\rangle\\&=E_a+\langle T\rangle+\langle V_d\rangle+\langle V_s\rangle+\langle V_0\rangle\\&\quad+E_{\text{image}}+E_c-E_{\text{LO}}-\sum_\sigma E_{I\sigma}.\end{aligned} \tag{20}$$

The transformation with U_1 is essential for the weak electron-phonon coupling case to obtain a lower energy. However, it was neglected in a previous paper.[12]

In Eq. (20),

$$E_a=\frac{\hbar^2K_\parallel^2}{2m^*_\parallel}+\frac{\hbar^2\gamma^2}{8m_\parallel}, \tag{21}$$

of which the first term is the kinetic energy corresponding to the free-polaron limit. For a bound polaron, this term is taken to be zero. $m^*_\parallel$ is the free-polaron effective mass parallel to the x-y plane and is given by

$$m^*_\parallel=m_\parallel\left(1+\Delta m_{\text{LO}}+\sum_\sigma\Delta m_{I\sigma}\right). \tag{22}$$

The average electron-band mass parallel to the x-y plane in Eqs. (21) and (22) is defined as $m_\parallel=m_{\parallel1}m_{\parallel2}/(m_{\parallel1}\overline{P}_2+m_{\parallel2}\overline{P}_1)$. Here $\overline{P}_1=\int_0^\infty|\zeta_A(z)|^2dz$ and $\overline{P}_2=\int_{-\infty}^0|\zeta_B(z)|^2dz$ are, respectively, the electron probabilities of being in material 1 and 2. The contributions from LO and IO phonons to the effective mass are given by

$$\Delta m_{\text{LO}}=2\frac{\hbar^2}{m_\parallel}\sum_{\mathbf{k}}\frac{|\phi_B(k,z_0,\gamma)_{\gamma\to0}|^2k_\parallel^2\cos^2(\theta)}{\left(\hbar\omega_{L1}\overline{P}_1+\hbar\omega_{L2}\overline{P}_2+\dfrac{\hbar^2k_\parallel^2}{2m_\parallel}+\dfrac{\hbar^2k_z^2}{2m_\perp}\right)^3}, \tag{23}$$

and

$$\Delta m_{I\sigma}=2\frac{\hbar^2}{m_\parallel}\sum_{\mathbf{q}}\frac{|\phi_G(\sigma,q,z_0,\gamma)_{\gamma\to0}|^2q^2\cos^2(\theta)}{\left(\hbar\omega_\sigma+\dfrac{\hbar^2q^2}{2m_\parallel}\right)^3}, \tag{24}$$

where θ is the angle between $\mathbf{K}_\parallel$ and $\mathbf{k}_\parallel$ or $\vec{q}$. In Eq. (20),

$$\langle T\rangle=\frac{\hbar^2}{2}\left[(Bb)^2(1+\beta-\beta^2/2)/2m_{\perp1}-(B'b')^2/4m_{\perp2}\right], \tag{25}$$

$$\langle V_d\rangle=4\pi e^2N_d\{-B'^2/b'\epsilon_{02}+B^2[(6+4\beta+\beta^2)/b\epsilon_{01}]\}, \tag{26}$$

$$\langle V_s\rangle=4\pi e^2N_s[B'^2(1-B'^2/2)/b'\epsilon_{02}+B^4(33+50\beta+34\beta^2+12\beta^3+2\beta^4)/4b\epsilon_{01}], \tag{27}$$

$$\langle V_0\rangle=V_0B'^2, \tag{28}$$

and

$$E_{\text{image}}=\frac{e^2(\epsilon_{\infty1}-\epsilon_{\infty2})}{4\epsilon_{\text{eff}}(\epsilon_{\infty1}+\epsilon_{\infty2})}B^2b[1+2\beta]. \tag{29}$$

In Eq. (26), N_d denotes the areal concentration of the fixed-depletion charges.[18] For the Coulomb interaction contribution in Eq. (20) we first perform a Fourier transformation then simplify it and obtain

$$E_c=-\left\langle \psi\left|\frac{e^2}{\epsilon(z,z_0)[x^2+y^2+(z-z_0)^2]^{1/2}}\right|\psi\right\rangle$$
$$=-\left\langle \psi\left|\frac{e^2}{\epsilon(z,z_0)}\sum_{\mathbf{Q}}\frac{4\pi}{Q^2}\exp[i\mathbf{Q}\cdot(\mathbf{r}-\mathbf{z}_0)]\right|\psi\right\rangle$$
$$=-e^2\gamma^3\int_0^\infty dq\,\frac{1}{(\gamma^2+q^2)^{3/2}}$$
$$\times\left\langle \zeta(z)\left|\frac{1}{\epsilon(z,z_0)}\exp(-|z-z_0|q)\right|\zeta(z)\right\rangle, \quad (30)$$

where the integrations over ρ and q_z have been carried out with definitions $\mathbf{r}=(\boldsymbol{\rho},z)$, $\mathbf{Q}=(\mathbf{q},q_z)$, and $q=\sqrt{q_x^2+q_y^2}$.

The last two terms of Eq. (20) are the self-trapping energies of the polaron due to the contribution from LO and IO phonons, respectively, and are given by

$$E_{\mathrm{LO}}=\sum_{\mathbf{k}}\frac{|\phi_B(k,z_0,\gamma)|^2}{\hbar\omega_{L1}\overline{P}_1+\hbar\omega_{L2}\overline{P}_2+\dfrac{\hbar^2k_\parallel^2}{2m_\parallel}+\dfrac{\hbar^2k_z^2}{2m_\perp}}, \quad (31)$$

and

$$E_{I\sigma}=\sum_{\mathbf{q}}\frac{|\phi_G(\sigma,q,z_0,\gamma)|^2}{\hbar\omega_\sigma+\dfrac{\hbar^2q^2}{2m_\parallel}}. \quad (32)$$

In the above equations, we have adopted the following notations:

$$\phi_B(k,z_0,\gamma)$$
$$=\sum_\lambda\left\langle \zeta(z)\left|\frac{B_\lambda(z)\sin(k_z|z|)e^{ik_zz}}{k}\right|\zeta(z)\right\rangle$$
$$-\frac{\gamma^3}{(\gamma^2+k_\parallel^2)^{3/2}}\left\langle \zeta(z)\left|\frac{B_{\lambda'}(z_0)\sin(k_z|z_0|)e^{ik_zz}}{k}\right|\zeta(z)\right\rangle, \quad (33)$$

and

$$\phi_G(\sigma,q,z_0,\gamma)=\left\langle \zeta(z)\left|\frac{G_\sigma e^{-q|z|}}{\sqrt{q}}\right|\zeta(z)\right\rangle$$
$$-\frac{\gamma^3}{(\gamma^2+q^2)^{3/2}}\frac{G_\sigma e^{-q|z_0|}}{\sqrt{q}}. \quad (34)$$

It should be pointed out that the second term on the right-hand side of Eq. (33) is the contribution from the impurity LO phonon interaction. Only when z and z_0 have the same sign is the contribution defined to be nonzero.

Minimizing $E(b,b',\gamma)-\langle V_s\rangle/2$ with respect to the variational parameters, respectively,[18] we obtain b, b', and γ. By inserting them into $E(b,b',\gamma)$ the bound-polaron ground-state energy E_{bp} can be obtained.

The ground-state energy E_{fp} for a free polaron in the absence of the donor can be derived by choosing $H_c=0$ in Eq. (1), subsequently, $E_c=0$ in Eq. (20). By repeating the above process, the variational parameter γ approaches 0 and the trial function in Eq. (15) becomes a plane wave. We note that the $\gamma\to0$ limit has to be done carefully since the wave function of Eq. (15) is normalized. The normalization constant is what gives rise to the γ factor in front of the exponential. The normalization constant is different in the limit of $\gamma\to0$. On the other hand, equivalent results can be reached by just replacing Eq. (15) with $\phi(\rho)=\exp(i\mathbf{K}_\parallel\cdot\boldsymbol{\rho})/\sqrt{A}$; in addition, one also removes H_c and the impurity-phonon coupling terms in Eqs. (6). The resulting expectation energy in Eq. (20) is exactly the sum of the previous terms with $\gamma=0$. Thus, for the free polaron we only have two independent-variational parameters b and b'.

The bound-polaron binding energy for the ground state can be written as

$$E_B=E_{\mathrm{fp}}-E_{\mathrm{bp}}. \quad (35)$$

B. Displacement-oscillator transformation without the coupling in the z direction (DOT)

We turn next to the second-unitary transformation of Eq. (19) but without the phase factor:

$$U_2=\exp\left[\sum_{\mathbf{k}}(f_ka_{\mathbf{k}}^\dagger-f_k^*a_{\mathbf{k}})+\sum_{\mathbf{q},\sigma}(g_{q\sigma}b_{\mathbf{q}\sigma}^\dagger-g_{q\sigma}^*b_{\mathbf{q}\sigma})\right], \quad (36)$$

and repeat the procedure described in Sec. II A. For this case, the only difference in the results is in the formulas concerning the contributions from LO phonons. Equation (23) is replaced by

$$\Delta m_{\mathrm{LO}}=2\frac{\hbar^2}{m_\parallel}\sum_{\mathbf{k}}\frac{|\phi_B(k,z_0,\gamma)_{\gamma\to0}|^2k_\parallel^2\cos^2(\theta)}{\left(\hbar\omega_{L1}\overline{P}_1+\hbar\omega_{L2}\overline{P}_2+\dfrac{\hbar^2k_\parallel^2}{2m_\parallel}\right)^3}. \quad (37)$$

Equation (31) is replaced by

$$E_{\mathrm{LO}}=\sum_{\mathbf{k}}\frac{|\phi_B(k,z_0,\gamma)|^2}{\hbar\omega_{L1}\overline{P}_1+\hbar\omega_{L2}\overline{P}_2+\dfrac{\hbar^2k_\parallel^2}{2m_\parallel}}. \quad (38)$$

Equation (33) is given by

$$\phi_B(k,z_0,\gamma)$$
$$=\sum_\lambda\left\langle \zeta(z)\left|\frac{B_\lambda(z)\sin(k_z|z|)}{k}\right|\zeta(z)\right\rangle$$
$$-\frac{\gamma^3}{(\gamma^2+k_\parallel^2)^{3/2}}\left\langle \zeta(z)\left|\frac{B_{\lambda'}(z_0)\sin(k_z|z_0|)}{k}\right|\zeta(z)\right\rangle. \quad (39)$$

The corresponding results can be obtained by combining the equations in Sec. II A with Eqs. (37)–(39).

C. VCA and effective phonon-mode approximation

To obtain the various parameters of the $Al_xGa_{1-x}As$ system used in the present paper the VCA is adopted.[18] Let Q_A

TABLE I. Parameters used in computation.

Quantities	GaAs	$Al_xGa_{1-x}As$	AlAs
a (Å)	5.64[a]	$5.64(1-x)+5.66x$[b]	5.66[a]
E_Γ (eV)	1.52[a]	$1.52(1-x)+3.05x$[b]	3.05[a]
E_X (eV)	1.98[a]	$1.98(1-x)+2.36x$[a]	2.36[a]
ϵ_0	13.18[a]	$13.18(1-x)+10.06x$[b]	10.06[a]
ϵ_∞	10.89[a]	$10.89(1-x)+8.16x$[b]	8.16[a]
m (m_e)	0.067[a]	$0.067(1-x)+0.15x$[b]	0.15[a]
$\hbar\omega_L$ (meV)	36.25[c]	$36.25+1.83x+17.12x^2-5.11x^3$[d]	50.09[c]
$\hbar\omega_T$ (meV)	33.29[c]	$33.29+10.7x+0.03x^2+0.86x^3$[d]	44.88[c]

[a]Reference 19.
[b]The VCA (Refs. 18 and 19).
[c]Reference 16.
[d]The EPMA (Ref. 16).

and Q_B be the quantities associated with GaAs (A) and AlAs (B), respectively, the quantities associated with $Al_xGa_{1-x}As$ can be written as

$$Q_{Al_xGa_{1-x}As}=(1-x)A+xB. \tag{40}$$

The energy-band gap, the dielectric constants, and the electron-band mass of $Al_xGa_{1-x}As$ will be calculated using the VCA.

As for the phonon frequencies of $Al_xGa_{1-x}As$, an empirical interpolation [effective phonon-mode-approximation (EPMA)][16] is used to represent the two LO and TO modes with the respective effective one LO and TO modes. We adopt the EPMA in our calculation and give the formulas in Table I.

III. NUMERICAL RESULTS AND DISCUSSION

The Hamiltonian components Eqs. (5) and (6) are strictly suitable to the heterojunction of which the semiconductors are one-mode LO or TO phonons. Here we perform the computation on the GaAs/$Al_xGa_{1-x}As$ heterojunction adopting the EPMA to simplify the LO and TO phonon modes of the barrier material $Al_xGa_{1-x}As$. The parameters needed are listed in Table I. The band mass of the electron has been considered as isotropic: $m_\parallel=m_\perp$ since the electrons are mainly confined within GaAs.

We focus our attention on the Al concentration within the range $x_l \leqslant x \leqslant x_c$, where $x_c \approx 0.4$ is the critical value,[18] below which the $Al_xGa_{1-x}As$ is a direct band-gap semiconductor. The lower bound x_l is the point of the concentration below which we do not expect the impurity near the interface to be properly treated within the present formalism. A value of $x_l=0.2$ is used here. The barrier height V_0 needed in the computation, according to the 60:40 rule[22] in Eq. (28), is given by

$$V_0=0.6(E_{\Gamma 2}-E_{\Gamma 1})x \quad \text{for } x<x_c. \tag{41}$$

For the given Al concentration $x=0.3$ and areal electronic density $N_s=4\times10^{11}/\text{cm}^2$, the energy level of a bound polaron at ground state vs z_0 is calculated by using the displacement-oscillator transformation coupling (DOTC) and the DOT respectively. The DOT gives an energy level lower than that given by the DOTC when $z_0<30$ Å and the difference is within 2% of the energy-level height. The results are opposite when $z_0>30$ Å, but the difference is negligibly small. It indicates that the result by the DOT is more reasonable when the impurity is closer to the interface ($|z_0|<30$ Å). In Fig. 1(a), the bound-polaron binding energies E_B^A and E_B^B calculated by using the DOTC and the DOT are shown, respectively, along with the binding energy E_B^N, which excludes the influence of phonons. It can be seen that the polaronic effect always decreases the binding energy E_B. The phonon influence reaches its maximum about 7% of E_B, when the impurity is located in the channel side around $z_0=50$ Å. The offset of E_B at $z_0=0$ is due to the abruptness in the dielectric constants of the Coulomb contribution in Eq. (4).

The net-phonon contributions to E_B are defined as

$$\Delta E_{\text{LO}}=-E_{\text{LO}}\ (\text{free-polaron})+E_{\text{LO}}\ (\text{bound polaron}) \tag{42}$$

for the LO phonon mode and

$$\Delta E_{I\sigma}=-E_{I\sigma}\ (\text{free-polaron})+E_{I\sigma}\ (\text{bound polaron}) \tag{43}$$

for the σth IO phonon mode, respectively. The free-polaron results are computed in the limit of $K_\parallel=0$. ΔE_{I+} and ΔE_{I-} are given in Fig. 1(b). Both of them are negative and decay when the impurity is located far away from the interface. The LO phonon contributions ΔE_{LO}^A and ΔE_{LO}^B, respectively, by the DOTC and by the DOT, are also plotted in Fig. 1(b) for comparison. It can be seen that IO phonons give a larger contribution when the impurity is located in the barrier side, where the LO phonon contribution is small. On the other hand, both the IO and LO phonons are important and give a negative contribution when the impurity is in the channel side. The phonon contribution is due to the competition between the electron and impurity polarization. When the impurity is located in the barrier side, the LO phonon contribution to E_B is mainly from the electron-phonon coupling. The contribution is small because there is not an obvious difference of the electron-phonon interactions between before and after the bound polaron is ionized. The impurity polarization and the weakness of the phonon effect, compared to the 3D bulk GaAs, make the bound polaron become ''shallow.''

The electron-average distance to the interface $\langle z_{\text{ph}}\rangle$, $\langle z\rangle=B^2(6+4\beta+\beta^2)/b-B'^2/b'$ and the in-plane average distance between the electron and the impurity $\langle\rho_{\text{ph}}\rangle$, $\langle\rho\rangle=2/\gamma$ with and without the influence of the phonons by the DOT, as functions of the impurity position z_0, are plotted in Fig. 1(c). It shows us that $\langle\rho\rangle$ is always less than $\langle\rho_{\text{ph}}\rangle$ and that the phonon influence becomes weaker as the impurity gets near the interface. $\langle z_{\text{ph}}\rangle$ is lower than $\langle z\rangle$ when the impurity is located on the barrier side. When the impurity is on the channel side, $\langle z_{\text{ph}}\rangle>\langle z\rangle$ for $z_0<60$ Å and $\langle z_{\text{ph}}\rangle<\langle z\rangle$ for $z_0>60$ Å. Generally speaking, the phonon influence on $\langle\rho\rangle$ and $\langle z\rangle$ is small due to the weak electron-phonon, impurity-phonon coupling, and the strong confinement of the heterojunction potential.

For the given Al concentration and impurity position, both $\langle\rho_{\text{ph}}\rangle$ and $\langle z_{\text{ph}}\rangle$ monotonically decrease with increasing N_s. $\langle z_{\text{ph}}\rangle$ is less than the free-polaron value $\langle z_F\rangle$. When $x=0.3$, $\langle z_F\rangle$ decreases from 120 Å to 59 Å with increasing

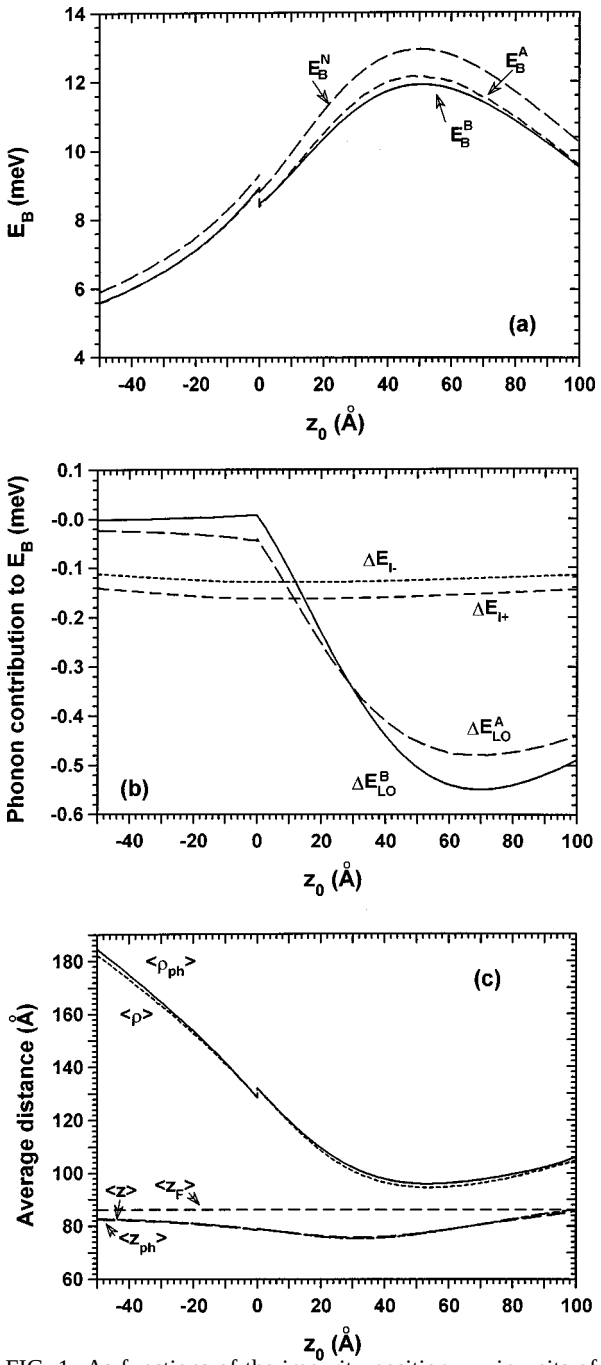

FIG. 1. As functions of the impurity position z_0, in units of Å, for a given areal-electronic density $N_s=4\times10^{11}/\mathrm{cm}^2$, the following quantities are presented corresponding to Al concentration $x=0.3$. (a) The bound-polaron binding energy E_B in units of meV. E_B^N is the result without the influence of phonons. E_B^A (E_B^B) is the result with the influence of phonons calculated by the DOTC (DOT). The effective Rydberg energy $E_R=m_1e^4/2\epsilon_{\infty1}^2\hbar^2=6.35$ meV for GaAs bulk material. (b) The phonon contribution, in units of meV, to E_B. ΔE_{I+} and ΔE_{I-} are the net contributions from IO phonon modes with higher and lower frequencies, respectively. ΔE_{LO}^A (ΔE_{LO}^B) is the net contribution from LO phonon modes calculated by the DOTC (DOT). (c) The electron-average distance to the interface $\langle z_{\mathrm{ph}}\rangle,\langle z\rangle$ and the in-plane-average distance between the electron and the impurity $\langle\rho_{\mathrm{ph}}\rangle,\langle\rho\rangle$, in units of Å, with and without the influence of phonons calculated by the DOT. The average distance of the electron to the interface $\langle z_F\rangle$ for the free-polaron case is also given for comparison. The effective Bohr radius $a_B=\epsilon_{\infty1}\hbar^2/m_1e^2=85.9$ Å for GaAs bulk material.

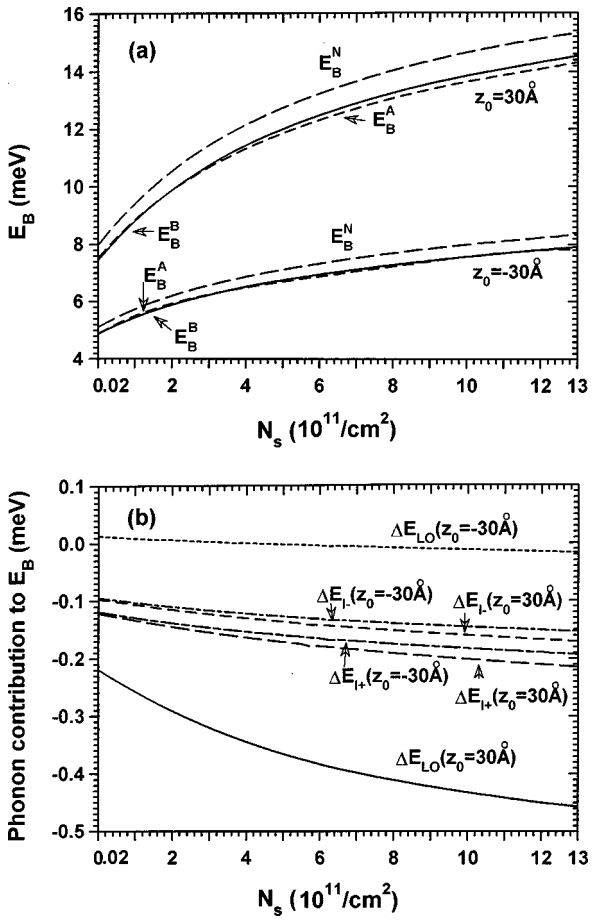

FIG. 2. As functions of the areal-electron density N_s, in units of cm^{-2}, the following quantities are given for Al concentration $x=0.3$, corresponding to the impurity position $z_0=-30$ and 30 Å, respectively. (a) The bound-polaron binding energy E_B in units of meV. E_B^N is the binding energy without the influence of phonons. E_B^A and E_B^B are the ones with the influence of phonons calculated by the DOTC and by the DOT. (b) The phonon contribution, in units of meV, to E_B calculated by the DOT. ΔE_{I+} and ΔE_{I-} are the net contributions from IO phonon modes with higher and lower frequencies, respectively. E_{LO} is that from the LO phonon modes.

N_s. However, z_{ph} decreases from 100(112) to 54(57) Å, corresponding to $z_0=30(-30)$ Å. This interface effect causes the binding energy E_B to gain a negative contribution from phonons as one increases N_s, as shown in Figs. 2(a) and 2(b) for $z_0=\pm30$ Å, respectively. In this case, the bound-polaron energy level calculated by the DOT is lower than that of the DOTC at most values of N_s. But the difference is less than 1% of the energy-level height. The binding energies E_B's calculated by the DOTC and by the DOT, respectively, are presented for comparison. It can be seen that in the contribution to E_B the IO phonon modes ($\Delta E_{I\sigma}$) play a dominant role for $z_0=-30$ Å. The difference between E_B^A and E_B^B is negligibly small.

The phonon contribution, when the impurity is located at $z_0=30$ Å decreases the binding energy, especially for large N_s, because the impurity LO phonon contribution becomes more important. At the same time, there is a non-negligible difference between the results obtained by the DOTC and by the DOT [Fig. 2(a)].

For the given $N_s=4\times10^{11}$ cm^{-2} and $z_0=-30(30)$ Å,

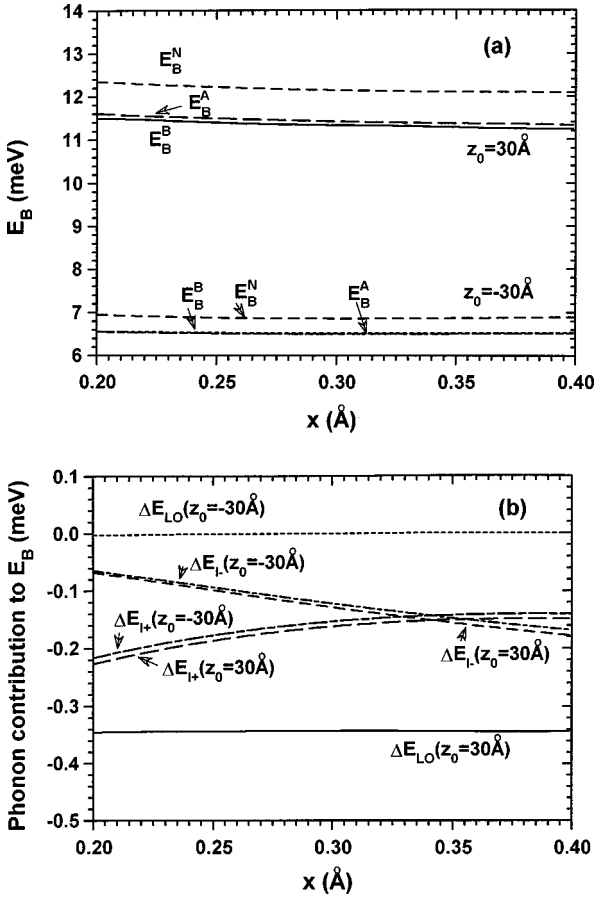

FIG. 3. As functions of Al concentration x, the following quantities are plotted for the given areal-electron density $N_s=4\times10^{11}/\mathrm{cm}^2$, corresponding to the impurity $z_0=30$ and -30 Å, respectively. (a) The bound-polaron binding energy E_B in units of meV. E_B^N is the binding energy without the influence of phonons. E_B^A and E_B^B are the ones with the influence of phonons calculated by the DOTC and the DOT, respectively. (b) The phonon contribution, in units of meV, to E_B calculated by the DOT. ΔE_{I+} and ΔE_{I-} are the net contributions from IO phonon modes with higher and lower frequencies, respectively. ΔE_{LO} is that from the LO phonon modes.

the bound-polaron energy-level height increases with x, with $\langle\rho_{\mathrm{ph}}\rangle$ and $\langle z_{\mathrm{ph}}\rangle$ decreasing slowly. Due to the small change of $\langle\rho_{\mathrm{ph}}\rangle$ and $\langle z_{\mathrm{ph}}\rangle$, and in addition to the fact that the impurity is not so close to the interface, E_B is insensitive to x. E_B, as a function of x, with and without the phonon influence is given in Fig. 3(a). For $z_0=30$ Å, both the LO and IO phonons are important to decrease the binding energy. Only the IO phonons are important for $z_0=-30$ Å, as shown in Fig. 3(b). In the contribution to E_B from the two branches of IO phonon modes, ΔE_{I+} increases and ΔE_{I-} decreases with increasing x. As a superposition result, the total contribution is insensitive to x.

In general, the polaron effect would increase with the reduction in dimensionality. For our quasi-2D system, the phonon effect is weaker in comparison with the bulk GaAs. This behavior is reminiscent of a similar result, albeit for a scattering investigation;[23] nevertheless, this surprising property needs further investigation.

The more complicated screening-effect influence on the bound-polaron properties is out of the scope of the present paper and will be the subject of future investigation.

IV. CONCLUSION

A variational theory has been developed to investigate the ground state of an optical polaron bound to a donor impurity near the interface of a polar semiconductor heterojunction. In particular, the influence of a realistic heterojunction potential is considered. A modified LLP intermediate-coupling method is adopted to deal with the electron-phonon and impurity-phonon interactions, including the effect of half-space bulk longitudinal and interface-optical phonon modes. The bound-polaron binding energy vs impurity position, depletion-electron density, and Al concentration is computed for a $\mathrm{GaAs/Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ $(0.2<x<0.4)$ heterojunction system. It is found that the impurity-phonon interaction is important and that the phonon contribution to the binding energy is negative. Both the bulk-longitudinal and interface-phonon modes give an important contribution to the binding energy when the impurity is located in GaAs. The interface-phonon modes are more important than the bulk-phonon modes when the impurity is located in $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$.

ACKNOWLEDGMENTS

S.L.B. was supported by the China Scholarship Council and cordially thanks the Department of Physics at the State University of West Georgia for the hospitality during his visit. The authors wish to thank Professor X. X. Liang and Professor X. Wang for helpful discussions.

*Permanent address: Department of Physics, Inner Mongolia University, Hohhot 010021, People's Republic of China.

[1] P. M. Platzman, Phys. Rev. **125**, 1961 (1962).
[2] Y. C. Li, L. F. Zheng, and S. W. Gu, Phys. Rev. B **38**, 4096 (1988).
[3] B. A. Mason and S. Das Sarma, Phys. Rev. B **33**, 8379 (1986).
[4] S. Sil and A. Chatterjee, J. Phys.: Condens. Matter **3**, 9401 (1991).
[5] Z. J. Shen, X. Z. Yuan, G. T. Shen, and B. C. Yang, Phys. Rev. B **49**, 11 035 (1994).
[6] M. H. Degani and O. Hipólito, Phys. Rev. B **33**, 4090 (1986).
[7] J. D. Levine, Phys. Rev. **140**, A586 (1965).
[8] M. Bhattacharya, S. Mukhopadhyay, and T. K. Mitra, Phys. Status Solidi B **120**, 555 (1983).
[9] A. Chartterjee and S. Sil, Phys. Rev. B **48**, 15 438 (1993).
[10] D. M. Hollox and P. R. Antoniewicz, Phys. Rev. B **33**, 8558 (1986).
[11] S. W. Gu and R. S. Zheng, Phys. Rev. B **36**, 3280 (1987).
[12] G. A. Farias, M. H. Degani, and O. Hipólito, Phys. Rev. B **43**, 4113 (1991).
[13] T. Ando, J. Phys. Soc. Jpn. **51**, 3900 (1982).
[14] H. Nakayama and Y. Kayanuma, Solid State Commun. **95**, 573 (1995).
[15] T. D. Lee, F. E. Low, and D. Pines, Phys. Rev. **90**, 297 (1953).
[16] S. Adachi, J. Appl. Phys. **58**, R1 (1985).
[17] X. X. Liang and J. S. Yang, Solid State Commun. **100**, 629 (1996).
[18] J. E. Hasbun, V. Singh, and L. Roth, Phys. Rev. B **35**, 2988

(1987); J. E. Hasbun and L. M. Roth, *ibid.* **37**, 2829 (1988), and references therein.
[19] J. E. Hasbun, Phys. Rev. B **52**, 11 989 (1995).
[20] S. L. Ban, X. X. Liang, and R. S. Zheng, Phys. Lett. A **192**, 110 (1994).
[21] M. H. Degani and G. A. Farias, Phys. Rev. B **41**, 3572 (1990).
[22] Y. Fu and K. A. Chao, Phys. Rev. B **43**, 4119 (1991).
[23] J. E. Hasbun and S. L. Ban, Phys. Rev. B **58**, 2102 (1998).