Polaron properties in quantum wells

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The Lee-Low-Pines variational method is used to investigate the properties of a polaron in a quantum well (QW). The electron wave function in a finite-height potential barrier has been used for the calculation. Therefore, the influence of the barrier height on the polaron properties is taken into account. GaAs/Al_xGa_{1-x}As QW is chosen as an example to calculate the polaron energy and effective mass. Our results indicate that the barrier height has an important influence on the polaron properties in a QW.

I. INTRODUCTION

Recently, various theoretical methods have been used to investigate the polaron properties in quantum well (QW) structures.[1–8] For example, Das Sarma and Stopa[1] calculated the binding energy and effective mass of an electron in a GaAs/Al_xGa_{1-x}As heterostructure by using three-dimensional (3D) bulk optical (BO) phonon modes. Comas, Trallero-Giner, and Riera[2] investigated the binding energy of a polaron in a QW only including the interaction of the electron with the confined-slab BO phonons. Degani and Hipolito[3] incorporated interface optical (IO) phonons and confined-slab BO phonons to study the polaron energy and effective mass in a heterostructure and a QW. Zheng, Ban, and Liang[4] used the Lee-Low-Pines (LLP) variational method to calculate the self-energy of a confined polaron in a QW. In all the above work, it has been assumed that the electron is confined in a QW with an infinite-height barrier. However, for most practical QW systems, a polar crystal slab is embedded in two semi-infinite substrates made of other polar material. In these systems, the electron can penetrate through the interfaces to go into the substrates. The phonons in the substrates can interact with the electron. This interaction is important for very narrow QW's because of the remarkable penetration effect. In addition, the interaction of the electron with the slab BO and IO phonons may be different from that in infinite height QW's. For example, for GaAs/Al_xGa_{1-x}As QW's when x, the Al concentration, equals 0.1, the barrier height $V=71.6$ meV.[9] If the well width $N=10$ (in units of lattice constant), the probability of the electron in the substrates is 0.32. In this case, the infinite-height QW model in which the electron is assumed to be wholly confined in the slab is obviously unrealistic. Hai, Peeters, and Devreese[5] reported a detailed investigation of the polaron properties in QW's with various potentials using the standard perturbation theory. For the finite barrier QW it is practically difficult to sum over all intermediate states in their calculation.[5] So they had to use the so-called leading-term approximation for calculation. But they found that there are not any contributions of the substrate material to the polaron energy and effective mass. Obviously this result is not satisfactory. In short, the infinite-height QW model is not adequate for a low-barrier QW. How does the barrier height of QW's affect the properties of the polaron? Is there any new phenomenon when the penetration effect is taken into account? So far there have been few reports involving the influence of barrier height on the polaron properties.

In the present paper, we use the LLP variational method[10] to calculate the polaron energy and effective mass in a QW with a finite-height barrier. In order to consider the influence of the substrate BO phonon on the polaron properties, we apply the exact electron wave function in a finite-height potential well. First, we give the general derivation of the energy and effective mass of the confined polaron. Then we give the numerical results for GaAs/Al_xGa_{1-x}As QW. Finally, we give a detailed discussion about the influences of the slab BO phonons, the IO phonons, and the substrate BO phonons on the polaron properties.

II. HAMILTONIAN

We assume that a slab with thickness $2d$ is made of a polar crystal and is surrounded by another kind of polar crystal as substrate. The linear scale of the slab in the x and y directions is taken to be much larger than $2d$. If the isotropic effective-mass approximation is adopted, the Hamiltonian of the system consisting of an electron, the BO phonons, and the IO phonons may be written as:[6]

$$H=H_e+H_{\rm ph}+H_{e-\rm BO}+H_{e-\rm IO}, \tag{1}$$

where

$$H_e=\begin{cases} -\left(\dfrac{\hbar^2}{2m_1^*}\right)\left(\dfrac{\partial^2}{\partial z^2}+\nabla_\rho^2\right), & |z|\leqslant d \\ -\left(\dfrac{\hbar^2}{2m_2^*}\right)\left(\dfrac{\partial^2}{\partial z^2}+\nabla_\rho^2\right)+V, & |z|>d \end{cases} \tag{2}$$

where m_1^* and m_2^* are the band masses of the electron in the slab and in the substrates, respectively, V is the height of the barrier, and ρ is the position vector of the electron in the x-y plane.

$$H_{\rm ph}=H_{\rm BO}^i+H_{\rm BO}^0+H_{\rm IO}, \tag{3}$$

$$H_{\rm BO}^i=\sum_{\mathbf{k},pm}\hbar\omega_{L1}\alpha_{pm}^+(\mathbf{k})\alpha_{pm}(\mathbf{k}), \tag{4}$$

$$H_{\mathrm{BO}}^{0}=\sum_{\mathbf{k},p,q}\hbar\omega_{L2}\alpha_{qp}^{+}(\mathbf{k})\alpha_{qp}(\mathbf{k}), \tag{5}$$

$$H_{\mathrm{IO}}=\sum_{\mathbf{k},p,\sigma}\hbar\omega_{\sigma}^{p}(\mathbf{k})\alpha_{p\sigma}^{+}(\mathbf{k})\alpha_{p\sigma}(\mathbf{k}), \tag{6}$$

where $\alpha_{mp}^{+}(\mathbf{k})$ and $\alpha_{mp}(\mathbf{k})$ are the creation and annihilation operators of the slab BO phonons with the frequency ω_{L1} and the wave vector $(\mathbf{k},m\pi/2d)$. $\mathbf{k}$ is the projection of the wave vector on the x-y plane. $\alpha_{qp}^{+}(\mathbf{k})$, $\alpha_{qp}(\mathbf{k})$ are the creation and annihilation operators of the substrate with frequency ω_{L2} and the wave vector $(\mathbf{k},q)$. q is the z component of phonon wave vector, and it is continuous since the substrate is infinite. $\alpha_{p\sigma}^{+}(\mathbf{k})$, $\alpha_{p\sigma}(\mathbf{k})$ are the creation and annihilation operators, respectively, of the IO phonons with the frequency ω_{σ}^{p} and the wave vector $\mathbf{k}$, where $\sigma=+$ or $-$. According to Wendler and Pechstedt's result,[6] there are four interface phonon mode corresponding frequencies, $\omega_{+}^{A},\omega_{-}^{A},\omega_{+}^{S},\omega_{-}^{S}$. The subscript p is the parity with respect to the mirror symmetry of the x-y plane for $z=0$. For BO phonons in the slab, it should be illustrated that for even parity (represented by S) m is odd, while for odd parity (represented by A), m is even. We take N as the slab thickness in units of the lattice constant a, namely, $Na=2d$. Being limited by the Brillouin-zone boundary, m may be any integer within the range $1\leqslant m\leqslant N/2$.

The IO phonon frequencies can be written as

$$\omega_{\pm}^{p}(k)=\left\{\frac{1}{2(\varepsilon_{1}^{p}+\varepsilon_{2}^{p})}\{\varepsilon_{1}^{p}(\omega_{L1}^{2}+\omega_{T2}^{2})+\varepsilon_{2}^{p}(\omega_{L2}^{2}+\omega_{T1}^{2})\pm[(\varepsilon_{1}^{p}(\omega_{L1}^{2}+\omega_{T2}^{2})+\varepsilon_{2}^{p}(\omega_{L2}^{2}+\omega_{T1}^{2}))^{2}-4(\varepsilon_{1}^{p}+\varepsilon_{2}^{p})(\varepsilon_{1}^{p}\omega_{L1}^{2}\omega_{T2}^{2}+\varepsilon_{2}^{p}\omega_{L2}^{2}\omega_{T1}^{2})]^{1/2}\}\right\}^{1/2}, \tag{7}$$

where $\varepsilon_{1}^{p}=\varepsilon_{\infty1}[1-\gamma_{p}\exp(-2kd)]$, $\varepsilon_{2}^{p}=\varepsilon_{\infty2}[1+\gamma_{p}\exp(-2kd)]$, $\gamma_{s}=1,\gamma_{A}=-1,\omega_{T1},\omega_{T2}$ are the transverse-optical phonon frequencies of the slab and the substrate, respectively, and ε_{01}, $\varepsilon_{\infty1}$, and ε_{02}, $\varepsilon_{\infty2}$ are the static and the optical dielectric constants of the slab and the substrate, respectively. $H_{e-\mathrm{BO}}$ and $H_{e-\mathrm{IO}}$ in Eq. (1) are the interaction Hamiltonians of the electron with the BO phonons and the IO phonons. We can express them in general form,

$$H_{e-i}=\sum_{i}\sum_{k}e^{i\mathbf{k}\cdot\rho}\Gamma_{i}(\mathbf{k},z)[\alpha_{i}(\mathbf{k})+\alpha_{i}^{+}(-\mathbf{k})], \tag{8}$$

where i represents various phonon modes, and $\Gamma_{i}(\mathbf{k},z)$ is the corresponding coupling functions.[6] For the slab BO phonons,

$$\Gamma_{L1}^{m}(\mathbf{k},z)=\left\{\frac{4\pi\hbar^{2}\omega_{L1}\alpha_{1}}{2Ad}\left[\frac{2\hbar\omega_{L1}}{m_{1}^{*}}\right]^{1/2}\right\}^{1/2}\times\begin{cases}0, & z>d\\ \dfrac{\sin[q_{1}^{m}(z+d)]}{\sqrt{k^{2}+(q_{1}^{m})^{2}}}, & |z|\leqslant d\\ 0, & z<-d\end{cases} \tag{9}$$

where $q_{1}^{m}=m\pi/2d$, $\alpha_{1}=(\varepsilon_{\infty1}^{-1}-\varepsilon_{01}^{-1})(m_{1}^{*}e^{4}/2\hbar^{3}\omega_{L1})^{1/2}$, and A is the interface area of the slab. Similarly, for the substrate BO phonons,

$$\Gamma_{L2}(k,q,z)=-\left\{\frac{4\pi\hbar^{2}\omega_{L2}\alpha_{2}}{V_{G}}\left[\frac{2\hbar\omega_{L2}}{m_{2}^{*}}\right]^{1/2}\right\}^{1/2}\times\begin{cases}\dfrac{\sin[q(z-d)]}{\sqrt{k^{2}+q^{2}}}, & z>d\\ 0, & |z|\leqslant d\\ \dfrac{\sin[(q(z+d)]}{\sqrt{k^{2}+q^{2}}}, & z<-d\end{cases} \tag{10}$$

where V_{G} is the volume of the substrate and $\alpha_{2}=(\varepsilon_{\infty2}^{-1}-\varepsilon_{02}^{-1})(m_{2}^{*}e^{4}/2\hbar^{3}\omega_{L2})^{1/2}$. When $d=0$ the electron-substrate-phonon interaction Hamiltonian (Wendler Hamiltonian) given by Eqs. (8) and (10) is not identical with the Frohlich Hamiltonian, since it is proportional to $\sin qz$ not e^{iqz}. The reason for the difference is that the interface confinement requires the amplitude of lattice vibration corresponding to the substrate BO phonon modes to be zero at the interfaces. Thus the interface confinements brings out an additional half-wave loss for the lattice wave. Therefore, the Wendler Hamiltonian is not wholly satisfactory when $d=0$. But if we calculate the polaron energy shifts and effective mass only to the first-order term of α_{2}, the Wendler Hamiltonian can give the same results as the Frohlich one does. Hence when $d=0$ if the high-order terms of α_{2} are ignored, the Wendler Hamiltonian can be regarded as equivalent to the Frohlich Hamiltonian. For IO phonons the coupling function is

$$\Gamma_{\pm}^{p}(\mathbf{k},z)=-\left(\frac{2\pi e^{2}\hbar}{A\omega_{\pm}^{p}(\mathbf{k})}\right)^{1/2}\frac{C_{\pm}^{p}}{k}\times\begin{cases}e^{-k(z-d)}, & z>d\\ f_{p}(k,z), & |z|\leqslant d\\ \gamma_{p}e^{k(z+d)}, & z<-d\end{cases} \tag{11}$$

where

$$C_{\pm}^{p}=\left\{\frac{k(1+\gamma_{p}e^{-2kd})}{2}\left[\frac{[\omega_{T1}^{2}-\omega_{\pm}^{p}(\mathbf{k})^{2}]^{2}[\omega_{T2}^{2}-\omega_{\pm}^{p}(\mathbf{k})^{2}]^{2}}{\varepsilon_{1}^{p}(\omega_{L1}^{2}-\omega_{T1}^{2})[\omega_{T2}^{2}-\omega_{\pm}^{p}(\mathbf{k})^{2}]^{2}+\varepsilon_{2}^{p}(\omega_{L2}^{2}-\omega_{T2}^{2})[\omega_{T1}^{2}-\omega_{\pm}^{p}(\mathbf{k})^{2}]^{2}}\right]\right\}^{1/2}, \tag{12}$$

and

$$f_S(k,z)=\frac{\cosh(kz)}{\cosh(kd)},\quad f_A(k,z)=\frac{\sinh(kz)}{\sinh(kd)}. \tag{13}$$

Certainly, we can also define a dimensionless coupling constant in analogy to the bulk polaron. That is, $\alpha_I=[m_1^*(eC_{\pm}^p)^4/8(\omega_{\pm}^p)^5\hbar^2]^{1/2}$, by which we can transform the coupling function $\Gamma_{\pm}^p(\mathbf{k},z)$ into a new form similar to that of the bulk phonon coupling function. But α_I is dependent on the wave vector $\mathbf{k}$.

From Eqs. (1)–(6) and (9)–(11) it can be seen easily that only the polaron momentum component parallel to the interface commutes with the Hamiltonian in Eq. (1). Therefore, we can define a unitary transformation U_1 which removes the coordinates ρ.

$$U_1=\exp\left\{-i\rho\left[\sum_{kmp}\mathbf{k}\alpha_{mp}^+(\mathbf{k})\alpha_{mp}(\mathbf{k})+\sum_{kp\sigma}\mathbf{k}\alpha_{p\sigma}^+(\mathbf{k})\alpha_{p\sigma}(\mathbf{k})+\sum_{kqp}\mathbf{k}\alpha_{qp}^+(\mathbf{k})\alpha_{qp}(\mathbf{k})\right]\right\}. \tag{14}$$

Obviously the transformed Hamiltonian $H_1=U_1^{-1}HU_1$ is still dependent on the electronic coordinates z through the coupling functions. Now we introduce the second unitary transformation,

$$U_2=\exp-\sum_{kmp}F_{kmp}(z)[\alpha_{mp}(\mathbf{k})-\alpha_{mp}^+(\mathbf{k})]-\sum_{kqp}G_{kq}(z)\times[\alpha_{qp}(\mathbf{k})-\alpha_{qp}^+(\mathbf{k})]-\sum_{k\sigma p}h_{k\sigma p}[\alpha_{p\sigma}(\mathbf{k})-\alpha_{p\sigma}^+(\mathbf{k})]\}, \tag{15}$$

where $F_{kmp}(z)$ and $G_{kq}(z)$, the BO phonon distribution functions, are assumed to be dependent on the electronic coordinates, z and $h_{k\sigma p}$, the distribution function of the IO phonons, is independent of z since the IO phonons have an important effect only when the electron is very close to the interfaces. The Hamiltonian H_1 can be transformed into

$$H_2=U_2^{-1}H_1U_2. \tag{16}$$

III. THE ENERGY AND EFFECTIVE MASS

The phonon part of the trial wave function of the Hamiltonian H_2 can be chosen as the vacuum state $|0\rangle$ since we only pay attention to the low-temperature limiting state, and the electron part can be chosen as the wave function of the electron in a finite-height potential well if the coupling between the electron and the phonons is very weak. The total trial wave function is taken as

$$\Psi=\Phi|0\rangle, \tag{17}$$

where

$$\Phi=\begin{cases}B_0\cos(k_ez), & |z|\leqslant d\\ B_0\cos(k_ed)\exp[-k_{e1}(|z|-d)], & |z|>d,\end{cases} \tag{18a}$$

$k_e=(2m_1^*E_0)^{1/2}/\hbar$, and $k_{e1}=[2m_2^*(V-E_0)]^{1/2}/\hbar$; the normalization constant B_0 is given by

$$B_0=\left[\frac{2k_e}{2k_ed+\sin(2k_ed)+2k_e\cos^2(k_ed)/k_{e1}}\right]^{1/2}. \tag{18b}$$

E_0 is the ground-state energy of the bare electron in the finite-height potential well and can be obtained by solving the following equation:

$$\tan(k_ed)=\left[\frac{m_1^*(V-E_0)}{m_2^*E_0}\right]^{1/2}. \tag{19}$$

The total ground-state energy of the electron-phonon system can be expressed as

$$E=\langle\Psi|H_2|\Psi\rangle. \tag{20}$$

If we diagonalize approximately the Hamiltonian H_2 to determine the phonon distribution functions, we can get two differential equations about $F_{kmp}(z),G_{kq}(z)$. But the equations are very difficult to solve.[7,8] Therefore, we use the following approximation method to determine the phonon distribution functions.[4,11] We assume the BO phonon distribution functions have the following forms:

$$F_{kmp}(z)=f_{kmp}\sin k_m(z+d), \tag{21}$$

$$G_{kq}(z)=g_{kq}\sin q(z+d), \tag{22}$$

where $k_m=m\pi/2d$ and f_{kmp},g_{kq} are independent of z; they can be determined by minimizing the energy. From the variational conditions $\delta E/\delta g_{kq}=\delta E/\delta h_{k\sigma p}=\delta E/\delta f_{kmp}=0$ we can obtain

$$f_{kmp}=-\frac{V_{kmp}\theta_1}{\left[\frac{\hbar^2k^2}{2m_1^*}+\hbar\omega_{L1}\right]\theta_1+\frac{\hbar^2k_m^2}{2m_1^*}\theta_2-\frac{\mathbf{p}_\parallel\cdot\mathbf{k}}{m_1^*}\theta_1}, \tag{23}$$

$$g_{kq}=-\frac{X_{kq}\nu_1}{\left[\frac{\hbar^2k^2}{2m_2^*}+\hbar\omega_{L2}\right]\nu_1+\frac{\hbar^2q^2}{2m_2^*}\nu_2-\frac{\mathbf{p}_\parallel\cdot\mathbf{k}}{m_2^*}\nu_1}, \tag{24}$$

$$h_{k\sigma S}=-\frac{W_{k\sigma S}}{\left[\frac{\hbar^2k^2}{2m_1^*}\xi_1+\frac{\hbar^2k^2}{2m_2^*}\xi_2\right]+\hbar\omega_{\sigma p}-\hbar\mathbf{p}_\parallel\cdot\mathbf{k}\left(\frac{\xi_1}{m_1^*}+\frac{\xi_2}{m_2^*}\right)}, \tag{25}$$

$$h_{k\sigma A}=0, \tag{26}$$

where

$$\theta_1=\int_{\text{slab}}\sin^2k_m(z+d)\Phi^2dz,$$

$$\theta_2=\int_{\text{slab}}\cos^2k_m(z+d)\Phi^2dz,$$

$$\nu_1=\int_{\text{sub}}\sin^2q(z+d)\Phi^2dz,$$

$$\nu_2=\int_{\text{sub}}\cos^2q(z+d)\Phi^2dz,$$

$$\xi_1=\int_{\text{slab}}\Phi^2dz,\quad \xi_2=\int_{\text{sub}}\Phi^2dz,$$

$$W_{k\sigma S}=\int_{-\infty}^{\infty}\Gamma_\sigma^S(\mathbf{k},z)\Phi^2dz,$$

$$V_{kmp}=\left\{\frac{4\pi\hbar^2\omega_{L1}\alpha_1}{2Ad(k^2+k_m^2)}\left[\frac{2\hbar\omega_{L1}}{m_1^*}\right]^{1/2}\right\}^{1/2},$$

$$X_{kq}=\left\{\frac{4\pi\hbar^2\omega_{L2}\alpha_2}{V_G(k^2+q^2)}\left[\frac{2\hbar\omega_{L2}}{m_2^*}\right]^{1/2}\right\}^{1/2},$$

and $\mathbf{p}_\parallel$ is the component of the polaron momentum in the x-y plane. We can assume that $\mathbf{p}_\parallel$ is very small since we are only interested in the slow electron. Therefore, we expand f_{kmp}, g_{kq}, and $h_{k\sigma S}$ into power series of $\mathbf{p}_\parallel$, and substitute them into Eq. (20). Now we can obtain the total polaron energy:

$$E=E_0+\Delta E_{\text{slab}}+\Delta E_{\text{sub}}+\Delta E_{\text{IO}}+\frac{\mathbf{p}_\parallel^2}{2M},\tag{27}$$

where ΔE_{slab}, ΔE_{sub}, and ΔE_{IO} are the polaron energy shifts in QW's due to the interaction of the electron with the slab BO phonons, the substrate BO phonons, and the IO phonons, respectively, and M is the effective mass of the polaron:

$$\Delta E_{\text{slab}}=-\sum_{kmp}\frac{V_{kmp}^2\theta_1^2}{\left[\frac{\hbar^2k^2}{2m_1^*}+\hbar\omega_{L1}\right]\theta_1+\frac{\hbar^2k_m^2}{2m_1^*}\theta_2},\tag{28}$$

$$\Delta E_{\text{sub}}=-\sum_{kq}\frac{X_{kq}^2\nu_1^2}{\left[\frac{\hbar^2k^2}{2m_2^*}+\hbar\omega_{L2}\right]\nu_1+\frac{\hbar^2q^2}{2m_2^*}\nu_2},\tag{29}$$

$$\Delta E_{\text{IO}}=-\sum_{k\sigma}\frac{W_{k\sigma S}^2}{\left[\frac{\hbar^2k^2}{2m_1^*}\xi_1+\frac{\hbar^2k^2}{2m_2^*}\xi_2\right]+\hbar\omega_\sigma^S},\tag{30}$$

$$\frac{1}{M}=\frac{\xi_1}{m_1^*}+\frac{\xi_2}{m_2^*}-\eta_1-\eta_2-\eta_3,\tag{31}$$

$$\eta_1=\sum_{kmp}\frac{2V_{kmp}^2\theta_1^4\hbar^2k^2\cos^2\beta}{\left[\left(\frac{\hbar^2k^2}{2m_1^*}+\hbar\omega_{L1}\right)\theta_1+\frac{\hbar^2k_m^2}{2m_1^*}\theta_2\right]^3m_1^{*2}},\tag{32}$$

$$\eta_2=\sum_{kq}\frac{2X_{kq}^2\nu_1^4\hbar^2k^2\cos^2\beta}{\left[\left(\frac{\hbar^2k^2}{2m_2^*}+\hbar\omega_{L2}\right)\nu_1+\frac{\hbar^2q^2}{2m_2^*}\nu_2\right]^3m_2^{*2}},\tag{33}$$

$$\eta_3=\sum_{k\sigma}\frac{2W_{k\sigma S}^2\hbar^2k^2\cos^2\beta\left[\frac{\xi_1}{m_1^*}+\frac{\xi_2}{m_2^*}\right]^2}{\left[\left(\frac{\hbar^2k^2}{2m_1^*}\xi_1+\frac{\hbar^2k^2}{2m_2^*}\xi_2\right)+\hbar\omega_\sigma^S\right]^3},\tag{34}$$

where β is the angle between $\mathbf{p}_\parallel$ and $\mathbf{k}$. When the well width tends to infinity, the electron energy E_0 tends to zero, and k_ed tends to $\pi/2$ [Eq. (19)], hence $\theta_1=\theta_2=1$. From Eq. (28) we can easily find that ΔE_{slab} and M tend to their 3D limiting value of the slab material. When the well width $N=0$, ΔE_{slab} and ΔE_{IO} are both equal to zero since $\theta_1=\theta_2=W_{k\sigma S}=0$, but ΔE_{sub} is equal to the 3D value of the substrate material since $\nu_1=\nu_2=1$ [see Eq. (29)]. Similarly, $\eta_1=\eta_3=0$ for $N=0$; hence the polaron effective mass reaches the 3D value of the substrate material. This result is reasonable since the QW has become an infinite polar crystal of the substrate material when the well width is zero. The infinite-height barrier model concludes that when N tends to zero, ΔE_{slab} tends to zero and ΔE_{IO} tends to the 2D limiting value of the slab material, which does not conform obviously to the actual situation of the QW system. To sum up, when $N=0$ and $N=\infty$ the correct limiting values of the polaron energy and effective mass have been obtained analytically, which indicates that our choice of the variational parameters is reasonable.

If we replace the electron wave function in Eqs. (28)–(34) by that of its first excited state, we can obtain the polaron properties for the electron in the first excited state. The difference of polaron energies for the electron in the ground state and the first excited state is interesting since it can be directly measured by experiment. The bare electron first excited state wave function is

$$\Phi_1=\begin{cases}B_1\sin(k_ez), & |z|\leqslant d\\ \tau B_1\sin(k_ed)\exp[-k_{e1}(|z|-d)], & |z|>d\end{cases}\tag{35}$$

where $\tau=1$ for $z>0$ and $\tau=-1$ for $z<0$. The electron energy E_1 in the bound first excited state can be determined by

$$-\left[\frac{m_1^*(V-E_1)}{m_2^*E_1}\right]^{1/2}=\cot\left[\frac{(2m_1^*E_1)^{1/2}d}{\hbar}\right].\tag{36}$$

IV. THE RESULT AND DISCUSSION

In order to understand the details of the polaron properties in a QW, we choose the GaAs/Al_xGa_{1-x}As QW as a typical example to perform our numerical calculation. All parameters used in the calculation are taken from Ref. 5. $\alpha=0.068$ for GaAs, for $Ga_xAs_{1-x}Al$ α is dependent on the Al concentration x, $\alpha=0.068+0.058x$.[12] Obviously, the barrier height of the GaAs/Al_xGa_{1-x}As QW is dependent on x. Lee *et al.*[9] give the variation of the band gap with x. According to the assumption of Sanders and Bajaj,[13] the well potential profiles for the electron are obtained by assuming that 60% of the band-gap variation is accommodated by the conduction band. We have

$$V=0.6\times(1.155x+0.37x^2)eV.\tag{37}$$

From Eqs. (28)–(30) we can calculate ΔE_{slab}, ΔE_{sub}, and ΔE_{IO}, respectively. The total polaron energy shift $\Delta E=\Delta E_{\text{slab}}+\Delta E_{\text{sub}}+\Delta E_{\text{IO}}$. From Eqs. (31)–(34) we can obtain the numerical result of the polaron effective mass M.

The energy shift ΔE_{slab} as a function of the well width N (in units of the lattice constant a of GaAs and $a=0.5654$ nm) is plotted in Fig. 1. We have also given the result of ΔE_{slab} obtained by the infinite-height QW model in Fig. 1 for comparison. First, we can find that the absolute value of ΔE_{slab} for the finite-height QW model is obviously smaller than that

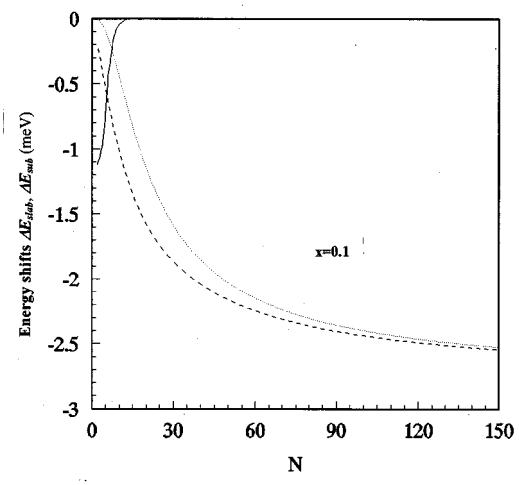

FIG. 1. Polaron energy shifts ΔE_{slab} as functions of the well width N for GaAs/Al_xGa_{1-x}As QW with $x=0.1$. Dotted and dashed curves correspond to the results of the finite- and infinite-height potential well models, respectively. The solid curve represents the energy shift ΔE_{sub}.

obtained by the infinite-height QW model when $N<60$. The more narrow the QW, the more apparent the difference is. This is due to the probability that the electron in the slab is smaller than that of the infinite-height QW (for infinite-height QW the electron is wholly confined in the slab). When the QW is very wide, the ground-state energy of the bare electron is very close to the well bottom. So the electron is almost wholly confined in the slab. The two results of ΔE_{slab} (infinite- and finite-height barrier models) are almost identical. Second, from Fig. 1 we can also find that ΔE_{slab} tends to the 3D limiting value ($\alpha_1\hbar\omega_{L1}=2.46$ meV) when the well is very wide. In Fig. 1 we also give the change of the energy shift ΔE_{sub} with N. It can be found that ΔE_{sub} is important only for very small N.

The total polaron energy shifts ΔE corresponding to $x=0.1$, 0.3, and 0.45, respectively, are showed in Fig. 2 (we

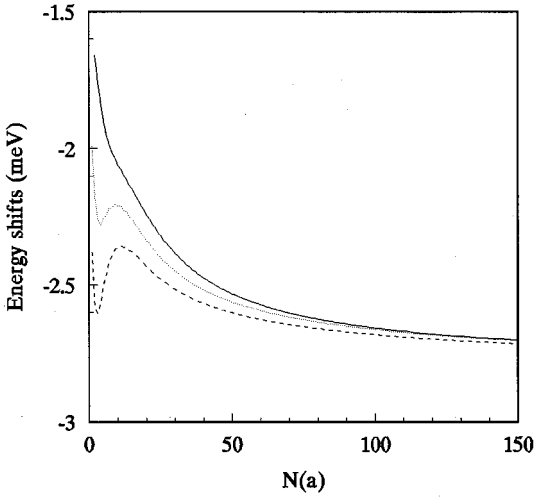

FIG. 2. The total polaron energy shifts as functions of the well width N. Solid, dotted, and dashed curves correspond to the results for $x=0.1$, 0.3, and 0.45, respectively.

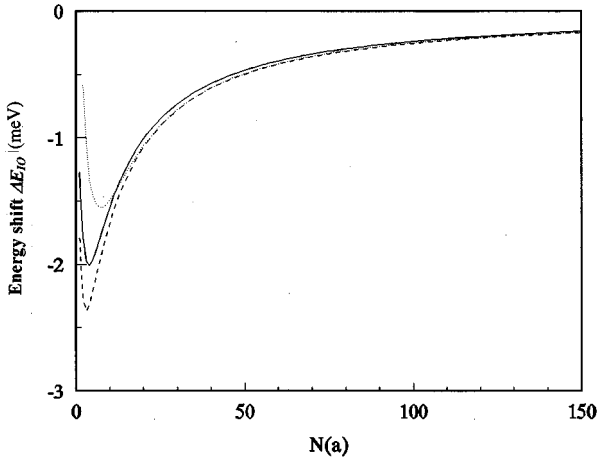

FIG. 3. The energy shifts ΔE_{IO} as functions of the well width N. The solid, dashed, and dotted curves correspond to the results for $x=0.3$, 0.45, and 0.1, respectively.

limit our discussion within the range $x\leqslant 0.45$ since the substrate is not a direct gap semiconductor when $x>0.45$). The three curves are different when N is small. When $x=0.45$ the total energy shift is approximately constant in spite of the small fluctuation when N is very small. The main reason is the dramatic influence of the Al concentration in the substrate material on ΔE_{IO}. We have given ΔE_{IO} as a function of the well width N in Fig. 3. We can find from Fig. 3 that ΔE_{IO} is very small for small x (e.g., $x=0.1$). When x becomes small the difference between the slab and the substrate material is not very remarkable. It is reasonable that the influence of IO phonon modes on the confined polaron properties becomes weak. When $x=0.1$, ΔE_{slab} is the dominant contribution to the total energy shift. Therefore, with the decrease of N the total energy shift tends to zero. When $x=0.45$, ΔE_{IO} and ΔE_{slab} are comparable if the QW is not very wide. When N becomes very small the decrease of the absolute value of ΔE_{slab} is complemented by the contribution of the IO phonons. Therefore, the total energy shift is ap-

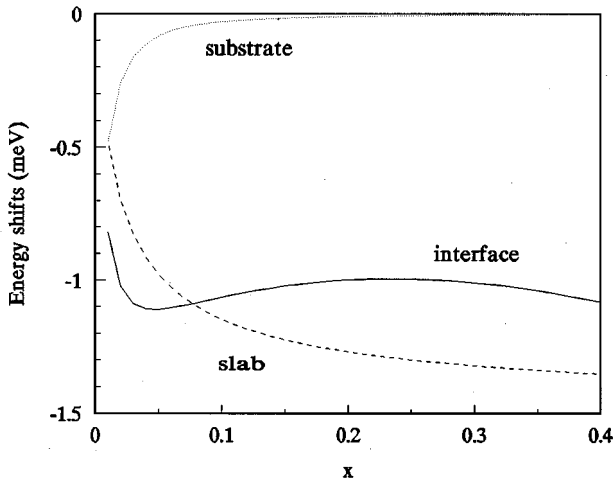

FIG. 4. The energy shifts as functions of x for the well width $N=20$.

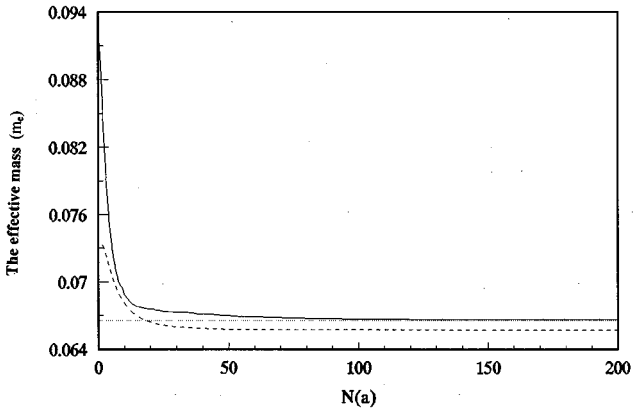

FIG. 5. The polaron effective mass as a function of the well width for $x=0.3$. The dotted line represents the 3D value. The dashed line represents the electron bare mass as a function of the well width.

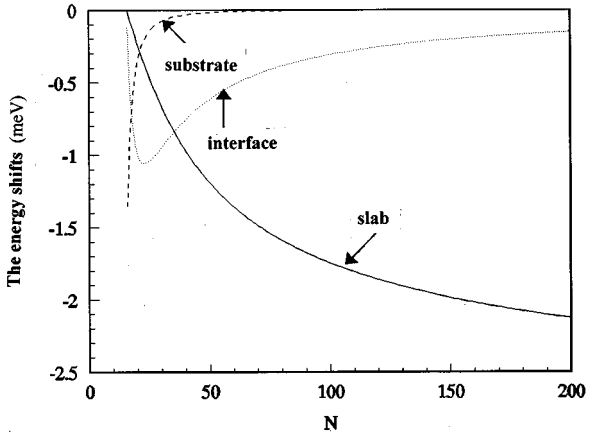

FIG. 7. The polaron energy shifts ($x=0.1$) for the electron in the first excited state versus the well width.

proximately constant for $x=0.45$. From Fig. 3, we can also find that the curve of ΔE_{IO} has a minimum at a certain N, which has also been obtained by Hai, Peeters, and Devreese[5] although a different theoretical model was used in their work. On one hand, the interface effect becomes obvious with the decrease of N; on the other hand, the electron can easily penetrate the interface for small N, which may lower the effect of IO phonons on the polaron properties. The two competitive factors may cause the occurrence of the minimum on the ΔE_{IO} curves.

In Fig. 4 we give the changes of the energy shifts with x for well width $N=20$. With the decrease of x (the barrier height V becomes small), ΔE_{slab} becomes small; in contrast with that, ΔE_{sub} becomes large since the probability of the electron in the substrate material is enlarging and comparable with that in the slab. The change of ΔE_{IO} with x is complicated since x influences not only the barrier height but also the coupling function of the electron with the IO phonons.

In Fig. 5 we give the effective mass of the polaron in a QW as a function of the well width N. In Eq. (31), η_1, η_2, and η_3 represent the contribution of the electron-phonon interaction to the polaron effective mass. The reciprocal of the term $\xi_1/m_1^*+\xi_2/m_m^*$ is the bare mass of the electron in the QW, and the bare mass is a combination of the two band masses of the electron in the slab and the substrate. Therefore, the electron bare mass changes with the well width due to the electron penetration effect. We also plot the electron bare mass as a function of N ion order to show more obviously the polaron effect. From Fig. 5 it can easily be found that (1) due to the electron-phonon interaction the effective mass of the polaron is larger than the electron bare mass and when N is small the difference is very obvious; (2) the effective mass of the confined polaron tends to the 3D limiting value when N is very large; on the other hand, when N is small the effective mass becomes larger than the 3D limiting value. This is due to the fact that the IO phonon effect is dominant for small N (Fig. 6). Considering the 3D polaron effective mass of the substrate material, $M_2=m_2^*(1+\alpha_2/6)=0.093m_e$ (for $x=0.3$).[14] We can find in Fig. 5 the polaron effective mass tends to M_2 indeed, which coincides wit the above analytical conclusion. In Fig. 6 we give the contributions of the slab BO phonons, the substrate BO

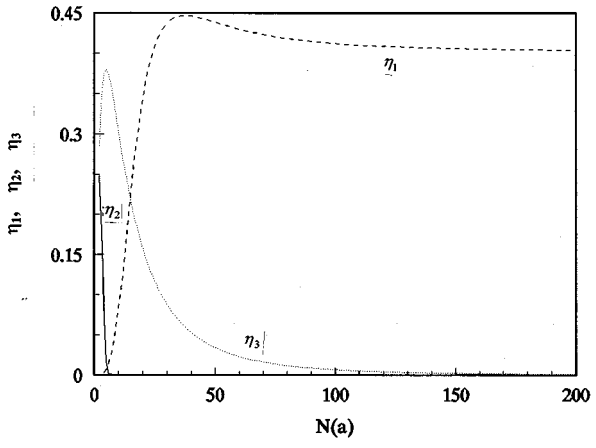

FIG. 6. The contributions of the three phonon modes to the effective mass of the polaron for $x=0.3$. The solid, dashed, and dotted curves represent the contributions of the bulk phonon in the substrate, slab, and interface phonon, respectively.

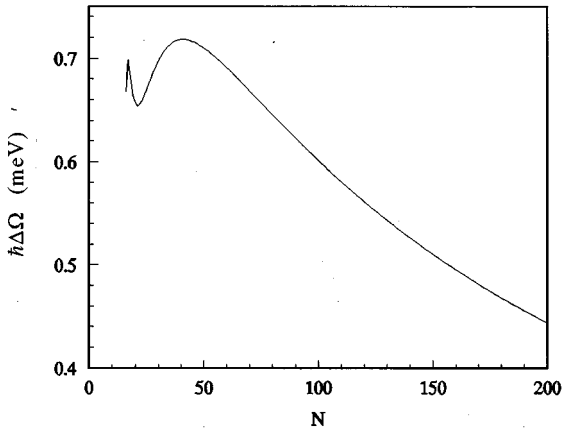

FIG. 8. The polaron correction to the electron energy-level difference ($x=0.1$).

phonons, and the IO phonons to the effective mass. From Fig. 6 we also can find that η_3, the interface contribution to the polaron effective mass, diminishes for very small N, but η_2 increases rapidly with the decrease of N. It is just the effect of η_2 guarantees the growth of the polaron effective mass as N approaches zero.

Using Eqs. (35) and (36), we can calculate the polaron energy shifts for the electron in the first excited state. In Fig. 7 we plot these energy shifts versus the well width N. We can find from Fig. 7 that the absolute values of the energy shifts $\Delta E_{\rm sub}$ and $\Delta E_{\rm IO}$ are larger, but that of $\Delta E_{\rm slab}$ is smaller, than those for the electron in the ground state. This implies that the electron penetration effect becomes more obvious when the electron is in the first excited state. E_1, the unperturbed electron energy in the first excited state, can be determined numerically by solving Eq. (36). When $[(2m_1^* V)^{1/2}/\hbar]d \leqslant \pi/2, E_1$ is higher than the height of the barrier. There fore, under this condition the bound first-excited state does not exist, and the electron energy spectrum will be continuous. We define the special well width as the threshold N_m. Only when $N > N_m$, the first-excited state is the bound state. For example, when $x=0.1$ and $V=71.3$ meV, $N_m=15$. The polaron ground-state energy $E_p^0 = E_0 + \Delta E_0$ and the first excited state energy $E_p^1 = E_1 + \Delta E_1$. They are functions of the well width. The polaron energy difference between two levels can be measured directly. And the polaron effect can give a correction to the electron energy difference by

$$\hbar \Delta\Omega = (E_p^1 - E_p^0) - (E_1 - E_0), \tag{38}$$

which is plotted in Fig. 8. It can be seen that $\hbar\Delta$ changes obviously with N, and has an oscillatory character for small-size QW.

In conclusion, we have used the LLP variational method to study the polaron properties in a QW with finite-height barrier. We find that (1) the contributions of the slab BO phonons and the IO phonons to the polaron properties is obviously dependent on the barrier height and very different from the results obtained by the infinite-height QW model. (2) The effect of the substrate phonons is important only when the QW is very narrow. (3) There is a threshold, N_m, of the well width. When the well width $N < N_m$, there is no bound excited state. Therefore, there is no discrete optical spectral line corresponding to the electron transition. The electron penetration effect is more obvious for the first excited state.

APPENDIX

Now we give the closed form of the Hamiltonian H_2 when $|z| \leqslant d$,

$$\begin{aligned} H_2 = {} & \frac{1}{2m_1^*}\left\{ \hat{P}_z^2 - i\hbar \sum_{kmp} [\alpha_{mp}^+(\mathbf{k}) - \alpha_{mp}(\mathbf{k})]\left(\frac{\partial F_{kmp}}{\partial z}\hat{P}_z + \hat{P}_z \frac{\partial F_{kmp}}{\partial z} \right) + \hbar^2 \left[\sum_{kmp} [\alpha_{mp}^+(\mathbf{k}) - \alpha_{mp}(\mathbf{k})]\left(\frac{\partial F_{kmp}}{\partial z} \right) \right]^2 \right\} \\ & + \frac{1}{2m_1^*}\left\{ \hat{P}_\parallel - i\hbar \sum_{kmp} \mathbf{k}[\alpha_{mp}^+(\mathbf{k}) + F_{kmp}][\alpha_{mp}(\mathbf{k}) + F_{kmp}] - i\hbar \sum_{k\sigma p} \mathbf{k}[\alpha_{p\sigma}^+(\mathbf{k}) + h_{k\sigma p}][\alpha_{p\sigma}(\mathbf{k}) + h_{k\sigma p}] \right\}^2 \\ & + \sum_{kmp} \hbar\omega_{L1}[\alpha_{mp}^+(\mathbf{k}) + F_{kmp}][\alpha_{mp}(\mathbf{k}) + F_{kmp}] + \sum_{k\sigma p} \hbar\omega_{\sigma p}[\alpha_{p\sigma}^+(k) + h_{k\sigma p}][\alpha_{p\sigma}(k) + h_{k\sigma p}] \\ & + \sum_{kmp} [\Gamma_{L1}^m \alpha_{mp}(\mathbf{k}) + \Gamma_{L1}^m \alpha_{mp}^+(\mathbf{k}) + 2F_{kmp}^2] + \sum_{k\sigma p} [\Gamma_\sigma^p \alpha_{p\sigma}(\mathbf{k}) + \Gamma_\sigma^p \alpha_{p\sigma}^+(\mathbf{k}) + 2h_{k\sigma p}^2], \end{aligned} \tag{A1}$$

when $|z| > d$

$$\begin{aligned} H_2 = {} & \frac{1}{2m_2^*}\left\{ \hat{P}_z^2 - i\hbar \sum_{kqp} [\alpha_{qp}^+(\mathbf{k}) - \alpha_{qp}(\mathbf{k})]\left(\frac{\partial G_{kq}}{\partial z}\hat{P}_z + \hat{P}_z \frac{\partial G_{kq}}{\partial z} \right) + \hbar^2 \left[\sum_{kqp} [\alpha_{qp}^+(\mathbf{k}) - \alpha_{qp}(\mathbf{k})]\left(\frac{\partial G_{kq}}{\partial z} \right) \right]^2 \right\} \\ & + \frac{1}{2m_2^*}\left[\hat{P}_\parallel - i\hbar \sum_{kqp} \mathbf{k}[\alpha_{qp}^+(\mathbf{k}) + G_{kq}][\alpha_{qp}(\mathbf{k}) + G_{kq}] - i\hbar \sum_{k\sigma p} \mathbf{k}[\alpha_{p\sigma}^+(\mathbf{k}) + h_{k\sigma p}][\alpha_{p\sigma}(k) + h_{k\sigma p}] \right]^2 \\ & + \sum_{kqp} \hbar\omega_{L2}[\alpha_{qp}^+(\mathbf{k}) + G_{kq}][\alpha_{qp}(\mathbf{k}) + G_{kq}] + \sum_{k\sigma p} \hbar\omega_{\sigma p}[\alpha_{p\sigma}^+(\mathbf{k}) + h_{k\sigma p}][\alpha_{p\sigma}(\mathbf{k}) + h_{k\sigma p}] \\ & + \sum_{kqp} [\Gamma_{L2}\alpha_{qp}(k) + \Gamma_{L2}\alpha_{qp}^+(\mathbf{k}) + 2G_{kq}^2] + \sum_{k\sigma p} [\Gamma_\sigma^p \alpha_{p\sigma}(\mathbf{k}) + \Gamma_\sigma^p \alpha_{p\sigma}^+(\mathbf{k}) + 2h_{k\sigma p}^2]. \end{aligned} \tag{A2}$$

Obviously the Hamiltonian H_2 includes the one-order terms, the two-order terms, and the high-order terms of the phonon operators. Therefore if we made the coefficient of the one-order terms equal to zero, we can only quasidiagonalize the Hamiltonian H_2 since there are still the high-order terms. Fortunately for the weak coupling case, the high-order term can be ignored.[15,16] To make the coefficient of the one-order terms equal to zero we can obtain two differential equations:

$$-\frac{d^2F_{kmp}}{dz^2}-\frac{1}{|\Phi|^2}\frac{d|\Phi|^2}{dz}\frac{dF_{kmp}}{dz}+\left[k^2+\frac{2m_1^*\omega_{L1}}{\hbar}\right]F_{kmp}=\frac{2m_1^*}{\hbar^2}\Gamma_{L1}^m \tag{A3}$$

$$-\frac{d^2G_{kq}}{dz^2}-\frac{1}{|\Phi|^2}\frac{d|\Phi|^2}{dz}\frac{dG_{kq}}{dz}+\left[k^2+\frac{2m_2^*\omega_{L2}}{\hbar}\right]G_{kq}=\frac{2m_2^*}{\hbar^2}\Gamma_{L2}. \tag{A4}$$

But the two equations are very difficult to solve. Therefore, we have to use the approximate method to determine the variational parameters.

The Hamiltonians (A1) and (A2) include the one-order, two-order, and high-order terms of the phonon creation or annihilation operator. The one-order terms can be eliminated by the suitable choice of the variational parameters. In the present paper only the double linear terms are considered for the calculation of the polaron energy and effective mass, and we have obtained the correct limiting values for well width $N=0$ and ∞. In fact, the high-order terms also have their contribution to the polaron properties though it is smaller than that of the linear terms. The high-order terms can be regarded as perturbation for the further calculation. Here we only take an extreme case, i.e., $d=0$, as an example for the perturbation calculation.

When $d=0$, the bare electron wave function can be taken as the plane wave form. The double-phonon term in Hamiltonian (A2) is

$$H'=\frac{\hbar^2}{2m_2^*}\sum_{kqp}\mathbf{k}\cdot\alpha_{qp}^+(\mathbf{k})G_{kq}(z)\cdot\sum_{k'qp}\mathbf{k}'\cdot\alpha_{qp}^+(\mathbf{k}')G_{k'q}(z)+\frac{\hbar^2}{2m_2^*}\sum_{kqp}q\cdot\alpha_{qp}^+(\mathbf{k})\frac{\partial G_{kq}(z)}{\partial z}\cdot\sum_{k'qp}q'\cdot\alpha_{qp}^+(\mathbf{k}')\times\frac{\partial G_{k'q'}(z)}{\partial z}+\mathrm{Hc}. \tag{A5}$$

The contribution of the double-phonon term to the polaron energy is given by the second-order perturbation theory,

$$\Delta E'=-\left(\frac{\hbar^2}{2m_2^*}\right)^2\sum_{kq}\sum_{k'}\frac{(\mathbf{k}\cdot\mathbf{k}'+q^2)^2(g_{kq}g_{k'q})^2}{2\hbar\omega_{L2}+\frac{\hbar^2}{2M_2}(\mathbf{k}+\mathbf{k}')^2}. \tag{A6}$$

As noted in Sec. II, when $d=0$ the QW system becomes an infinite semiconductor which can be described by the well-known Frohlich Hamiltonian. We give the expression of the second-order contribution to the polaron energy by using the Frohlich Hamiltonian[17]

$$\Delta E'=-\left(\frac{\hbar^2}{2m_2^*}\right)^2\times\sum_{kq}\sum_{k'q'}\frac{(\mathbf{k}\cdot\mathbf{k}'+q\cdot q')^2|f(\mathbf{k},q)|^2|f(\mathbf{k}',q')|^2}{2\hbar\omega_{L2}+\frac{\hbar^2}{2M_2}(\mathbf{k}+\mathbf{k}')^2+\frac{\hbar^2}{2M_2}(q+q')^2}, \tag{A7}$$

where $f(\mathbf{k},q)$ is the 3D variational parameter. By comparing Eqs. (A6) and (A7), we can find that the second-order-term contributions to the polaron energy obtained by the Wendler Hamiltonian and the Frohlich Hamiltonian are obviously different. Therefore, when the well width is zero the Wendler Hamiltonian used by us is not identical with the Frohlich Hamiltonian though they can give the same result if the high-order terms are ignored.

[1] S. Das Sarma and M. Stopa, Phys. Rev. B **36**, 9595 (1987).
[2] F. Comas, C. Trallero-Giner, and R. Riera, Phys. Rev. B **39**, 5907 (1989).
[3] M. H. Degani and O. Hipolito, Phys. Rev. B **35**, 7717 (1987).
[4] R. S. Zheng, S. L. Ban, and X. X. Liang, Phys. Rev. B **49**, 1796 (1994).
[5] G. Q. Hai, F. M. Peeters, and J. T. Devreese, Phys. Rev. B **42**, 11 063 (1990).
[6] L. Wendler and R. Pechstedt, Phys. Status Solidi B **141**, 129 (1987).
[7] J. Sak, Phys. Rev. B **6**, 3981 (1972).
[8] D. Ninno and G. Iadonisi, Phys. Rev. B **38**, 3803 (1988).
[9] H. J. Lee, L. Y. Juravel, J. C. Wolley, and A. J. Springthorpe, Phys. Rev. B **21**, 659 (1980).
[10] T. D. Lee, F. E. Low, and D. Pines, Phys. Rev. **90**, 297 (1953).
[11] E. Evans and D. L. Mills, Phys. Rev. B **8**, 4004 (1973).
[12] S. Adachi, J. Appl. Phys. **58**, R1 (1985).
[13] G. D. Sanders and K. K. Bajaj, Phys. Rev. B **36**, 4849 (1987).
[14] J. Callaway, *Quantum Theory of the Solid State*, 2nd ed. (Academic, New York, 1991), p. 711.
[15] S.-W. Gu, Y.-C. Li, and L.-F. Zheng, Phys. Rev. B **39**, 1346 (1989).
[16] E. Haga, Prog. Theor. Phys. (Jpn.) **11**, 449 (1954).
[17] D. Pines, *Polarons and Excitons* (Plenum, New York, 1963).