Polarons in quasi-two-dimensional structures

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A theory of quasi-two-dimensional (2D) polarons in semiconductor quantum wells is presented. We have derived analytical expressions for the energy-gap shift and effective polaron mass in the small-well-width limit. The analytical results agree exactly with those obtained for an ideal 2D system in the limit of zero well width. For larger quantum-well widths, we have numerically evaluated the values for the energy-gap shift and effective mass of a polaron.

I. INTRODUCTION

There is currently great interest in the study of electron-phonon interaction in semiconductor quantum-well structures.[1-4] This is because of the effect of lattice vibrations on the physical properties of low-dimensional systems which are known for industrial applications[5-7] in optoelectronic devices. The usual materials for fabricating the semiconductor quantum-well structures are weakly ionic III-V compounds such as GaAs-$Al_xGa_{1-x}As$ in which the interaction of electrons with optical phonons is an important mechanism that needs to be studied in detail.

It is well established[8] that when an electron becomes surrounded by phonons due to the distortion of lattice induced by the electric field of the electron, a polaron is formed. The subsequent behavior of the electron accompanied by phonons (polaron) is then modified depending on its strength of interaction with the phonon cloud. It is also well established[9] that the energy of a polaron is lower and its effective mass heavier than those of a free electron in bulk crystals. In a semiconductor quantum well, the thickness of the well layer is comparable to the de Broglie wavelength λ, confining polarons to a very thin layer. Hence their transport essentially becomes two dimensional with characteristics not exhibited in bulk semiconductors. The study of the properties of a polaron modified by its confinement in a quantum well and the relation between polarons in two- and three-dimensional systems have been investigated in the last few years.[10,11] Devreese[10] has reviewed the behavior of two-dimensional as well as three-dimensional polarons. In this paper we present the calculation of the effective mass and energy of polarons in a quantum well as functions of the quantum-well width. Using a unitary transformation, first we diagonalize the Hamiltonian consisting of the electron, phonon, and electron-phonon interaction energy operators in a quasi-two-dimensional (2D) system, and then we calculate the energy of a polaron using variational methods.

A rigorous treatment of the electron-phonon interaction involves an accurate determination of the various phonon normal modes which exist within a quantum well. As has been shown by several researchers,[2,4,12] there is a variety of phonon modes arising from the anisotropy of quantum wells, e.g., bulklike phonon modes,[13] slab modes,[11] and interface or surface modes[13] which exist in a GaAs-$Al_xGa_{1-x}As$ system. It is important to note that although various phonon modes have been used to treat the problem of electron-phonon interaction in quasi-two-dimensional systems, the results have not been consistent with each other,[13] especially for the well width dependence of the electronic properties. In this paper we have assumed that the coupling of confined electrons to bulk phonons plays the dominant role, and that the bulk phonons are unaffected by the one-dimensional potentials of a quantum-well system. The contribution of the slab phonon modes is assumed to be negligible. This is justified because the interactions of electrons with bulklike phonons is the most important one as the lattice and dielectric constants of GaAs and $Al_xGa_{1-x}As$ are nearly the same. It is further supported by Mori and Ando,[2] who have applied a sum rule which states that the sum of interactions of an electron with the various phonon modes is approximately the same as the interaction with the bulk phonon modes. Thus it is expected that the simple bulk-phonon model should project the dependence of polaron properties on the quantum-well width quite accurately. The energy of a polaron thus calculated here is found to be lower than that of a free electron, and it depends on the quantum-well width. The effective mass of a polaron in a quantum well is found to increase in comparison with that of a free electron, and is also a function of the quantum-well width.

II. ENERGY OF POLARON IN A QUANTUM WELL

The electron wave function in a quantum well differs from that in the bulk because of the effects of the confinement. The state vector of an electron interacting with phonons in a quantum well can be expressed as $|\mathbf{K}_\parallel, m; n(\mathbf{q})\rangle$ which describes an energy state m of an electron with linear momentum $\hbar\mathbf{K}_\parallel$ in the XY plane interacting with optical phonons, $|n(\mathbf{q})\rangle = |n_{q_1}, n_{q_2}, \ldots\rangle$ is the phonon state vector, and n_q is the occupation number of phonons. Here we consider that the XY plane is the plane of confinement, and all vectors in this plane are denoted with a subscript $\parallel$.

The energy of a quasi-2D polaron can be calculated by

solving the following Schrödinger equation:

$$\hat{H}|\mathbf{K}_{\parallel},m;n(\mathbf{q})\rangle = E(\mathbf{K}_{\parallel},m)|\mathbf{K}_{\parallel},m;n(\mathbf{q})\rangle \ , \tag{1}$$

where the Hamiltonian $\hat{H}$ is given by

$$\hat{H}=\hat{H}_{\rm el}+\hat{H}_{\rm ph}+\hat{H}_I \ , \tag{2}$$

$\hat{H}_{\rm el}$ is the energy operator of an electron confined within a potential well and written in the first quantization as

$$\hat{H}_{\rm el}=\frac{\mathbf{p}_{\parallel}^2}{2m_e^*}+\frac{\mathbf{p}_z^2}{2m_e^*}+V(z) \ , \tag{3}$$

where $\mathbf{p}_{\parallel}$ and $\mathbf{p}_z$ are the momentum operators of the electron in the XY plane and in the z direction, respectively, and m_e^* is the effective mass of the electron which is assumed to be the same in the transverse direction (XY plane) as well as the z direction. $V(z)$ is the potential-energy operator which confines the electron within the quantum well in the z direction. From here on, we consider the infinite well approximation[14] for a quantum well of width L_z, where

$$V(z)=\begin{cases}0 \ , & |z|\le L_z \\ \infty \ , & |z|\ge L_z \ ,\end{cases} \tag{4}$$

and the potential $V(z)$ is assumed to be well defined at the geometrical interface.

$\hat{H}_{\rm ph}$ is the optical-phonon-energy operator given by

$$\hat{H}_{\rm ph}=\sum_{\mathbf{q}}\hbar\omega b_{\mathbf{q}}^{\dagger}b_{\mathbf{q}} \ , \tag{5}$$

where $\hbar\omega$ is the energy of an optical phonon, and for simplfication the zero-point energy term is omitted in Eq. (5). $\hat{H}_I$ is the electron-phonon interaction energy operator in a quasi-2D system involving LO-phonon modes, and it is given by[9]

$$\hat{H}_I=\sum_{\mathbf{q}}(V_{\mathbf{q}}b_{\mathbf{q}}e^{i\mathbf{q}_{\parallel}\cdot\mathbf{r}_{\parallel}+iq_zz}+V_{\mathbf{q}}^{*}b_{\mathbf{q}}^{\dagger}e^{-i\mathbf{q}_{\parallel}\cdot\mathbf{r}_{\parallel}-iq_zz}) \ , \tag{6}$$

where

$$|V_{\mathbf{q}}|^2=\frac{4\pi\alpha(\hbar\omega)^2}{AL_z(q_{\parallel}^2+q_z^2)}\left[\frac{\hbar}{2m_e^*\omega}\right]^{1/2} \ , \tag{7}$$

and α and A are the electron-phonon-coupling constant which depends on the material of the quantum well and the surface area, respectively.

In an exact 2D case, $q_z=0$, and $|V_{\mathbf{q}}|^2$ is given by[15]

$$|V_{\mathbf{q}}|^2=\frac{2\pi\alpha(\hbar\omega)^2}{Aq_{\parallel}}\left[\frac{\hbar}{2m_e^*\omega}\right]^{1/2} \ . \tag{8}$$

As the interaction operator $\hat{H}_I$ in Eq. (6) is not in a diagonal form, it is difficult to solve the Schrödinger Eq. (1) exactly. First of all, we try to eliminate the dependence of $\hat{H}_I$ on the electronic coordinate $\mathbf{r}_{\parallel}$ by applying a unitary transformation U_1 given by[16]

$$U_1=\exp\left[-i\sum_{\mathbf{q}}\mathbf{q}_{\parallel}\cdot\mathbf{r}_{\parallel}b_{\mathbf{q}}^{\dagger}b_{\mathbf{q}}\right] \ . \tag{9}$$

Applying U_1, one obtains[17]

$$U^{-1}b_{\mathbf{q}}^{\dagger}U=b_{\mathbf{q}}^{\dagger}\exp(i\mathbf{q}_{\parallel}\cdot\mathbf{r}_{\parallel}) \ , \tag{10a}$$

$$U^{-1}b_{\mathbf{q}}U=b_{\mathbf{q}}\exp(-i\mathbf{q}_{\parallel}\cdot\mathbf{r}_{\parallel}) \ , \tag{10b}$$

$$U_1^{-1}\mathbf{p}_{\parallel}U_1=\mathbf{p}_{\parallel}-i\sum_{\mathbf{q}}\hbar\mathbf{q}_{\parallel}b_{\mathbf{q}}^{\dagger}b_{\mathbf{q}} \ . \tag{10c}$$

Using Eqs. (10a), (10b), and (10c), we obtain the transformed Hamiltonian as

$$\begin{aligned}\hat{H}'&=U_1^{-1}\hat{H}U_1 \\ &=\frac{1}{2m_e^*}\left[\mathbf{p}_{\parallel}-\sum_{\mathbf{q}}\hbar\mathbf{q}_{\parallel}b_{\mathbf{q}}^{\dagger}b_{\mathbf{q}}\right]^2+\frac{\mathbf{p}_z^2}{2m_e^*}+V(z) \\ &\quad+\sum_{\mathbf{q}}\hbar\omega b_{\mathbf{q}}^{\dagger}b_{\mathbf{q}}+\sum_{\mathbf{q}}(V_{\mathbf{q}}b_{\mathbf{q}}e^{iq_zz}+V_{\mathbf{q}}^{*}b_{\mathbf{q}}^{\dagger}e^{-iq_zz}) \ .\end{aligned} \tag{11}$$

By expanding the first term in (11), $\hat{H}'$ becomes

$$\begin{aligned}\hat{H}'&=\frac{\mathbf{p}_{\parallel}^2}{2m_e^*}+\sum_{\mathbf{q}}\left[\hbar\omega+\frac{\hbar^2\mathbf{q}_{\parallel}^2}{2m_e^*}-\frac{\hbar\mathbf{p}_{\parallel}\cdot\mathbf{q}_{\parallel}}{m_e^*}\right]b_{\mathbf{q}}^{\dagger}b_{\mathbf{q}} \\ &\quad+\frac{\mathbf{p}_z^2}{2m_e^*}+V(z)+\sum_{\mathbf{q}}(V_{\mathbf{q}}e^{iq_zz}b_{\mathbf{q}}+V_{\mathbf{q}}^{*}e^{-iq_zz}b_{\mathbf{q}}^{\dagger}) \\ &\quad+\frac{1}{2m_e^*}\sum_{\mathbf{q},\mathbf{q}'}\hbar^2\mathbf{q}_{\parallel}\cdot\mathbf{q}_{\parallel}'b_{\mathbf{q}}^{\dagger}b_{\mathbf{q}'}^{\dagger}b_{\mathbf{q}}b_{\mathbf{q}'} \ .\end{aligned} \tag{12}$$

The last two terms in Eq. (12) are not in diagonal forms, but these can be partially diagonalized by applying a second unitary transformation given by[16]

$$U_2=\exp\left[\sum_{\mathbf{q}}f(\mathbf{q})b_{\mathbf{q}}^{\dagger}-f^{*}(\mathbf{q})b_{\mathbf{q}}\right] \ , \tag{13}$$

where $f(\mathbf{q})$ is a variational parameter to be determined below. Using Eq. (13), we obtain[16,17]

$$U_2^{-1}\mathbf{p}_{\parallel}U_2=\mathbf{p}_{\parallel} \ , \tag{14a}$$

$$U_2^{-1}b_{\mathbf{q}}U_2=b_{\mathbf{q}}+f(\mathbf{q}) \ , \tag{14b}$$

$$U_2^{-1}b_{\mathbf{q}}^{\dagger}U_2=b_{\mathbf{q}}^{\dagger}+f^{*}(\mathbf{q}) \ . \tag{14c}$$

and then the transformed Hamiltonian $U_2^{-1}\hat{H}'U_2$ can be obtained easily. The energy eigenvalue of the ground state $E_{\rm pol}(0)$ [with zero-phonon population, i.e., $n(\mathbf{q})=0$] can be evaluated using the transformed Hamiltonian thus obtained as

$$\begin{aligned}E_{\rm pol}(0)&=\langle n(\mathbf{q});l,\mathbf{K}_{\parallel}|U_2^{-2}\hat{H}'U_2|\mathbf{K}_{\parallel},m,n(\mathbf{q})\rangle \\ &=\frac{\hbar^2\mathbf{K}_{\parallel}^2}{2m_e^*}+\sum_{\mathbf{q}}\left[\hbar\omega+\frac{\hbar^2\mathbf{q}_{\parallel}^2}{2m_e^*}-\frac{\hbar^2\mathbf{K}_{\parallel}\cdot\mathbf{q}_{\parallel}}{m_e^*}\right]f(\mathbf{q})f^{*}(\mathbf{q}) \\ &\quad+\sum_{\mathbf{q}}V_{\mathbf{q}}^{*}f^{*}(\mathbf{q})\langle l|e^{-iq_zz}|m\rangle+E_{z,m} \\ &\quad+\frac{\hbar^2}{2m_e^*}\sum_{\mathbf{q},\mathbf{q}'}\mathbf{q}_{\parallel}\cdot\mathbf{q}_{\parallel}'f(\mathbf{q})f(\mathbf{q}')f^{*}(\mathbf{q})f^{*}(\mathbf{q}') \ ,\end{aligned} \tag{15}$$

where $E_{z,m}$ is the energy of discrete electronic states due to electron motion in the z direction. Using Eq. (4), the energy $E_{z,m}$ is obtained as[14]

$$E_{z,m}=\frac{m^2\hbar^2\pi^2}{2m_e^*L_z^2} \ , \quad m=1,2,3\ldots,$$

Minimizing $E_{\rm pol}(0)$ with respect to $f^*(\mathbf{q})$, we can determine the parameter $f(\mathbf{q})$ as

$$f(\mathbf{q})=-\frac{V_{\mathbf{q}}^*\langle l|e^{-iq_z z}|m\rangle}{\left[\hbar\omega+\frac{\hbar^2}{2m_e^*}\mathbf{q}_\parallel^2-\frac{\hbar^2}{m_e^*}\mathbf{K}_\parallel\cdot\mathbf{q}_\parallel(1-\eta)\right]}, \tag{16}$$

where η is expected to be a fraction defined by

$$\eta\mathbf{K}_\parallel=\sum_q|f(\mathbf{q})|^2\mathbf{q}_\parallel . \tag{17}$$

Substituting $f(\mathbf{q})$ given in Eq. (16) into Eq. (15), $E_{\rm pol}(0)$ is obtained as

$$E_{\rm pol}(0)=\frac{\hbar^2\mathbf{K}_\parallel^2}{2m_e^*}(1-\eta^2)+E_{z,m}-I , \tag{18}$$

where

$$I=\sum_{\mathbf{q}}\frac{|V_{\mathbf{q}}|^2|\langle l|e^{-iq_z z}|m\rangle|^2}{\left[\hbar\omega+\frac{\hbar^2}{2m_e^*}\mathbf{q}_\parallel^2-\frac{\hbar^2}{m_e^*}\mathbf{K}_\parallel\cdot\mathbf{q}_\parallel(1-\eta)\right]} .$$

By converting the summation into an integration, I can be rewritten as

$$I=\frac{A}{2\pi^2}\sum_{q_z}\int_0^\infty\int_0^{2\pi}d\theta\,dq_\parallel q_\parallel\frac{|V_{\mathbf{q}}|^2|\langle l|e^{-iq_z z}|m\rangle|^2}{\left[\hbar\omega+\frac{\hbar^2}{2m_e^*}\mathbf{q}_\parallel^2-\frac{\hbar^2}{m_e^*}\mathbf{K}_\parallel\cdot\mathbf{q}_\parallel(1-\eta)\right]} . \tag{19}$$

Using the infinite well approximation as given in Eq. (4), the electron wave function can be expressed[14] as

$$\psi_m(z)=\frac{e^{\mathbf{K}_\parallel\cdot\mathbf{r}_\parallel}}{\sqrt{A}}\left[\frac{2}{L_z}\right]^{1/2}\sin\left[\frac{m\pi z}{L_z}\right], \quad m=1,2,3\ldots \tag{20}$$

for $0\le z\le L_z$. Using Eq. (20), one can define $|m\rangle=|\psi_m(z)\rangle$, and then $|\langle l|e^{-iq_z z}|m\rangle|^2$ in Eq. (19) can be evaluated for the case of $l=m=1$ as

$$G(q_zL_z)=|\langle l|e^{-iq_z z}|m\rangle|^2=\frac{\pi^2}{\pi^2-(q_zL_z)^2}\exp\left[\frac{-iq_zL_z}{2}\right]\frac{\sin\left[\frac{q_zL_z}{2}\right]}{\left[\frac{q_zL_z}{2}\right]} . \tag{21}$$

Using Eq. (21) in Eq. (19) we obtain

$$I=\frac{\alpha}{\pi}(\hbar\omega)^2\left[\frac{\hbar}{2m_e^*\omega}\right]^{1/2}\int_0^\infty\frac{dq_\parallel q_\parallel F(q_\parallel,L_z)}{\left\{\left[\hbar\omega+\frac{\hbar^2q_\parallel^2}{2m_e^*}\right]^2-\left[\frac{\hbar^2}{m_e^*}K_\parallel q_\parallel(1-\eta)\right]^2\right\}^{1/2}} , \tag{22}$$

where $F(q_\parallel,L_z)$ is given by

$$F(q_\parallel,L_z)=\int_0^\infty\frac{dq_z|G(q_zL_z)|^2}{(q_\parallel^2+q_z^2)^2} . \tag{23}$$

Assuming $[\hbar\omega+(\hbar^2q_\parallel^2/2m_e^*)]\gg(\hbar^2/m_e^*)K_\parallel q_\parallel(1-\eta)$, the denominator of the integrand in Eq. (22) can be expanded, and then the integral I can be split into two terms as

$$I\approx I_1+I_2 , \tag{24}$$

where I_1 and I_2 are given by

$$I_1=\frac{\alpha}{\pi}(\hbar\omega)^2\left[\frac{\hbar}{2m_e^*\omega}\right]^{1/2}\int_0^\infty\frac{dq_\parallel q_\parallel F(q_\parallel,L_z)}{\left[\hbar\omega+\frac{\hbar^2q_\parallel^2}{2m_e^*}\right]} \tag{25}$$

and

$$I_2=\frac{\alpha}{\pi}(\hbar\omega)^2\left[\frac{\hbar}{2m_e^*\omega}\right]^{1/2}\left[\frac{\hbar^2K_\parallel(1-\eta)}{m_e^*}\right]^2\times\int_0^\infty\frac{dq_\parallel q_\parallel^3F(q_\parallel,L_z)}{\left[\hbar\omega+\frac{\hbar^2q_\parallel^2}{2m_e^*}\right]^3} . \tag{26}$$

The integrals in Eqs. (25) and (26) can be evaluated numerically for any general L_z, but one can evaluate these analytically only for very small L_z, approximating $F(q_\parallel,L_z)$ as

$$F(q_\parallel,L_z)\simeq\frac{\pi}{(1+q_\parallel L_z)q_\parallel} , \tag{27}$$

which is known to be a good approximation[18] having an error of about 5% for values of $q_\parallel$ up to $q_\parallel=4/L_0$ where

$L_0=\sqrt{\hbar/2m_e^*\omega}$. Then, using Eq. (27) in Eqs. (25) and (26), I_1 and I_2 can be evaluated analytically to give

$$I_1=\frac{\alpha\hbar\omega\left[\frac{\pi}{2}+L^*\ln L^*\right]}{(1+L^{*2})} \tag{28}$$

and

$$I_2=\frac{\hbar^2K_\parallel^2}{2m_e^*}\alpha(1-\eta)^2\left[\frac{\pi}{8}-\frac{L^*}{2}\right], \tag{29}$$

where $L^*=L_z/4L_0$.

Using Eqs. (24), (28), and (29) in Eq. (18), the ground-state energy of a quasi-2D polaron at small well widths is thus obtained as

$$E_{\rm pol}(0)=E_{\rm pol}^{\rm KE}+E_{z,m}-\Delta E\ , \tag{30}$$

where

$$E_{\rm pol}^{\rm KE}=\frac{\hbar^2K_\parallel^2}{2m_e^*}\left[(1-\eta^2)-\alpha(1-\eta)^2\left[\frac{\pi}{8}-\frac{L^*}{2}\right]\right] \tag{31}$$

and

$$\Delta E=\alpha\hbar\omega\frac{\left[\frac{\pi}{2}+L^*\ln L^*\right]}{(1+L^{*2})}\ , \tag{32}$$

where $E_{\rm pol}^{\rm KE}$ and ΔE represent the kinetic energy and energy-gap shift for a polaron, respectively. Writing $E_{\rm pol}^{\rm KE}=\hbar^2K_\parallel^2/2m_p^*$, we obtain the effective mass of the quasi-2D polaron from Eq. (31) as

$$m_p^*=\frac{m_e^*}{\left[(1-\eta^2)-\alpha(1-\eta)^2\left[\frac{\pi}{8}-\frac{L^*}{2}\right]\right]}\ . \tag{33}$$

It is obvious from Eqs. (32) and (33) that both ΔE and m_p^* depend explicitly on the quantum-well width. The kinetic energy $E_{\rm pol}^{\rm KE}$ of the polaron is less than that of a free electron, and the total polaron energy is lowered by an amount ΔE. The decrease in the kinetic energy is accounted for by the increase in its effective mass as given in Eq. (33).

III. RESULTS AND DISCUSSION

Here we have calculated the energy and effective mass of a polaron in 2D quantum wells. As in the case of bulk crystals, the energy of a polaron as obtained in $E_{\rm pol}(0)$ [Eq. (30)] is less and the effective mass heavier than those of a free electron. However, there are some notable differences obtained in the properties of polarons in bulk crystals and quantum wells. The energy of a polaron in bulk (3D) is obtained as[9]

$$E_{\rm pol}^{\rm 3D}=\frac{\hbar^2K^2}{2m_e^*}\left[(1-\eta_{\rm 3D}^2)-\frac{\alpha}{6}(1-\eta_{\rm 3d})^2\right]-\alpha\hbar\omega\ , \tag{34}$$

which give the polaron effective mass as

$$m_p^{\rm 3D}=\frac{m_e^*}{\left[(1-\eta_{\rm 3D}^2)-\frac{\alpha}{6}(1-\eta_{\rm 3D})^2\right]}\ , \tag{35}$$

where $\eta_{\rm 3D}$ is defined for bulk material in the same way as η in Eq. (17). The essential difference between $E_{\rm pol}^{\rm 3D}$ in Eq. (34) and $E_{\rm pol}(0)$ in Eq. (18) is that the latter depends not only on α and η, but also on the quantum-well width. The expression for η in Eq. (17) cannot be evaluated analytically for general quantum-well widths. However, for an ideal 2D system with a zero quantum-well width, Eq. (17) can be evaluated analytically to give $\eta_{\rm 2D}=\pi\alpha/8$. On the other hand, for bulk crystals, $\eta_{\rm 3D}$ is obtained approximately as[16] $\eta_{\rm 3D}\approx(\alpha/6)/(1+\alpha/6)$. It is interesting to note that although $\eta_{\rm 3D}$ is never greater than unity, $\eta_{\rm 2D}$ may become larger than one for $\alpha\geq 2.5$. This means that $\eta_{\rm 2D}=\pi\alpha/8$ is valid only for very weak coupling with $\alpha\leq 2.5$. This agrees very well with the values of $\alpha\ll 0.5$, known for semiconductor materials.

For any general quantum-well width, the energy-gap shift ΔE and increase in polaronic mass given by $\Delta m_p^*/m_e^*=[(m_p^*/m_e^*)-1]\times 100\%$ can only be calculated numerically using Eqs. (25) and (26). For numerical evaluation, we consider the case of electrons in a GaAs-$Al_{x\,1-x}As$ system, and the values of the physical parameters are taken as[19] $m_e^*=0.067m_e$, $\alpha=0.068$, and $\hbar\omega=36.8$ meV. The energy-gap shift ΔE is plotted as a function of the quantum-well width in Fig. 1. It can be seen that ΔE decreases monotonically with increasing well width. For example, ΔE decreases by 23% at a well width of 30 Å, by 33% at a well width of about 90 Å, and by approximately 35% at well widths $\geq$200 Å. From Fig. 1, it is also obvious that in the two limiting situations of $L_z\to 0$ and ∞, ΔE approaches the well known values for ideal 2D and 3D (bulk) systems, respectively.

In Fig. 2, the increase in polaron mass $\Delta m_p^*/m_e^*$ is plotted as a function of the quantum-well width. Like ΔE in Fig. 1, $\Delta m_p^*/m_e^*$ decrease monotonically with increasing well width. Here we find that the decrease in polaron mass is by 50% at a well width of 30 Å, and by approximately 44% for well widths $\geq$180 Å. The polaron mass also approaches its values for ideal 2D and 3D systems for $L_z\to 0$ and ∞, respectively. The approxima-

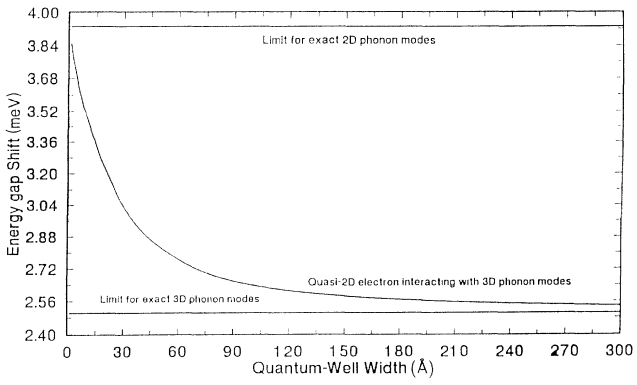

FIG. 1. Polaron energy-gap shift as a function of quantum-well width.

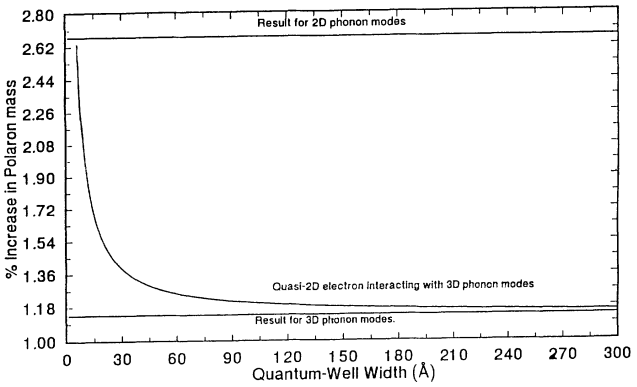

FIG. 2. Increase in polaron mass as a function of quantum-well width.

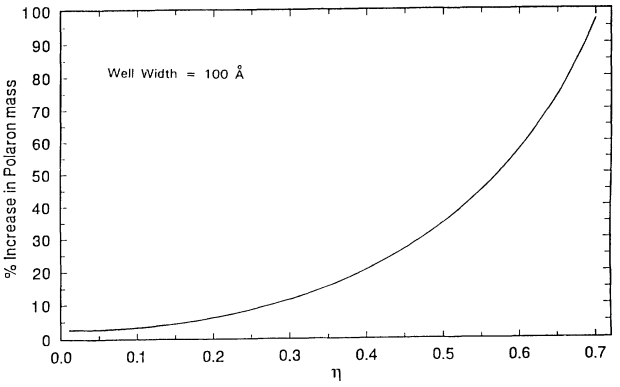

FIG. 3. Increase in polaron mass as a function of η.

tion in Eq. (27) proved to be very useful, because it enables one to obtain an analytical expression for the energy-gap shift and an increase in polaronic mass at small quantum well widths.

From our calculation, it is found that analytical values and numerically computed values for ΔE and $\Delta m_p^*/m_e^*$ agree very well for $L_z \leq 30$ Å . Moreover, as stated above, $\eta \rightarrow \pi\alpha/8$ for an ideal 2D system and, for such a system, η is expected to be very small ($\eta \ll 1$). Using this result in (33), we find that

$$m_p^* \approx (1+\eta_{2D}) m_e^* , \tag{36}$$

which leads to the increase in polaron mass as

$$\frac{\Delta m_p^*}{m_e^*} \approx \eta_{2D} = \frac{\pi\alpha}{8} . \tag{37}$$

The energy-gap shift can also be estimated for an ideal 2D system in a similar way. We thus obtain

$$\Delta E_{2D} = \frac{\pi\alpha}{2}\hbar\omega . \tag{38}$$

The expressions obtained in Eqs. (37) and (38) are well-known results for an ideal two-dimensional system.[15,20]

Recently Mori *et al.*[21] have measured $\Delta m_p^*/m_e^*$, and found it to be about 13% for a well width of 100 Å in GaAs-$Al_xGa_{1-x}As$ systems. This value is much larger than even the maximum possible value of $\pi\alpha/8$ for $\Delta m_p^*/m_e^*$ obtained in the exact 2D case, as shown in Fig. 1. In order to explain such a large discrepancy between experimental and theoretical results, we have calculated the increase in polaronic mass $\Delta m_p^*/m_e^*$ as a function of η, using Eq. (33) for a particular value of $L_z = 100$ Å, and shown it in Fig. 3. From Fig. 3, we find that $\Delta m_p^*/m_e^* = 14\%$ for $L_z = 100$ Å and $\eta = 0.35$. This is a much larger value for η than what one obtains from $\pi\alpha/8$ for $\alpha \sim 0.068$.[19] Hence the analytical result $\eta \sim \pi\alpha/8$ obtained for parabolic bands may not be applicable for quantum wells. The point that the above discrepancy may be due to nonparabolic characteristics of the electron energy band has also been suggested earlier.[22]

As stated earlier, we have calculated the polaron energy using only the bulk-phonon modes and assuming that the contribution of the surface modes is negligible. Liang, Gu, and Lin[11] have calculated the polaron energy using both types of phonon modes, and the results show the contribution of the surface modes to be much less than that of the bulk modes. In addition, the results also show that the contribution of the surface modes does not decrease monotonically like that of the bulk modes, which represents a qualitative behavior brought about by surface phonon modes. Our results agree very well with those of Liang, Gu, and Lin obtained for bulk modes, which makes the maximum contribution to the polaronic effect. Also, recent theories[13] seem to suggest that bulk-phonon modes play the most significant role in determining the properties of an electron interacting with phonons in a quantum well. In this view, our assumption to neglect the surface-phonon modes seems quite appropriate.

We have calculated the polaron energy by considering that the height of the quantum-well potential is infinite. This is a common approach to the problem of an electron confined in a single quantum well and interacting with phonons.[11] However, the assumption of an infinite quantum well implies that it is not possible for an electron to escape the potential well if the well width is reduced. The effect of the electron escaping may be important to consider in the case of a superlattice, but it seems to be of no consequence for a single quantum well.

In conclusion, we have obtained expressions for the energy-gap shift and the increase in polaronic mass in quantum wells. It is shown that, for small well widths, one can obtain analytical expressions for ΔE and $\Delta m_p^*/m_e^*$; however, for larger quantum-well widths, these values can only be obtained numerically. We have also addressed the problem that the assumption of a parabolic electron energy band may not be very suitable for quantum wells.

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