Effects of interface defects on polaron states in GaAs-$Ga_{1-x}Al_xAs$ quantum wells

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Effects of interface defects on polaron states in GaAs-$Ga_{1-x}Al_xAs$ quantum wells (QW's) are investigated theoretically by introducing a coordinate transformation that transforms QW's with defect interfaces to those with planar interfaces with an effective potential associated with the interface defects. The interface defects are idealized as an infinite track or a cylindrical hollow protruding into the barrier material on one of the interfaces. Polaron ground-state energies are calculated variationally as functions of the defect lateral sizes. For GaAs-$Ga_{1-x}Al_xAs$ QW's with well width d less than 150 Å, the changes in polaron ground-state energies due to interface defects are expected to lead to sizable effects on optical experiments, such as broadening of the luminescence, absorption, and excitation spectra of GaAs-$Ga_{1-x}Al_xAs$ QW's, but our calculation predicts smaller spectrum broadenings than those predicated by a previous theory for the same interface disorder. Changes in polaron self-energies and polaron effective masses caused by interface defects are negligible for materials with weak electron–LO-phonon interactions, such as GaAs for which the Fröhlich coupling constant α_{LO} is less than 0.1. Effects of interface defects on exciton states in QW's are discussed qualitatively.

I. INTRODUCTION

Modern material growth techniques such as molecular-beam epitaxy (MBE) and metal organic chemical vapor deposition have made possible the realization of high-quality semiconductor layer structures, e.g., quantum wells (QW's) and superlattices (SL's). Electron motions in these systems are quantized in directions perpendicular to the interfaces, while their in-plane motions are still free-electron-like.[1] This quasi-two-dimensional (2D) behavior in electron motions is also seen in other electronic systems such as semiconductor heterostructures or metal-oxide-semiconductor (MOS) inversion layers. Electron–optical-phonon interactions, e.g., the polaron effects, in these systems are enhanced relative to those in the bulk systems.[2] In recent years the problem of surface or interface polarons has received renewed interest both experimentally and theoretically because unusual polaron effects are observed in these quasi-2D systems. Line splitting of cyclotron resonance[3] (CR) and oscillations of the cyclotron effective mass[4] in heterostructures in the quantum limit have been reported. Strong narrowing and a positional shift of CR in Si MOS structures in the quantum limit have been observed.[5] And pronounced current oscillations in the experiment of Hickmott *et al.*[6] in 2D systems has been predicted theoretically due to a strong oscillation in the 2D electron density of states induced by strong electron–optical-phonon interactions in 2D systems.[7]

In realistic quasi-2D systems, such as QW's, SL's, heterostructures, and MOS structures, it is almost impossible to produce ideally planar interfaces due to environmental fluctuations and mechanical controlling inaccuracy in the growth process. Experimental studies have shown that the interface roughness in Si-SiO_2 interfaces in Si MOS structures are about several monolayers in height, ranging from 5 to 10 Å, and with about 50-Å periodicity,[8] while the electron wave-function extension perpendicular to the interfaces are about 50 Å for Si MOS structure inversion layers.[9] The interface roughness is not negligibly small compared with the electron extension perpendicular to the interfaces. The interface roughness in MBE-grown QW's or SL's is considerably less than that in MOS structures. In high-quality samples the mean interface defect depth is about one monolayer ($\cong 2.86$Å in GaAs) and its lateral extension is about 300 Å.[10] With improved growth techniques (growth interruption), the interface roughness of QW's can be further reduced.[11,12] But the interface roughness still produces sizable effects on optical experiments in thin QW's or SL's with the well width d ranging from 50 to 150 Å. The main effects so far observed due to the interface roughness are the following: (i) Exciton-line width broadening in the excitation spectrum of the luminescence line in GaAs-$Ga_{1-x}Al_xAs$ QW's;[13,14] (ii) red shift (Stokes shift) of the photoluminescence spectrum with respect to the excitation spectrum maximum in GaAs-$Ga_{1-x}Al_xAs$ QW's, due to exciton trapping on interface defects;[15,16] (iii) the shift of the energy position of the intensity maximum of the excitonic transition as the delay time increased in the time-resolved photoluminescence of the excitonic transition of GaAs-$Ga_{1-x}Al_xAs$ QW's;[17] and (iv) the temperature dependence of the exciton population in the emission spectra of GaAs single QW's.[18]

On the theoretical side, effects of interface defects on exciton trapping in QW's have been studied theoretically by Bastard *et al.*[15] They modeled QW's with rough interfaces by QW's with planar interfaces and added an empirical potential energy associated with interface defects to the Hamiltonian. Schwarz and Ting[10] and Leo[20] have recently investigated effects of fluctuations in the well width on electron transport in a semiconductor SL when an electric field is applied perpendicular to the wells. However, effects of interface defects on the polaron in-plane motions in quasi-2D systems have not been studied previously. In this paper, we present a theoretical investigation on effects of interface defects on polaron states in GaAs-$Ga_{1-x}Al_xAs$ QW's. Our purpose is twofold. First, following the basic theory presented in this paper, we plan to investigate whether rough interfaces will produce any sizable effects on experiments associated with polaron properties in quasi-2D systems. For instance, we are interested in knowing whether the trapping of polarons on interface defects will cause detectable changes in cyclotron resonance, etc. Second, we intend to set up a theory to study effects of rough interfaces on excitons in QW's which starts from the commonly accepted Hamiltonian without introducing an additional empirical potential energy. In fact, we shall derive an effective potential associated with the interface defects from the theory presented in this paper. To simplify the calculation, we are going to study effects of interface defects on polaron states in GaAs-$Ga_{1-x}Al_xAs$ QW's with an idealized defect—an infinite track or a cylindrical hollow protruding into the barrier material on one of the QW interfaces.

II. POLARONS IN QW's WITH DEFECT INTERFACES

A. Polaron Hamiltonian

The QW with defect interfaces we are considering consists of two lattice-matched semiconductors, e.g., GaAs and $Al_xGa_{1-x}As$ with rather similar lattice dielectric properties, which enables us to make the approximation that the electron in the QW interacts only with the bulk LO phonons of GaAs. The second approximation we made is that the QW interfaces represent infinitely high potential barriers, which for QW's with well width $d > 50$ Å is a good approximation. The electron is confined within the QW and its wave function vanishes on the interfaces. Within the above approximations, the polaron Hamiltonian for the QW reads[21,22]

$$H_{\text{pol}} = -\frac{\hbar^2}{2m_e}\nabla_{\mathbf{r}}^2 + \sum_{\mathbf{k}} \hbar\omega_{\text{LO}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \sum_{\mathbf{k}} (V_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}} a_{\mathbf{k}}^\dagger + \text{H.c.}) \qquad (1)$$

The eigenenergy E of the polaron states is given by the equation

$$H_{\text{pol}}\psi = E\psi \qquad (2)$$

with the polaron wave function ψ satisfying the boundary condition

$$\psi|_{z=d} = 0, \quad \psi|_{z=f(x,y)} = 0 , \qquad (3)$$

where m_e is the electron band mass, $a_{\mathbf{k}}^\dagger$ creates a bulk LO phonon with wave vector $\mathbf{k}$ and frequency ω_{LO}, $z = f(x,y)$ gives the interface defect which is assumed to be on the interface at $z = 0$, d is the width of the QW, and

$$V_{\mathbf{k}} = -i\left[\frac{2\pi\hbar\omega_{\text{LO}}e^2}{V_0}\left[\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\right]\right]^{1/2} \qquad (4)$$

is the electron–LO-phonon interaction constant with V_0 ($V_0 \to \infty$) the volume of the QW system (the well plus the cladding materials), and ϵ_∞ and ϵ_0 the high-frequency and static dielectric constants of the QW material, respectively.

In solving the polaron problem of H_{pol} (1) with the boundary condition (3), the obstacle to overcome is that it is difficult to find a trial wave function that satisfies the boundary condition on the defect interface. We avoid this obstacle by introducing a coordinate transformation that transforms the QW with defect interfaces to that with planar interfaces. Though the transformation will complicate H_{pol} (1), this is usually easy to handle in numerical calculations.

B. Coordinate transformation

The defect on the QW interface we are considering is idealized as an infinite track along the y axis as shown in Fig. 1(a) or a cylindrical hollow centered on the $\hat{z}$ axis as

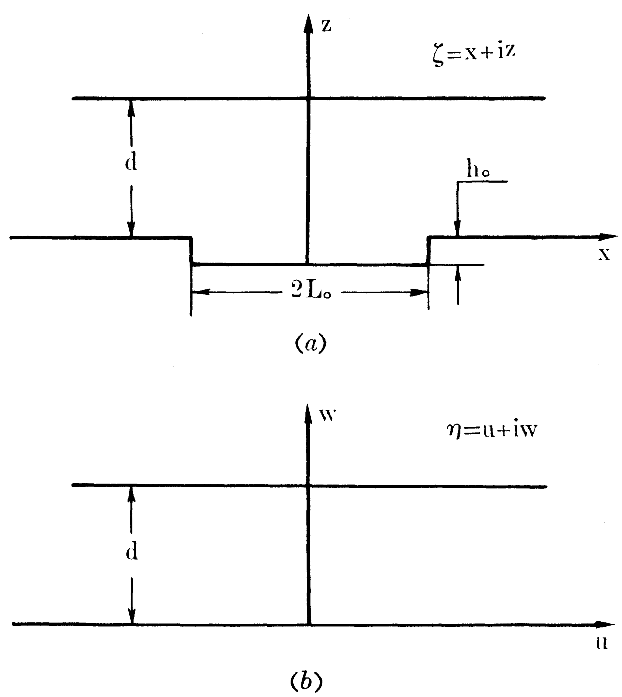

FIG. 1. (a) A section the x-z plane of the QW with an infinite track along the y axis and protruding into the barrier material on one of the QW interfaces. (b) A section on the u-w plane of the QW in (a) after the coordinate transformation introduced in the text.

TABLE I. The corresponding transforming points used to determine the coordinate transformation from ξ to η planes, with $2L_0$ and h_0 the width and height of the track [see Fig. 1(a)], respectively. L and h are determined from L_0 and h_0 in the text.

Original points in the $\xi=x+iz$ plane				Transformed points in the $\eta=u+iw$ plane			
A	B	C	D	A'	B'	C'	D'
$-L_0$	$-L_0-ih_0$	L_0-ih_0	L_0	$-L-h$	$-L$	L	$L+h$

shown in Fig. 4(a) protruding into the barrier material. Because of the geometric symmetry, we can consider the system on any x-z plane with y fixed for the infinite-track defect or on any $\tilde{\rho}$-$\tilde{z}$ plane with $\tilde{\varphi}$ fixed for the cylindrical hollow defect. The profiles of the defective interfaces look the same on these two section planes. So in what follows, we consider only the infinite-track defect. The coordinate transformation derived here can also be used for the cylindrical-hollow defect.

If we consider the x-z plane in Fig. 1(a) as a complex plane $\xi=x+iz$, the coordinate transformation that transforms the QW with an infinite track on one of its interfaces in complex plane $\xi=x+iy$ to the QW with planar interfaces in complex plane $\eta=u+iv$ [as shown in Fig. 1(b)] can be obtained by a Schwarz transformation,[23] which transforms the region within the QW in Fig. 1(a) to the upper half-space, followed by a logarithmic transformation, which transforms the upper half-space to the region within the QW with planar interfaces as shown in Fig. 1(b). In Table I, we list the corresponding transforming points used to determine the transformation, which is given by

$$\xi=A\int_{\exp[-\pi(L+h)/d]}^{\exp(\pi\eta/d)} t^{-1}\left[\frac{t-\exp[-\pi(L+h)/d]}{t-\exp[-\pi L/d]}\right]^{1/2}\left[\frac{t-\exp[\pi(L+h)/d]}{t-\exp[\pi L/d]}\right]^{1/2} dt-L_0 \tag{5}$$

with the constant A determined by the condition that when $\eta=-L$, we must have $\xi=-L_0-ih_0$, where L and h are determined by requiring that as $|\mathrm{Re}\eta|\to\infty$, Eq. (5) should reduce to $\xi=\eta$, as can be seen from Figs. 1(a) and 1(b).

For the case where $\exp(-2\pi L_0/d)\ll 1$ (that is, $L_0\geq d$), to first order in h_0 we have

$$\xi=\eta-\frac{h_0}{\pi}\ln\left[\frac{\sinh[(\pi/2d)(\eta-L)]}{\sinh[(\pi/2d)(\eta+L)]}\right] \tag{6}$$

or

$$x=u+\delta x(u,w)=u-\frac{h_0}{2\pi}\ln\left[\frac{\sin^2(\pi w/2d)+\sinh^2[(\pi/2d)(u-L)]}{\sin^2(\pi w/2d)+\sinh^2[(\pi/2d)(u+L)]}\right], \tag{6a}$$

$$z=w+\delta z(u,w)=\begin{cases} w-\dfrac{h_0}{\pi}\left\{\arctan\left[\tan\left[\dfrac{\pi w}{2d}\right]\coth\left[\dfrac{\pi}{2d}\left(|u|-L\right)\right]\right]\right. \\ \qquad \left.-\arctan\left[\tan\left[\dfrac{\pi w}{2d}\right]\coth\left[\dfrac{\pi}{2d}\left(|u|+L\right)\right]\right]\right\}, & \text{for } |u|>L \\ w-\dfrac{h_0}{\pi}\left\{\pi-\arctan\left[\tan\left[\dfrac{\pi w}{2d}\right]\coth\left[\dfrac{\pi}{2d}\left(|u|-L\right)\right]\right]\right. \\ \qquad \left.-\arctan\left[\tan\left[\dfrac{\pi w}{2d}\right]\coth\left[\dfrac{\pi}{2d}\left(|u|+L\right)\right]\right]\right\}, & \text{for } |u|<L\,, \end{cases} \tag{6b}$$

with

$$h=\frac{2h_0}{\pi}\left[1-\frac{h_0}{2d}\right],\quad L=L_0\frac{1+(h_0/\pi L_0)\ln(h_0/2d)}{1+h_0/d}\,. \tag{7}$$

From Eqs. (6a) and 6(b) it is easy to show that

$$z|_{w=d}=d,\quad z|_{w=0}=\begin{cases}0, & \text{for } |u|>L\\ -h_0 & \text{for } |u|<L\end{cases}\,. \tag{8}$$

The transformation (6) transforms the QW with an infinite track on one of its interfaces in ξ plane to that with planar interfaces in the η plane (see Fig. 1).

C. Ground-state energy of polarons in a QW with an infinite track on one of its interfaces

A section on the x-z plane of a QW with an infinite track along the axis y and protruding into the barrier material on one of its interfaces is shown in Fig. 1(a). The following coordinate transformation:

$$x=u+\delta x(u,w)\ , \tag{9a}$$

$$y=v\ , \tag{9b}$$

$$z=w+\delta z(u,w)\ , \tag{9c}$$

transforms the QW with the defective interface in space (x,y,z) to the QW with planar interfaces in space (u,v,w), where Eqs. (9a) and (9c) are given by Eqs. (6a) and (6b). A section on the u-w plane of the transformed QW is shown in Fig. 1(b). In space (u,v,w), the boundary condition (3) satisfied by the polaron wave function becomes

$$\psi\Big|_{w=d}=0,\quad \psi\Big|_{w=0}=0\ . \tag{10}$$

To first order in the track height h_0, the eigenvalue equation (2) for the polaron ground-state energy E_g becomes

$$H_{\rm eff}\psi=E_g\psi \tag{11}$$

with

$$\begin{aligned}H_{\rm eff}=&-\frac{\hbar^2}{2m_e}\left[\frac{\partial^2}{\partial u^2}+\frac{\partial^2}{\partial w^2}\right]\\&-\frac{\hbar^2}{2m_e}[1+\delta(u,w)]\frac{\partial^2}{\partial v^2}-E_g^{(0)}\delta(u,w)\\&+\sum_{\mathbf{k}}[1+\delta(u,w)]\hbar\omega_{\rm LO}a_{\mathbf{k}}^\dagger a_{\mathbf{k}}\\&+\sum_{\mathbf{k}}[\tilde V_{\mathbf{k}}(u,w)\exp(-i\mathbf{k}\cdot\mathbf{R})a_{\mathbf{k}}^\dagger+\text{H.c.}]\ ,\end{aligned} \tag{12}$$

where the position vector $\mathbf{R}=(u,v,w)$, $E_g^{(0)}$ is the polaron ground state energy for a QW with planar interfaces and width d,

$$\begin{aligned}\tilde V_{\mathbf{k}}(u,w)=&V_{\mathbf{k}}[1+\delta(u,w)]\\&\times\exp\{-i[k_x\delta x(u,w)+k_z\delta z(u,w)]\}\ ,\end{aligned} \tag{13}$$

and

$$\begin{aligned}\delta(u,w)&\\=\frac{h_0}{d}&\left[\frac{\sinh[(\pi/2d)(u+L)]\cosh[(\pi/2d)(u+L)]}{\sin^2(\pi w/2d)+\sinh^2[(\pi/2d)(u+L)]}\right.\\&\left.-\frac{\sinh[(\pi/2d)(u-L)]\cosh[(\pi/2d)(u-L)]}{\sin^2(\pi w/2d)+\sinh^2[(\pi/2d)(u-L)]}\right]\ .\end{aligned} \tag{14}$$

If the track height h_0 goes to zero, from Eqs. (12)–(14) together with the boundary condition (10), $H_{\rm eff}$ (12) reduces to the polaron Hamiltonian for a QW with planar interfaces. The third term in $H_{\rm eff}$ (12) is obviously an effective potential associated with the defect on the interface. It is easy to show that this effective potential goes to zero when $|u|\to\infty$ and it shows a potential well within the track in which the polaron will be trapped. Physically, this trapping is simple to understand. If we ignore the polaron effect, the first subband energy of the quantized electron motion perpendicular to the QW interfaces is $E_0=(\hbar^2/2m_e)(\pi/d)^2$ for a QW with width d and its interfaces representing infinitely high potential barriers. The electronic energy at places where the QW is wide is lower than where the QW is thin. This causes polaron trapping on parts of the QW where the interfaces protrude into the barrier material making the QW locally wide. For small defect ($h_0/d\ll 1$), the energy change caused by the defect is much smaller than the level spacing of the energy subbands of the quantized electron motion perpendicular to the interface, and so we assume that the electron motion remains in the first subband. The effective polaron Hamiltonian describing the polaron in-plane motion is obtained as follows. We first apply a unitary transformation U_1 to $H_{\rm eff}$ (12), with

$$U_1=\exp\left[-i\sum_{\mathbf{k}}[\mathbf{k}_\parallel\cdot\mathbf{P}+k_x\delta x(u,w)]\right] \tag{15}$$

where $\mathbf{k}_\parallel$ and $\mathbf{P}$ are the in-plane components of $\mathbf{k}$ and $\mathbf{R}$. Then we average the transformed $H_{\rm eff}$ over the electron distribution perpendicular to the interfaces, which is a technique often used in the polaron theory of quasi-2D systems.[2,22] Because we have assumed that the electron motion remains in the first subband, the electron distribution perpendicular to the interfaces may be taken as

$$\varphi_0(w)=\sqrt{2/d}\,\sin\left[\frac{\pi w}{d}\right]\ , \tag{16}$$

which ensures that the boundary condition (10) is satisfied. A second unitary transformation U_2 is applied to the averaged $H_{\rm eff}$, with

$$U_2=\exp\left[\sum_{\mathbf{k}}[a_{\mathbf{k}}^\dagger g_{\mathbf{k}}-a_{\mathbf{k}}g_{\mathbf{k}}^*]\right]\ , \tag{17}$$

where

$$g_{\mathbf{k}}(u)=-\frac{\langle\varphi_0(w)|V_{\mathbf{k}}\exp\{-ik_z[w+\delta z(u,w)]\}|\varphi_0(w)\rangle}{[1+\bar\delta(u)]^2(\hbar\omega_{\rm LO}+\hbar^2k_\parallel^2/2m_e)}\ , \tag{18}$$

And finally in the low-temperature limit, we decouple the electron–LO-phonon interaction by taking average of the transformed $H_{\rm eff}$ over the LO-phonon ground state Ψ_0. The effective polaron Hamiltonian describing the polaron in-plane motion reads

$$\overline{H}_{\rm pol}=\langle \Psi_0 U_2^{-1}\varphi_0(z)U_1^{-1}|H_{\rm eff}|U_1\varphi_0(z)U_2\Psi_0\rangle$$
$$=-\frac{\hbar^2}{2m_e}\left[1-\frac{2\hbar^2}{m_e}\sum_{\mathbf{k}}\frac{k_x^2|\overline{V}_{\mathbf{k}}(x)|^2}{[1+\overline{\delta}(x)]^2[\hbar\omega_{\rm LO}+(\hbar^2k_\parallel^2/2m_e)]^3}\right]\frac{d^2}{dx^2}+V_{\rm eff}(x)$$
$$+E_0-\sum_{\mathbf{k}}\frac{|\overline{V}_{\mathbf{k}}(x)|^2}{[1+\overline{\delta}(x)]^2[\hbar\omega_{\rm LO}+(\hbar^2k_\parallel^2/2m_e)]}+\overline{\delta}(x)\sum_{\mathbf{k}}\frac{|\overline{V}_{\mathbf{k}}(x)|^2}{\hbar\omega_{\rm LO}+(\hbar^2k_\parallel^2/2m_e)}\ , \tag{19}$$

with $V_{\rm eff}(x)=-E_0(h_0/d)\overline{\delta}(x)$,

$$\overline{\delta}(x)=\Theta(x+L)\left[1-\exp\left[-\frac{2\pi}{d}|x+L|\right]\right]$$
$$-\Theta(x-L)\left[1-\exp\left[-\frac{2\pi}{d}|x-L|\right]\right]$$

and

$$\overline{V}_{\mathbf{k}}(x)=\langle\varphi_0(z)|V_{\mathbf{k}}\exp\{-ik_z[z+\delta z(x,z)]\}|\varphi_0(z)\rangle\ ,$$

where $\Theta(x)$ is the unit-step function and $E_0=(\hbar^2/2m_e^*)(\pi/d)^2$.

For notational convenience we have redenoted $(u,v,w,)$ as (x,y,z). But one must keep in mind that we are working in the transformed space. In obtaining $\overline{H}_{\rm pol}$ (19), we have neglected the term $\partial^2/\partial v^2$ (or $\partial^2/\partial y^2$) for the ground state, which is assumed to be independent of v (or y), as can be seen from the geometric symmetry of the QW [Fig. 1(a)].

The last two terms in $\overline{H}_{\rm pol}$ (19) are the polaron self-energy due to the electron–LO-phonon interaction. To estimate the changes caused by the interface defect in the polaron self-energy, we calculate the self-energy at $|x|\to\infty$ and $x=0$. As $|x|\to\infty$, from Eqs. (6a) and (6b) we have $\delta x=0$ and $\delta z=0$. Substituting these into Eq. (19), we obtain that the polaron self-energy [the last two terms in $\overline{H}_{\rm pol}$ (19)] equals that of a QW with planar interfaces and width d. At $x=0$, we have $\delta x=0$ and $\delta z=(h_0/d)w-h_0$ (for $d/L_0\le 1$). The polaron self-energy equals that of a QW with planar interfaces and width $d+h_0$. The change in polaron self-energy caused by the interface defect is about $\alpha_{\rm LO}\hbar\omega_{\rm LO}(h_0/d)$. For weak-coupling materials, such as GaAs, the Frölich coupling constant $\alpha_{\rm LO}\le 0.1$, and when the QW is thin ($d<100$ Å), $\hbar\omega_{\rm LO}\le E_0$. The change in polaron self-energy is a negligible high-order perturbation. The same is true for the polaron renormalization mass due to the electron–LO-phonon interaction [the second term of the kinetic energy in $\overline{H}_{\rm pol}$ (19)]. The change in polaron renormalization mass caused by the interface defect is about $m_e\alpha_{\rm LO}(h_0/d)$. To the first order in h_0/d, we can set h_0 equal to zero in the calculation of the polaron self-energy and mass renormalization. $\overline{H}_{\rm pol}$ (19) can be further simplified to

$$\overline{H}_{\rm pol}=-\frac{\hbar^2}{2m_e^*}\frac{d^2}{dx^2}+V_{\rm eff}(x)+E_g^0 \tag{19'}$$

with

$$E_g^0=E_0-\frac{\pi}{2}\alpha_{\rm LO}\hbar\omega_{\rm LO},\quad m_e^*=\frac{m_e}{1+\pi\alpha_{\rm LO}/8}\ . \tag{20}$$

In the calculation of the polaron self-energy and polaron effective mass due to the electron–LO-phonon interaction in $\overline{H}_{\rm pol}$ (19′), we have assumed that the polaron is a strict 2D polaron.[2] This approximation does not affect our discussions on effects of interface defects on polaron states, because as discussed above the effects of interface defects on the electron–LO-phonon interaction can be neglected for weak-coupling materials. Examining $\overline{H}_{\rm pol}$ (19′) we find that when the terms of order $O(\alpha_{\rm LO}h_0/d)$ and higher are neglected, which is valid for weak-coupling materials, apart from an energy shift in E_g^0 and a small mass renormalization in m_e^* [see Eq. (20)], the problem of effects of interface defects of a QW on polaron state, such as its ground-state energy and the localization of the polaron motion in the plane parallel to the interface, can be treated as that for an electron in presence of interface defects.

The effective potential $V_{\rm eff}$ associated with the surface defect (an infinite track) in $\overline{H}_{\rm pol}$ (19′) is shown in Fig. 2 (solid line) for a GaAs-$Ga_{1-x}Al_xAs$ QW with an infinite track on one of its interfaces, where the width of the QW $d=70$ Å, the height of the track $h_0=5.72$ Å (about two

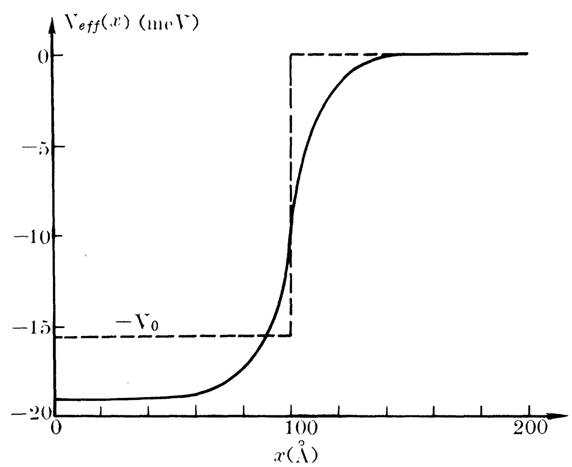

FIG. 2. Effective potential (solid line) associated with the surface defect—an infinite track as shown in Fig.1(a) in a GaAs-$Ga_{1-x}Al_xAs$ QW with the well width $d=70$ Å, the track height $h_0=5.72$ Å, and the track width $2L=200$ Å. The potential is an even function of x. The dashed line is the square potential well used in the text to determine the polaron trial wave function.

monolayers) and the width of the track $2L=200$ Å [see Fig. 1(a)]. V_{eff} is an even function of x, e.g., $V_{\text{eff}}(-x)=V_{\text{eff}}(x)$ and resembles a square potential well.

We calculate the ground-state energy of the trapped polaron variationally with the trial wave function taken as the ground-state wave function of a square potential well shown in Fig. 2 (dashed line). For a given potential depth V_0, the ground-state wave function is determined. So we introduce $\gamma=V_0/E_0$ as a variational parameter. The trial wave function $\varphi(\gamma,x)$ reads[24]

$$\varphi(\gamma,x)=\begin{cases} C\cos(\beta_0 x), & \text{for } |x|<L \\ C\cos(\beta_0 L)\exp[-\beta_1(|x|-L)] & \text{for } |x|>L \end{cases} \quad (21)$$

where C is the normalization constant, $\beta_1=[\gamma(\pi/d)^2-\beta_0^2]^{1/2}$, and β_0 satisfies the following equation:

$$\tan(\beta_0 L)=\beta_1/\beta_0 \quad (22)$$

with $\beta_0<\min\{\pi/2L, [\gamma(\pi/d)^2]^{1/2}\}$ to ensure that $\varphi(\gamma,x)$ (21) is the ground-state wave function.

The shift δE_g in the ground-state energy of the polaron caused by the interface defect relative to the ground-state energy E_g^0 of a QW with planar interfaces is obtained by minimizing the averaged $\overline{H}_{\text{pol}}$ (19′) with respect to γ,

$$\delta E_g=\min_{\gamma}[\langle\varphi(\gamma,x)|\overline{H}_{\text{pol}}-E_g^0|\varphi(\gamma,x)\rangle] . \quad (23)$$

The numerical results of δE_g as functions of the track half width L_0 are given in Fig. 3 (solid lines) with the track height $h_0=2.86$ Å (one monolayer) and 5.72 Å (two monolayers) for a GaAs-$Ga_{1-x}Al_xAs$ QW with a width $d=70$ Å [see Fig. 1(a)]. The experimental parameters are taken as $\alpha_{\text{LO}}=0.071$, $\hbar\omega_{\text{LO}}=36.8$ meV, and $m_e=0.66m_0$, which give $E_0=116.3$ meV and $E_g^0=112.2$ meV. The dashed lines in Fig. 3 correspond to δE_g with $L_0\to\infty$.

D. Ground-state energy of polarons in a QW with a cylindrical hollow on one of its interfaces

Though the cylindrical hollow is still an idealized interface defect, it is more realistic than the infinite track, for it is finite in all directions parallel to the interface. The coordinate transformation we need is obtained as follows. First, we introduce a coordinate space $(\tilde{\rho},\tilde{\varphi},\tilde{z})$, with $-\infty<\tilde{\rho}<\infty$, $0<\tilde{\varphi}<\pi$, and $-\infty<\tilde{z}<\infty$. It is related to coordinate space (x,y,z) by

$$x=\tilde{\rho}\cos\tilde{\varphi} , \quad (24a)$$

$$y=\tilde{\rho}\sin\tilde{\varphi} , \quad (24b)$$

$$z=\tilde{z} . \quad (24c)$$

Space $(\tilde{\rho},\tilde{\varphi},\tilde{z})$ is not the cylindrical coordinate system, for $\tilde{\rho}$ can be negative. Because of the cylindrical symmetry of the hollow, its profile looks the same on any section plane with $\tilde{\varphi}$ fixed. A section on the $\tilde{\rho}$-$\tilde{z}$ plane of a QW

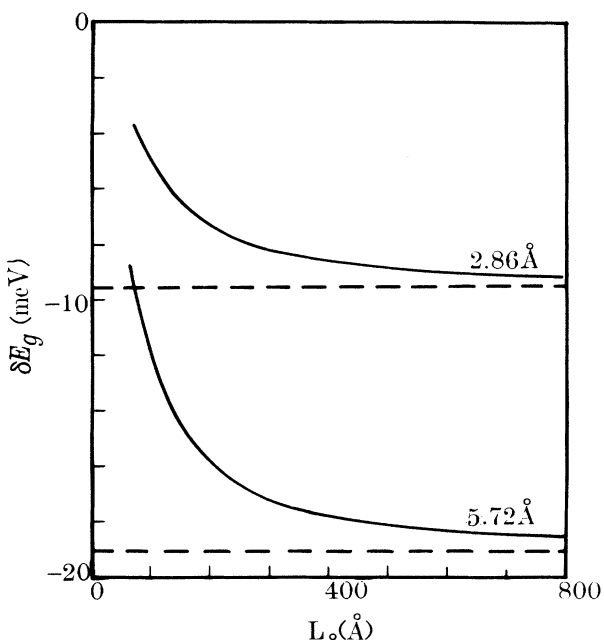

FIG. 3. Shift δE_g in the ground-state energy of the polaron, relative to that of a QW with planar interfaces, in a GaAs-$Ga_{1-x}Al_xAs$ QW with an infinite track on its interfaces. The results are given as functions of the track half width L_0 with the well width $d=70$ Å and the track height $h_0=2.86$ and 5.72 Å. The dashed lines correspond to δE_g with $L_0\to\infty$.

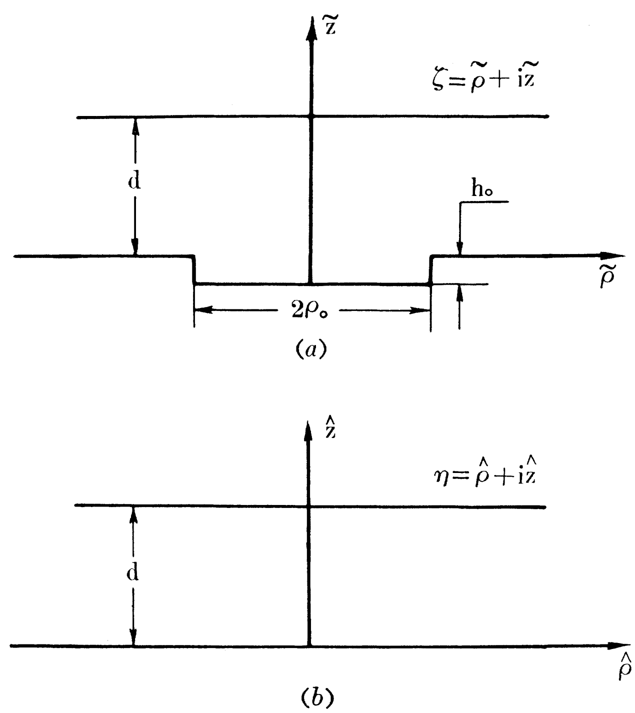

FIG. 4. (a) A section on the $\tilde{\rho}$-$\tilde{z}$ plane of the QW with a cylindrical hollow centered on the $\tilde{z}$ axis and protruding into the barrier material on one of the QW interfaces. (b) A section on the $\hat{\rho}$-$\hat{z}$ plane of the QW in (a) after the coordinate transformation introduced in the text.

with a cylindrical hollow centered on the $\tilde{z}$ axis and protruding into the barrier material on one of its interfaces is shown in Fig. 4(a). If we consider this section plane as a complex plane $\xi=\tilde{\rho}+i\tilde{z}$, the QW with the defect interface in complex plane ξ can be transformed to the QW with plane interfaces in complex plane $\eta=\hat{\rho}+i\hat{z}$ [as shown in Fig. 4(b)] by the coordinate transformation (6) we have obtained in Sec. II B. So we introduce the following transformation:

$$\tilde{\rho}=\hat{\rho}+\delta\tilde{\rho}(\hat{\rho},\hat{z}) , \tag{25a}$$

$$\tilde{\varphi}=\hat{\varphi} , \tag{25b}$$

$$\tilde{z}=\hat{z}+\delta\tilde{z}(\hat{\rho},\hat{z}) , \tag{25c}$$

with Eqs. (25a) and (25c) given by Eqs. (6a) and (6b). Finally, we introduce the cylindrical coordinate space (ρ,φ,z) given by

$$\rho=\hat{\rho} \text{ for } \hat{\rho}>0, \quad \rho=-\hat{\rho} \text{ for } \hat{\rho}<0 ; \tag{26a}$$

$$\varphi=\hat{\varphi} \text{ for } \hat{\rho}>0, \quad \varphi=\hat{\varphi}+\pi \text{ for } \hat{\rho}<0 ; \tag{26b}$$

$$z=\hat{z} \text{ for } \hat{\rho}>0, \quad z=\hat{z} \text{ for } \hat{\rho}<0 . \tag{26c}$$

The coordinate transformations (24)–(26) are what we need to transform the QW with the defective interfaces [Fig. 4(a)] to the QW with plane interfaces [Fig. 4(b)]. Substituting these transformation into the polaron Hamiltonian H_{pol} (1)–(3), and following the same manipulations as in Sec. II C, we obtain the effective polaron Hamiltonian describing the polaron in-plane motion

$$\overline{H}_{\text{pol}}=-\frac{\hbar^2}{2m_e^*}\left[\frac{d^2}{d\rho^2}+\frac{d\rho}{\rho d\rho}\right]+V_{\text{eff}}(\rho)+E_g^0 , \tag{27}$$

with m_e^* and E_g^0 being the same as those defined in Eq. (20) and

$$V_{\text{eff}}(\rho)=-E_0\frac{h_0}{d}\left\{\vartheta(\rho+\bar{\rho})\left[1-\exp\left[-\frac{2\pi}{d}|\rho+\bar{\rho}|\right]\right]-\vartheta(x-\bar{\rho})\left[1-\exp\left[-\frac{2\pi}{d}|\rho-\bar{\rho}|\right]\right]\right.$$
$$\left.+\frac{d}{2\pi\rho}\left[\exp\left[-\frac{2\pi}{d}|\rho+\bar{\rho}|\right]-\exp\left[-\frac{2\pi}{d}|\rho-\bar{\rho}|\right]\right]\right\} \tag{28}$$

where

$$\bar{\rho}=\rho_0\frac{1+(h_0/\pi\rho_0)\ln(h_0/2d)}{1+(h_0/d)} .$$

In obtaining $\overline{H}_{\text{pol}}$ (27), we have neglected high-order perturbations such as terms containing $(h_0/d)^2$ and $\alpha_{\text{LO}}(h_0/d)$, etc. We have also neglected the term $\partial^2/\partial\varphi^2$ in $\overline{H}_{\text{pol}}$ for the ground state, which is assumed to be independent of φ, as can be seen from the geometric symmetry of the QW [Fig. 4(a)].

The effective potential V_{eff} associated with the surface defect (a cylindrical hollow) in $\overline{H}_{\text{pol}}$ (27) is shown in Fig. 5 (solid line) for a GaAs-$Ga_{1-x}Al_x$As QW with a cylindrical hollow on one of its interfaces, where the width of the QW $d=70$ Å, the height of the hollow $h=5.72$ Å (about two monolayers) and the radius of the hollow $\bar{\rho}=100$ Å [see Fig. 4(a)]. V_{eff} resembles a 2D square potential well. The trial wave function $\varphi(\gamma,\rho)$ of the polaron ground state is taken as the ground-state wave function of a 2D square potential well shown in Fig. 5 (dashed line).

$$\varphi(\gamma,\rho)=\begin{cases} CJ_0(\beta_0\rho) & \text{for } \rho<\bar{\rho} \\ C\dfrac{J_0(\beta_0\bar{\rho})}{K_0(\beta_1\bar{\rho})}K_0(\beta_1\rho) & \text{for } \rho>\bar{\rho} \end{cases} \tag{29}$$

where J_n and K_n are the Bessel functions of the first kind and modified Bessel function of the second kind, respectively; C is the normalization constant, $\gamma=V_0/E_0$ is the variational parameter, $\beta_1=[\gamma(\pi/d)^2-\beta_0^2]^{1/2}$, and β_0 satisfies the following equation:

$$\beta_0\frac{J_1(\beta_0\bar{\rho})}{J_0(\beta_0\bar{\rho})}=\beta_1\frac{K_1(\beta_1\bar{\rho})}{K_0(\beta_1\bar{\rho})} \tag{30}$$

with

$$\beta_0<\min\{2.4048/\bar{\rho},\ [\gamma(\pi/d)^2]^{1/2}$$

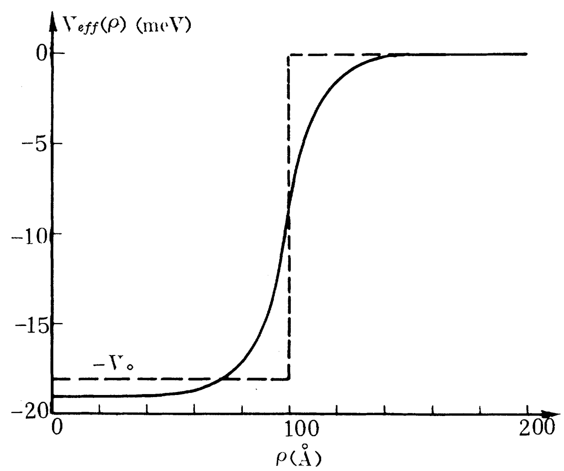

FIG. 5. Effective potential (solid line) associated with the surface defect—a cylindrical hollow as shown in Fig. 4(a) in a GaAs-$Ga_{1-x}Al_x$As QW with the well width $d=70$ Å, the hollow height $h_0=5.72$ Å, and the hollow radius $\bar{\rho}=100$ Å. The dashed line is the 2D square potential well used in the text to determine the polaron trial wave function.

to ensure that $\varphi(\gamma,x)$ (29) is the ground-state wave function.

The shift δE_g in the ground-state energy of the polaron caused by the interface defect relative to the ground-state energy E_g^0 of a QW with planar interfaces is obtained by

$$\delta E_g = \min[\langle \varphi(\gamma,\rho)|\overline{H}_{\rm pol} - E_g^0|\varphi(\gamma,\rho)\rangle] \ . \qquad (31)$$

The numerical results of δE_g as functions of the hollow radius ρ_0 is given in Fig. 6 (solid lines) with the hollow height $h_0 = 2.86$ Å (one monolayer) and 5.72 Å (two monolayers). Other parameters are the same as those defined in Fig. 3. The dashed lines in Fig. 6 correspond to δE_g with $\rho_0 \to \infty$.

III. DISCUSSION

As discussed in Sec. II C, polarons in QW's with defective interfaces will be trapped at places where the QW interfaces protrude into the barrier materials making the QW's locally wide. This is also shown clearly in the effective potential $V_{\rm eff}$ associated with the interface defects in Fig. 2 and 5 (solid lines). Because $V_{\rm eff}$ is inversely proportional to the mass of the particle (the electron) [see Eqs. (19) and (28)], the effective Hamiltonian $\overline{H}_{\rm pol} - E_g^0$ [see Eqs. (19′) and (27)], which determines the in-plane spatial distribution of the particle, is also inversely proportional to the mass of the particle. This implies that the wave function of the in-plane distribution of the particle is independent of its mass, that is, in one QW both the electron and hole will be trapped at the same place. This in-plane confinement of the electron and hole will increase the exciton binding energy just like the confinement of the electron and hole within the QW increases the exciton binding energy comparing with that in bulk materials.

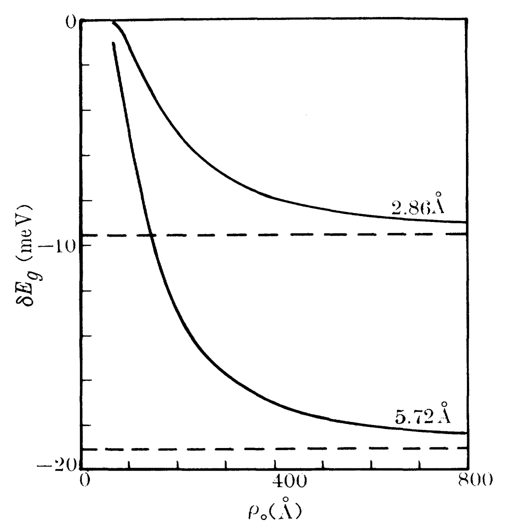

FIG. 6. Shift δE_g in the ground-state energy of the polaron, relative to that of a QW with planar interfaces, in a GaAs-$Ga_{1-x}Al_xAs$ QW with a cylindrical hollow on its interfaces. The results are given as functions of the hollow radius ρ_0 with the well width $d = 70$ Å and the hollow height $h_0 = 2.86$ and 5.72 Å. The dashed lines correspond to δE_g with $\rho_0 \to \infty$.

The numerical calculations show that the change δE_g in the polaron energy caused by the interface defects is a function of ρ_0/d and depends on the well width d through multiplication constants $E_0 = (\hbar^2/2m_e^*(\pi/d)^2$ and h_0/d. If we give the numerical results $\delta E_g/[(h_0/d)E_0]$ as a function of ρ_0/d, for QW's with different well width the curves in Figs. 3 and 6 (solid lines) change little as long as ρ_0/d is the same. It is seen clearly from Fig. 6 (solid lines) that the change δE_g in the polaron energy caused by the interface defects depends strongly on the lateral size of the defect when $\rho_0/d < 4$. For instance, when $\rho_0/d < 2$, δE_g is less than half of its maximum

$$\delta E_g^0 = \frac{\hbar^2}{2m_e^*}\left[\frac{\pi}{d}\right]^2 \frac{2h_0}{d} \ ,$$

which is the limit value of δE_g when $\rho_0 \to \infty$. In explaining a systematic increase of the linewidth of luminescence, absorption, and excitation spectra of undoped GaAs-$Ga_{1-x}Al_xAs$ multiquantum-well structures with decreasing layer thickness, Weisbuch *et al*,[13,14] have attributed this broadening to the islandlike structure of the QW interfaces. Their calculation agrees very well with the experiment for the well width d in the 80–150 Å range with a simple assumption that an interface defect with a height h_0 will shift the electron energy by

$$\delta E_g^0 = \frac{\hbar^2}{2m_e^*}\left[\frac{\pi}{d}\right]^2 \frac{2h_0}{d}$$

with well width fluctuations h_0 being about one or two monolayers. From the theory of Weisbuch *et al.*[13,14] and together with our numerical results in Fig. 6 (solid lines), we have the following two different conclusions: (i) If the well-width fluctuations are about one or two monolayers as suggested by Weisbuch *et al.*,[13,14] for their calculation to be correct, we must assume that the average radius of the interface defects ρ_0 is larger than $4d$ ($d = 80$–150 Å) to have $\delta E_g \to \delta E_g^0$ [see Fig. 6 (solid lines)], that is, the average lateral size of interface defects $2\rho_0$ is larger than 1000 Å, and (ii) if the lateral size of interface defects is about several hundred angstroms ($\simeq 400$ Å) as suggested by Weisbuch *et al.*[13] and other authors,[15,16] we have that the ratio $\rho_0/d = 200/d \simeq 2$ ($d = 80$–150 Å) and $\delta E_g \simeq 0.5\delta E_g^0$ [see Fig. 6 (solid lines)]. To observe the spectrum broadenings in the experiment of Weibuech *et al.*,[13,14] the well width fluctuations must be larger than one or two monolayers. At present, we are not able to decide which conclusion is correct, for we lack information on the detailed statistics of the shapes and heights of the interface defects. But one thing is certain: our calculation predicts smaller effect on the electronic states (such as broadenings of the luminescence, absorption, and excitation spectra) than that predicted by the theory of Weisbuch *et al.*[13,14] for the same QW interface disorder.

As discussed in Sec. II C, for materials with weak electron-phonon interaction, such as GaAs, where $\alpha_{\rm LO} < 0.1$, the changes in the polaron self-energy and polaron effective mass caused by interface defects are negligible. But for materials with strong electron-phonon coupling ($\alpha_{\rm LO}>1$), and when the width of the QW is not very thin so that $(\hbar^2/2m_e^*)(\pi/d)^2 \leq \hbar\omega_{\rm LO}$, the change in the polaron self-energy caused by interface defects is not negligible. The polaron self-energy depends on the position of the electron. This position dependent polaron self-energy is another effective potential acting upon the polaron in determining the in-plane motion of the polaron. Because the polaron self-energy at places where the QW is thin is lower than that where the QW is wide,[2] this effective potential partially cancels the effective potential $V_{\rm eff}$ we derived in Sec. II, since it shows potential barriers at places where $V_{\rm eff}$ shows potential wells. It might be possible that this cancellation is so overwhelming that the polaron would be trapped at places where interface defects make the QW locally thin.

In studying exciton trappings on QW interface defects, it is important to know how excitons are trapped. A correct picture of the exciton trapping is very helpful in giving correct estimations of ground-state energies of trapped excitons in experiments and determining the choice of the exciton trial wave functions in numerical calculations. One can view the trapping of excitons on interface defects with aid of the following two pictures: (i) The electron and hole are trapped on interface defects individually, and then they form the exciton by the Coulombic interaction, and (ii) the electron and hole form the exciton first, and then the exciton as a whole, or its mass center, is trapped on interface defects. Which picture is more favorable is determined by which one gives a lower exciton energy. With the present theory, we estimate the exciton energy with the following approximations: First, we assume that the Coulombic interaction energies $E_{\rm Coul}$ are the same for the two pictures. Second, we assume that the exciton can be treated as a point. Its mass center moves in a 2D effective potential which is the superposition of the electron and hole effective potentials given by Eq. (28). The latter approximation is valid for the case where the radius of the interface defect ρ_0 is larger than the exciton radius, which is about 150 Å in bulk GaAs. With the above approximations, we obtain the exciton energy for picture (i):

$$E_{\rm ex}=\frac{\hbar^2}{2m_e^*}\left[\frac{\pi}{d}\right]^2+\frac{\hbar^2}{2m_h^*}\left[\frac{\pi}{d}\right]^2+E_{\rm Coul}+\delta E_g^e+\delta E_g^h\,, \tag{32}$$

and for picture (ii)

$$E_{\rm ex}=\frac{\hbar^2}{2m_e^*}\left[\frac{\pi}{d}\right]^2+\frac{\hbar^2}{2m_h^*}\left[\frac{\pi}{d}\right]^2+E_{\rm Coul}+\delta E_g^c\,, \tag{33}$$

where $\delta E_g^{e(h)}$ is the energy of the electron (hole) in-plane motion determined by the effective Hamiltonian (27), and δE_g^c is the energy of the in-plane motion of the exciton

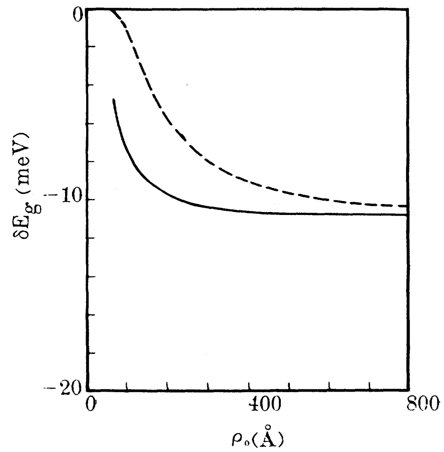

FIG. 7. The dashed line is the energy of the electron and hole in-plane motions in a GaAs-$Ga_{1-x}Al_xAs$ QW described in Fig. 6 when the electron and hole are trapped individually on the interface defect. The solid line is the energy of the in-plane motion of the exciton mass center in the same QW with the exciton treated as a point. The results are given as functions of the radius ρ_0 of the interface defect.

mass center. In Fig. 7, we give the numerical results of $\delta E_g^e+\delta E_g^h$ (dashed line) and δE_g^c (solid line) as functions of ρ_0 for a QW with a cylindrical hollow on one of its interfaces, where the well width $d=70$ Å and the height of the hollow $h_0=2.86$ Å. Obviously, the exciton will be trapped as a whole on interface defects, as suggested by some authors.[15,16] The results for $\rho_0<200$ Å in Fig. 7 is not very meaningful, because when $\rho_0<200$ Å, the radii of the defect and the exciton are about the same order of magnitude. Excitons can no longer be treated as points. Rigorous calculations including the Coulombic interaction between electrons and holes are needed to determine how excitons are trapped on interface defects.

Bastard *et al*,[15] have made a theoretical investigation on effects of interface defects on excitons in QW's. They modeled QW's with defective interfaces by QW's with planar interfaces and added an empirical potential energy associated with the interface defects to the Hamiltonian. The choice of the empirical potential energy is to some extent arbitrary. So the results obtained from the theory only qualitatively explained the effects of defective interfaces on excitons in QW's. Another approximation made by Bastard *et al.*[15] in their theory is the neglect of changes in Coulombic potential between the electron and hole when modeling QW's with defective interfaces by QW's with planar interfaces. While the theoretical calculations of Bastard *et al.*[25] have shown that the Coulombic energy of excitons in GaAs-$Ga_{1-x}Al_xAs$ QW's shows a strong dependence on the well width when the well width $d<150$ Å. These approximations are not necessary in the theory we presented. The potential energy associated with the interface defects are derived uniquely from the theory. And if we substitute the coordinate transformations derived in Sec. II into the Coulombic potential of the electron and hole, an additional term associated with the interface defects will appear. We think that it will be worthwhile reexamining the effects of interface defects on exciton in QW's using the theory we presented in this paper.

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