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Polaron ground state in a double heterostructure of polar crystals

D L Lin, R Chen and Thomas F George
Department of Physics and Astronomy, State University of New York at Buffalo, Buffalo, NY 14260, USA

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Abstract. The ground-state energy and effective mass of a polaron in the GaAs well of a GaAs/AlAs double heterostructure are calculated as functions of the well width. In considering electron–phonon interactions, we have included both the confined longitudinal optical (LO) as well as the interface phonon modes. The results differ qualitatively from what can be found in the literature, demonstrating the importance of interface modes as well as the confinement of LO modes.

1. Introduction

There have been extensive investigations in recent years on the electronic properties in heterostructures and superlattices of polar crystals. In particular, the importance of the interaction between electrons and the polarization field of longitudinal optical (LO) phonons has been well recognized as it strongly modifies the transport and optical properties of such microstructures of reduced dimensionality. In dealing with the electron–phonon interaction in heterostructures, however, most of the researchers have assumed the Frölich Hamiltonian for a confined electron interacting with bulk phonons.

The polaronic states in a slab of polar crystals have recently been calculated (Liang *et al* 1986) with both surface optical (SO) and LO phonons included. It is shown that the energy correction due to surface phonons can be very significant provided that the thickness of the slab is sufficiently small. In practice, however, measurements of quasi-two-dimensional polarons can only be made in quantum wells or superlattices which differ from an isolated slab by the presence of interfaces. The optical phonon modes in these structures are expected to be qualitatively different from those in a slab (Lassnig 1984, Sood *et al* 1985). As a matter of fact, optical phonon modes and their interactions with an electron in a single heterostructure (Wendler 1985) and semiconductor double heterostructure (DHS) (Lin *et al* 1990a, b, Chen *et al* 1990, Mori and Ando 1989) have been reported recently. In the case of a GaAs/AlGaAs DHS, it is found that near the centre of the first Brillouin zone, the interface phonon with longitudinal polarization in fact vibrates at a bulk TO frequency and vice versa (Lin *et al* 1990a). The interface phonon is also found (Lin *et al* 1990b, 1991) to be responsible for the pinning phenomenon observed in the transition-energy measurements of a magnetopolaron bound to a hydrogenic impurity in quantum wells (Chang *et al* 1988). Furthermore, significant effects of

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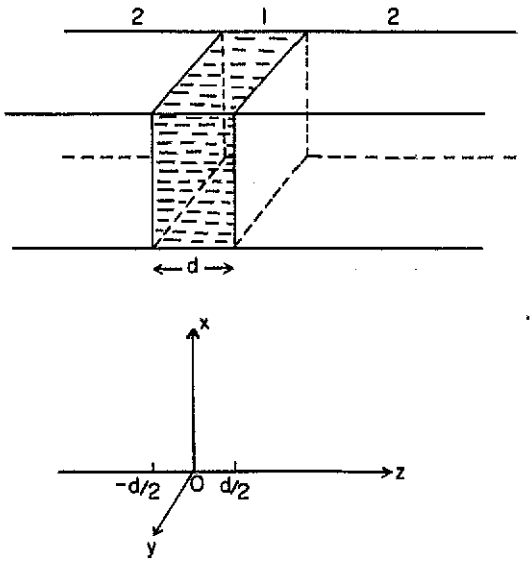

Figure 1. Geometry of the DHS composed of materials 1 and 2.

interface modes on the polaron mobility and magnetopolaron resonance have been obtained in theoretical calculations (Mori and Ando 1989).

The surface phonon contribution to polaron effects in a slab on the top of a substrate has already been considered (Degani and Hipolito 1988). We calculate in this paper the ground-state energy and effective mass for a polaron confined in a DHS with the interaction Hamiltonian derived previously (Lin *et al* 1990b). Both the binding energy and effective mass are calculated as functions of the well width d. Because of the presence of interface phonons, the variation of these quantities with d is shown to be qualitatively different from that found in the literature. The polaron binding energy starts with the bulk value of the side material when $d \approx 0$, increases rapidly to a maximum as d increases, drops back to a minimum, and then increases slowly to the limit of the bulk value of the central layer as d increases indefinitely. The effective mass, on the other hand, decreases slightly at first and then increases with increasing d.

After the total Hamiltonian is written down, the binding energy and effective mass of the polaron confined in the GaAs well of a GaAs/AlAs DHS are calculated. We then discuss our results and present conclusions.

2. The Hamiltonian

Consider a DHS of two different polar crystals as shown in figure 1. The central layer is labelled 1 and the side material is labelled 2. We introduce, for convenience, the two-dimensional vectors $\boldsymbol{\kappa}$ and $\boldsymbol{\rho}$ such that $\boldsymbol{k} = (\boldsymbol{\kappa}, q)$ and $\boldsymbol{r} = (\boldsymbol{\rho}, z)$ for the phonon momentum and electron position. In the effective mass approximation our problem is to solve the electron–phonon interaction in a square well of width d. Thus the total Hamiltonian may be written as

$$H = H_e + H_{ph} + H_{e\text{-}ph}. \tag{1}$$

The first term describes an electron in a finite square well and is given by

$$H_e = \begin{cases} p^2/2m_e & |z| < d/2 \\ p^2/2m_e + V_0 & |z| \geqslant d/2. \end{cases} \tag{2}$$

where m_e stands for the electron band mass. For simplicity, we assume throughout this paper the same m_e in both materials 1 and 2. Different band masses merely complicate the calculation, but no qualitative change of results is expected (Greene and Bajaj 1985). The second term in (1) is the free-phonon Hamiltonian which includes the travelling interface modes with wave vector κ in the xy plane and the confined modes with wave vector q in the z direction. As has been discussed in detail previously (Chen *et al* 1990), the confined modes in the central layer are quantized with discrete allowed values of the wave vector, $q = m\pi/d$, but remain continuous in the side layers. Thus,

$$H_{ph} = \sum_{q,\kappa,\nu} \hbar\omega_{L\nu}\,[a_q^\dagger(\kappa)a_q(\kappa) + \tfrac{1}{2}] + \sum_{\kappa,j} \{\hbar\omega_{sj}(\kappa)\,[a_{sj}^\dagger(\kappa)a_{sj}(\kappa) + \tfrac{1}{2}] + \hbar\omega_{aj}(\kappa)\,[a_{aj}^\dagger(\kappa)a_{aj}(\kappa) + \tfrac{1}{2}]\} \tag{3}$$

where $\omega_{L\nu}$ is the frequency of the bulk LO phonon in material ν ($\nu = 1, 2$) and ω_{sj} and ω_{aj} are the symmetric and antisymmetric interface phonon frequencies, respectively. The index $j = 1, 2$ labels the two branches of these modes. $a^\dagger$ and a are the corresponding phonon creation and annihilation operators. While $\omega_{L\nu}$ are constant, the interface modes are dispersive and are given by (Chen *et al* 1990)

$$\begin{aligned}\omega_{aj} = \{[\varepsilon_{\infty 2}(\omega_{T1}^2 + \omega_{L2}^2) + \varepsilon_{\infty 1}(\omega_{T2}^2 + \omega_{L1}^2)\coth(\kappa d/2) \pm \{\varepsilon_{\infty 2}^2(\omega_{T1}^2 - \omega_{L2}^2)^2 \\ + \varepsilon_{\infty 1}^2(\omega_{T2}^2 - \omega_{L1}^2)^2\coth^2(\kappa d/2) + 2\varepsilon_{\infty 1}\varepsilon_{\infty 2}[(\omega_{T1}^2 + \omega_{L2}^2)(\omega_{T2}^2 + \omega_{L1}^2) \\ - 2(\omega_{T2}^2\omega_{L1}^2 + \omega_{L2}^2\omega_{T1}^2)\coth(\kappa d/2)]\}^{1/2}\}^{1/2} \\ \times \{2[\varepsilon_{\infty 2} + \varepsilon_{\infty 1}\coth(\kappa d/2)]\}^{-1/2}\end{aligned} \tag{4a}$$

$$\begin{aligned}\omega_{sj} = \{[\varepsilon_{\infty}(\omega_{T1}^2 + \omega_{L2}^2) + \varepsilon_{\infty 1}(\omega_{T2}^2 + \omega_{L1}^2)\tanh(\kappa d/2) \pm \{\varepsilon_{\infty 2}^2(\omega_{T1}^2 - \omega_{L2}^2)^2 \\ + \varepsilon_{\infty 1}^2(\omega_{T2}^2 - \omega_{L1}^2)^2\tanh^2(\kappa d/d) + 2\varepsilon_{\infty 1}\varepsilon_{\infty 2}[(\omega_{T1}^2 + \omega_{L2}^2)(\omega_{T2}^2 + \omega_{L1}^2) \\ - 2(\omega_{T2}^2\omega_{L1}^2 + \omega_{T1}^2\omega_{L2}^2)]\tanh(\kappa d/2)\}^{1/2}\}^{1/2} \\ \times \{2[\varepsilon_{\infty 2} + \varepsilon_{\infty 1}\tanh(\kappa d/2)]\}^{-1/2}\end{aligned} \tag{4b}$$

where $j = 1$ (2) when one takes the + (−) sign in the second term.

The last term in (1) stands for the electron–phonon interaction, which can be written as

$$H_{e\text{-}ph} = H_{e\text{-}LO} + H_{e\text{-}IN}. \tag{5}$$

The confined LO modes have different frequencies on the adjacent layers. Hence $H_{e\text{-}LO}$ can be written as

$$H_{e\text{-}LO} = -\sum_{\kappa} e^{i\kappa\cdot\rho}\left\{\sum_{m=1,3,\ldots} B_m(\kappa)\cos[(m\pi/d)z][a_m(\kappa) + a_m^\dagger(-\kappa)] + \sum_{m=2,4,\ldots} B_m(\kappa)\sin[(m\pi/d)z][a_m(\kappa) + a_m^\dagger(-\kappa)]\right\} \tag{6a}$$

$$|B_m(\kappa)|^2 = (1/Ad)\,4\pi e^2\hbar\omega_{L1}/[\kappa^2 + (m\pi/d)^2](1/\varepsilon_{\infty 1} - 1/\varepsilon_{01}) \tag{6b}$$

for $|z| < d/2$, where the wave vector $q = m\pi/d$ is quantized and

$$H_{e\text{-}LO} = -\sum_{\kappa}\sum_{q>0} e^{i\kappa\cdot\rho} B_q(\kappa)\sin(q|z| - qd/2)[a_q(\kappa) + a_q^\dagger(-\kappa)] \tag{7a}$$

$$|B_q(\kappa)|^2 = (1/AD)\,4\pi e^2\hbar\omega_{L2}/(\kappa^2 + q^2)(1/\varepsilon_{\infty 2} - 1/\varepsilon_{02}) \tag{7b}$$

for $z > d/2$, where q is in the continuum and the thickness $D \to \infty$ is assumed at the end of the calculation. In (6*b*) and (7*b*), A stands for the interface area and $\varepsilon_{\infty\nu}$ and $\varepsilon_{0\nu}$ denote the optic and dielectric constants of material ν. The interaction of the electron with interface modes is given by (Lin *et al* 1990b).

$$H_{e\text{-}IN} = -\sum_{\kappa,j} e^{i\kappa\cdot\rho - \kappa(|z| - d/2)}\{B_{sj}(\kappa)[\hat{a}_{s,j}(\kappa) + \hat{a}_{s,j}^\dagger(-\kappa)]$$

$$- \operatorname{sgn}(z)B_{aj}(\kappa)[\hat{a}_{a,j}(\kappa) + \hat{a}_{a,j}^\dagger(-\kappa)]\} \qquad \text{for } |z| > d/2 \tag{8a}$$

$$H_{e\text{-}IN} = -\sum_{\kappa,j} e^{i\kappa\cdot\rho}\{B_{sj}(\kappa)\cosh(\kappa z)/\cosh(\kappa d/2)[\hat{a}_{s,j}(\kappa) + \hat{a}_{s,j}^\dagger(-\kappa)]$$

$$- B_{aj}(\kappa)[\sinh(\kappa z)/\sinh(\kappa d/2)][\hat{a}_{a,j}(\kappa) + \hat{a}_{a,j}^\dagger(-\kappa)]\} \tag{8b}$$

$$\text{for } |z| < d/2$$

$$|B_{sj}(\kappa)|^2 = (\pi e^2/A\kappa)\,\hbar\omega_{sj}(\kappa)/[\bar{\varepsilon}_1 \tanh(\kappa d/2) + \bar{\varepsilon}_2] \tag{9a}$$

$$|B_{aj}(\kappa)|^2 = (\pi e^2/A\kappa)\,\hbar\omega_{aj}(\kappa)/[\bar{\varepsilon}_1 \coth(\kappa d/2) + \bar{\varepsilon}_2] \tag{9b}$$

where we have defined the function $\operatorname{sgn}(z) = 1$ for $z > 0$ and -1 for $z < 0$. The function $\bar{\varepsilon}_\nu(\omega)$ is defined by

$$1/\bar{\varepsilon}_\nu(\omega) = 1/[\varepsilon_\nu(\omega) - \varepsilon_{0\nu}] - 1/[\varepsilon_\nu(\omega) - \varepsilon_{\infty\nu}] \tag{10}$$

with the dielectric function of materials, ν, given by

$$\varepsilon_\nu(\omega) = \varepsilon_{\infty\nu}(\omega_{L\nu}^2 - \omega^2)/(\omega_{T\nu}^2 - \omega^2). \tag{11}$$

3. Polaron ground-state energy

We now proceed to calculate the polaron binding energy by treating the interaction Hamiltonian, $H_{e\text{-}ph}$, as a perturbation on the eigenstates of the free Hamiltonian $H_e + H_{ph}$. The unperturbed ground state wave function is taken to be

$$|\psi_0\rangle = |k_\parallel, 0; n_{\kappa,\beta}\rangle = \frac{1}{\sqrt{A}} e^{ik_\parallel\cdot\rho} f(z)\,|n_{\kappa,\beta}\rangle \tag{12}$$

where use has been made of the fact that electron states are characterized by a plane wave $k_\parallel$ in the xy-plane and the ground state 0 in the z direction. The electron wave

vector is defined as $\boldsymbol{k}_e = (\boldsymbol{k}_\parallel, k_z)$ and the electron ground-state wave function in a quantum well is given by

$$f(z) = \begin{cases} C\cos(k_z d/2)\, e^{ik_z'(|z|-d/2)} & |z| \geqslant d/2 \\ C\cos(k_z z) & |z| < d/2. \end{cases} \tag{13}$$

The wave numbers k_z and k_z' are related to the electron subband energy E_l by

$$k_z = \sqrt{2m_e E_l/\hbar^2} \qquad k_z' = \sqrt{2m_e(V_0 - E_l)/\hbar^2} \tag{14}$$

with E_l determined by the transcendental equation

$$E_l = V_0 \cos^2[(d/2)\sqrt{2m_e E_l/\hbar^2}] \quad l = 1, 2, \ldots. \tag{15}$$

The normalization constant, C, is given by

$$C = \sqrt{2k_z'/(k_z' d + 2)}. \tag{16}$$

The phonon state $|n_{k,\beta}\rangle$ is specified by n phonons with wave vector $\boldsymbol{k} = (\boldsymbol{\kappa}, q)$ and index β labelling the phonon mode, which may be one of the interface or confined LO modes.

The unperturbed energy of the electron in the ground state (12) can be written as

$$\varepsilon_{k_e}^{(0)} = \frac{\hbar k_\parallel^2}{2m_e} + E_l + \sum_{\kappa,\beta} (n + \tfrac{1}{2})\hbar\omega_{\kappa,\beta}. \tag{17}$$

In the weak-coupling approximation, the corrections due to the electron–phonon interaction can be calculated by standard perturbation theory as

$$\varepsilon_{k_e} - \varepsilon_{k_e}^{(0)} = \sum_{\kappa,\beta} \frac{|\langle \boldsymbol{k}_\parallel, 1_{\kappa,\beta}|H_{e\text{-ph}}|\boldsymbol{k}_\parallel - \boldsymbol{\kappa}, 0_{\kappa,\beta}\rangle|^2}{\varepsilon_{k_\parallel}^{(0)} - \varepsilon_{k_\parallel - \kappa}^{(0)} - \hbar\omega_{\kappa,\beta}} \tag{18}$$

where we have assumed that transitions to or from a state with more than one phonon are negligible. This is true as long as the phonon energy $\hbar\omega_k \geqslant k_B T$, and the temperature does not have to be absolute zero. For simplicity, matrix elements corresponding to interband transitions are ignored in our calculation. This is a good approximation, in general, except for the two limiting cases $d \to 0$ and $d \to \infty$, where the whole subband spectrum including the continuum should be included because the subband energy spacings become arbitrarily small in these limits. We should emphasize here that leaving out any part of the electron energy spectrum would then not guarantee the correct limiting values. With these simplifications in mind, we can rewrite (18) as

$$\varepsilon_{k_e} - \varepsilon_{k_e}^{(0)} = \Delta E_1 + \Delta E_2 + \Delta E_3 \tag{19}$$

where ΔE_1 is the correction due to the confined LO modes in the central layer,

$$\Delta E_1 = \sum_{\kappa,m} \frac{|\langle \boldsymbol{k}_\parallel, 1_{\kappa,m}|H_{e\text{-LO}}|\boldsymbol{k}_\parallel - \boldsymbol{\kappa}, 0_{\kappa,m}\rangle|^2}{\hbar^2 k_\parallel^2/2m_e - \hbar^2(\boldsymbol{k}_\parallel - \boldsymbol{\kappa})^2/2m_e - \hbar\omega_{L1}}. \tag{20a}$$

ΔE_2 is caused by the confined LO modes in the side layers,

$$\Delta E_2 = \sum_{\kappa,q>0} \frac{|\langle \boldsymbol{k}_\parallel, 1_{\kappa,q}|H_{e\text{-LO}}|\boldsymbol{k}_\parallel - \boldsymbol{\kappa}, 0_{\kappa,q}\rangle|^2}{\hbar^2 k_\parallel^2/2m_e - \hbar^2(\boldsymbol{k}_\parallel - \boldsymbol{\kappa})/2m_e - \hbar\omega_{L2}} \tag{20b}$$

and ΔE_3 is due to the interface modes,

$$\Delta E_3 = \sum_{\kappa,j} \left\{ \frac{|\langle \boldsymbol{k}_\parallel, 1_{\kappa,sj}|H_{e\text{-IN}}|\boldsymbol{k}_\parallel, 0_{\kappa,q}\rangle|^2}{\hbar^2 k_\parallel^2/2m_e - \hbar^2(\boldsymbol{k}_\parallel - \boldsymbol{\kappa})^2/2m_e - \hbar\omega_{sj}} + \frac{|\langle \boldsymbol{k}_\parallel, 1_{\kappa,aj}|H_{e\text{-IN}}|\boldsymbol{k}_\parallel - \boldsymbol{\kappa}, 0_{\kappa,aj}\rangle|^2}{\hbar^2 k_\parallel^2/2m_e - \hbar^2(\boldsymbol{k}_\parallel - \boldsymbol{\kappa})^2/2m_e - \hbar\omega_{aj}} \right\}. \tag{20c}$$

It is noted that the second term in (20*c*) vanishes identically because the antisymmetric phonon wave function is an odd function while the electron ground state is an even function. With the Hamiltonian operators given by (6)–(8), and the wave function by (12), we find, after integration over the phonon momentum, that

$$\Delta E_1 = -\alpha_{L1}\hbar\omega_{L1} - (\hbar^2 k_\parallel^2/2m_e)\gamma_{L1} \tag{21a}$$

$$\Delta E_2 = -\alpha_{L2}\hbar\omega_{L2} - (\hbar^2 k_\parallel^2/2m_e)\gamma_{L2} \tag{21b}$$

$$\Delta E_3 = -\sum_j \int_0^\infty d\kappa\, \alpha_{IN}(\kappa)\hbar\omega_{\beta j}(\kappa) - (\hbar^2 k_\parallel^2/2m_e)\gamma_{IN}. \tag{21c}$$

The parameters α and γ are related to the Fröhlich-type coupling constants involving the particular phonon modes indicated by the subscripts. Explicitly, the α's are given by

$$\alpha_{L1} = \frac{4\alpha_{F1}}{K_{p1}d}|C|^4 \sum_{m=1,3,\ldots} \left(\frac{d}{m\pi}\right)^2 \left(1 + \frac{\cos(k_z d)}{1-(2k_z d/\mu\pi)^2}\right)^2 \left[\left(\frac{m\pi}{K_{p1}d}\right)^2 - 1\right]^{-1} \ln\left|\frac{m\pi}{K_{p1}d}\right| \tag{22a}$$

$$\alpha_{L2} = \frac{4\alpha_{F2}}{\pi K_{p2}^2}|C|^4 \cos^4(k_z d/2) \int_0^\infty dt \frac{t^2 \ln|t|}{[t^2 + 4(k_z'/K_{p2})^2]^2(t^2-1)} \tag{22b}$$

$$\alpha_{IN} = \alpha_{Fsj}(\kappa)\,|C|^4/K_{psj}(\kappa)Q^2(\kappa)[(\kappa/K_{psj}(\kappa))^2 + 1] \tag{22c}$$

and we have defined the function

$$Q^{-1}(\kappa) = 2\cos^2(k_z d/2)/(\kappa + 2k_z') + \tanh(\kappa d/2)/\kappa + 2k_z \sin(k_z d)/(\kappa^2 + 4k_z^2) + \kappa/(\kappa^2 + 4k_z^2)\tanh(\kappa d/2)\cosh(k_z d). \tag{23}$$

K_{p1}^{-1} and K_{p2}^{-1} measure the polaron size due to the LO phonon in materials 1 and 2, respectively, while α_{F1} (α_{F2}) denotes the usual LO-phonon–electron coupling constant of Frölich type in material 1 (2). They are given by

$$K_{p1} = \sqrt{2m_e\omega_{L1}/\hbar} \tag{24a}$$

$$K_{p2} = \sqrt{2m_e\omega_{L2}/\hbar} \tag{24b}$$

$$\alpha_{F1} = (e^2 K_{p1}/2\hbar\omega_{L1})(1/\varepsilon_{\infty 1} - 1/\varepsilon_{01}) \tag{25a}$$

$$\alpha_{F2} = (e^2 K_{p2}/2\hbar\omega_{L2})(1/\varepsilon_{\infty 2} - 1/\varepsilon_{02}). \tag{25b}$$

Although the corresponding quantities due to the interface phonon are not physically meaningful, they are nevertheless defined mathematically for convenience. Thus, we have

$$K_{psj}(\kappa) = \sqrt{2m_e\omega_{sj}(\kappa)/\hbar} \tag{25c}$$

$$\alpha_{Fsj}(\kappa) = [e^2 K_{psj}(\kappa)/2\hbar\omega_{sj}(\kappa)]\,1/[\varepsilon_1 \tanh(\kappa d/2) + \bar{\varepsilon}_2]. \tag{26}$$

It is emphasized that both K_{psj} and α_{Fsj} are not constant but depend on κ. Similarly, the γ's are given by

$$\gamma_{L1} = \frac{4\alpha_{F1}}{K_{p1}d}|C|^4 \sum_{m=1,3,\ldots} \left(\frac{d}{m\pi}\right)^2 \left(1 + \frac{\cos(k_z d)}{[1-(2k_z d/m\pi)^2]}\right)^2 \times \int_0^\infty dt \frac{t}{[t+(m\pi/K_{p1}d)^2](t+1)^3} \tag{27a}$$

$$\gamma_{L2} = \frac{\alpha_{F2}}{k_z' K_{p2}}|C|^4 \cos^4(k_z d/2) \int_0^\infty dt \frac{t}{(\sqrt{t}+2k_z'/K_{p2})^2(t+1)^3} \tag{27b}$$

$$\gamma_{IN} = \sum_j \int_0^\infty d\kappa \frac{2\kappa^2 \alpha_{Fsj}(\kappa)}{K_{psj}^3 Q^2(\kappa)[(\kappa/K_{psj})^2+1]^3}|C|^4. \tag{27c}$$

In calculating the energy corrections (21), we have expanded the denominators in (20) up to the second order in $k_\parallel$ and replaced the summations of $\boldsymbol{\kappa}$ and q by the integrals,

$$\sum_{\boldsymbol{\kappa}} \to [A/(2\pi)^2] \int d\boldsymbol{\kappa} \quad \text{and} \quad \sum_{q>0} \to (D/2\pi) \int dq.$$

Substituting (21) into (19) we find

$$\varepsilon_{k_e} - \varepsilon_{k_e}^{(0)} = -\alpha_{L1}\hbar\omega_{L1} - \alpha_{L2}\hbar\omega_{L2} - \sum_j \int_0^\infty d\kappa\, \alpha_{IN}(\kappa)\hbar\omega_{sj}(\kappa) - (\hbar^2 k_\parallel^2/2m_e)(\gamma_{L1}+\gamma_{L2}+\gamma_{IN}). \tag{28}$$

Combining (28) and the unperturbed energy (17), we obtain immediately the ground-state energy of the interacting electron–phonon system as

$$\varepsilon_{k_e} = \frac{\hbar^2 k_\parallel^2}{2m_e^*} + E_l + \sum_{\kappa,\beta} (n+\tfrac{1}{2})\hbar\omega_{\kappa,\beta} - \Delta E \tag{29}$$

where

$$m_e^* = m_e/(1-\gamma_{L1}-\gamma_{L2}-\gamma_{IN}) \tag{30}$$

is the polaron effective mass and

$$\Delta E = \alpha_{L1}\hbar\omega_{L1} + \alpha_{L2}\hbar\omega_{L2} + \sum_j \int_0^\infty d\kappa\, \alpha_{IN}(\kappa)\hbar\omega_{sj}(\kappa). \tag{31}$$

4. Results and discussion

Equations (30) and (31) are now employed to compute the effective mass and binding energy of a polaron in the GaAs quantum well of a GaAs/AlAs double heterostructure.

Table 1. Parameters used in the GaAs/AlAs DHS (m_0 is the rest mass of a free electron).

	m_e/m_0	$\varepsilon(0)$	$\varepsilon(\infty)$	ω_L (cm^{-1})	ω_T (cm^{-1})
GaAs	0.067	12.5	10.06	297	273
AlAs	—	10.6	8.16	403.7	361.7

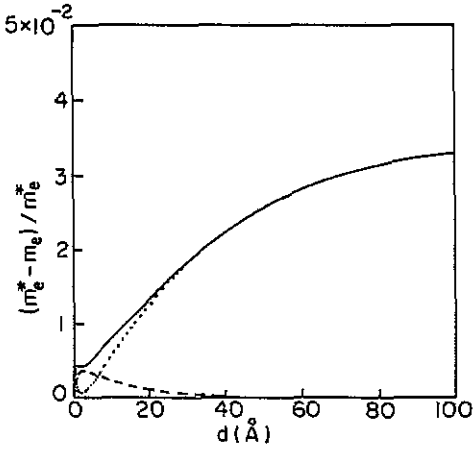

Figure 2. Polaron effective mass (full curve) as a function of the well width. The dotted curve represents the contribution from confined LO modes of phonons, and the broken curve represents the contributions from the interface modes.

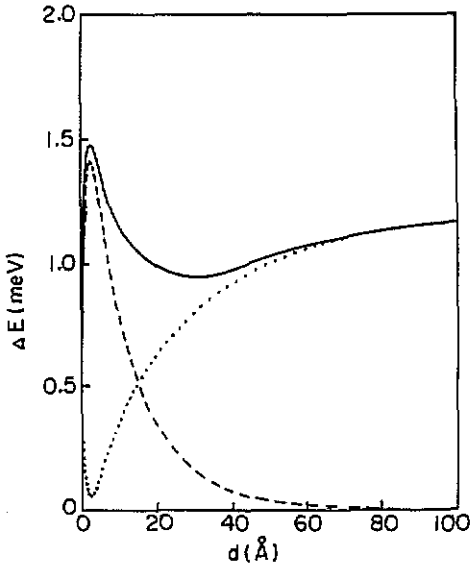

Figure 3. Polaron binding energy as a function of the well width. The dotted and broken curves represent the contributions from confined LO and interface modes, respectively.

The parameters used in our calculation are listed in table 1. The results are plotted as functions of the well width, d, in figures 2 and 3. In each case, contributions from the confined LO modes and interface modes are also shown by the dotted and broken curves, respectively.

Let us first look at the confined LO-mode contribution. This consists of two parts: one is from inside the well and the other from outside. The former starts from zero at $d \approx 0$ and increases monotonically with increasing d until the limiting value corresponds to that of the bulk GaAs, while the latter starts with the bulk value of AlAs and decreases with increasing d. This is, of course, expected because the effect of outside phonons on the electron in the well must diminish as the thickness of the central layer increases indefinitely.

The behaviour of the interface–phonon contribution can also be understood easily. It starts from zero, peaks quickly at about $d \sim 2.5$ Å, and then drops with increasing d. The effect of interface phonons essentially vanishes at $d \geqslant 60$ Å. While this is true in the present case of a free polaron, it is important to point out that the situation is totally

different in the case of a bound polaron under the influence of strong magnetic fields. (Chang *et al* 1988). In fact, the pinning effect observed in a quantum well of width $d =$ 100 Å can be completely accounted for by the interface phonon interaction with an electron which is bound to the hydrogenic impurity (Lin *et al* 1991). Such difference is understandable because the dynamics have been changed by the screened Coulomb force and the strong magnetic field, as well as the antisymmetric interface phonons which have no contribution to the free polaron.

When these contributions are combined, it is seen from figures 2 and 3 that both the calculated effective mass and binding energy of the polaron yield the correct limits. When $d \rightarrow 0$, the DHS becomes a bulk AlAs. As a consequence, the interface phonons disappear and the results must reduce to those of a polaron in the bulk AlAs. On the other hand, the interface phonon effect vanishes when $d \rightarrow \infty$ but the results reduce to those in a bulk GaAs.

It is perhaps of some interest to explain why the present results differ qualitatively from those in the literature. Liang *et al* (1986) have dealt with an isolated slab whose surfaces act like rigid walls. Thus the electron wave function is completely confined within the slab, and both the bulk LO and surface phonon contributions vanish when the slab width approaches zero. A slab with a free surface on one side and an interface on the other has been considered by Degani and Hipolito (1988). Unfortunately, an infinite square well was assumed in the z direction, making the small width results unreliable. More recently, Comas *et al* (1989) have considered only the bulk LO phonons interacting with the electron in an infinite square well. Therefore, their results are meaningful only for wells of sufficiently large width.

Acknowledgments

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References

Chang Y H, McCombe B D, Mercy J M, Reeder A A, Ralston J and Wicks G A 1988 *Phys. Rev. Lett.* **61** 1408
Chen R, Lin D L and George T F 1990 *Phys. Rev.* B **41** 1435
Comas F, Trallero-Giner C and Riera R 1989 *Phys. Rev.* B **39** 5907
Degani M H and Hipolito O 1988 *Surf. Sci.* **196** 459
Greene R and Bajaj K K 1985 *Phys. Rev.* B **31** 913
Lassnig R 1984 *Phys. Rev.* B **30** 7132
Liang X X, Gu S W and Lin D L 1986 *Phys. Rev.* B **34** 2807
Lin D L, Chen R and George T F 1990a *Solid State Commun.* **73** 799
—— 1990b *Quantum Well and Superlattice Physics II, SPIE Proc. 1283* p 273
—— 1991 *Phys. Rev.* B **43** 9328
Mori N and Ando T 1989 *Phys. Rev.* B **40** 6175
Sood A K, Menedez J, Cardona M and Ploog K 1985 *Phys. Rev. Lett.* **54** 2111; 2115
Wendler L 1985 *Phys. Status Solidi* b **129** 513