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Binding energy of a bound polaron in strong magnetic fields in low-dimensional semiconductor systems

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Abstract. Ionization energies of a shallow donor in a quantum well (Q2D), quantum well wire (Q1D) and quantum box (Q0D) of the GaAs/$Ga_{1-x}Al_xAs$ superlattice system in strong magnetic fields are obtained. The contributions from the electron–lattice coupling are also systematically investigated in all these systems. It is found that the ionization energy (E_{ion}) (i) decreases with an increase in well width in Q2D, Q1D and Q0D systems; (ii) increases with magnetic field for a given well width in all these systems, and (iii) increases as the spatial dimension is reduced for a given well width and magnetic field. The polaronic effect on E_{ion}, that is, $\Delta E_{e-1}(B)/E_{ion}(\alpha = 0, B)$ decreases when the magnetic field is increased in all three systems, showing a softening of the electron–lattice coupling. This decrease is more pronounced in Q2D than in Q1D or Q0D. The polaronic shift is also seen to be more important for systems with a smaller well width. The results are discussed in the light of the existing literature on these systems wherever available.

1. Introduction

The subject of semiconductors in intense magnetic fields has been a topic of great interest for a long time (Landwehr 1983). Recently there has been considerable interest both in the fabrication and in the physics of low-dimensional semiconductor systems (LDSSs) (Haug and Koch 1990, Ando *et al* 1982, Bastard *et al* 1991). Literature is rich with efforts on the study of impurity ionization energies in static electric fields (Bastard and Brum 1986, Sukumar and Navaneethakrishnan 1990a, El-said and Tomak 1990, 1992, Santiago *et al* 1992), in intense magnetic fields (Green and Bajaj 1985, Sukumar and Navaneethakrishnan 1990b), in crossed electric and magnetic fields (El-Said and Tomak 1990, Ilaiwi and Tomak 1990) and under hydrostatic pressures (Venkateswaran *et al* 1985, 1986, Sukumar and Navaneethakrishnan 1990b). Polaronic effects in a quantum well (Q2D) have been investigated by Mason and Das Sarma (1986), Ercelebi and Tomak (1985), Ercelebi and Saqqa (1988) and Elangovan and Navaneethakrishnan (1992a). Polaronic effects in a quantum well wire (Q1D) have been investigated by Degani and Hipolito (1988). In these investigations it is shown that the electron–longitudinal optical (LO) phonon interaction is appreciable in the computation of donor ionization energies. The polaronic effect in a quantum dot (Q0D) has not yet drawn much attention (Degani and Farias 1990).

In the present work we investigate systematically the polaronic effect on the donor ionization energy in the GaAs well of GaAs/$Ga_{1-x}Al_xAs$ superlattice system in the presence of strong magnetic fields. The theory is outlined in the next section while the results and discussion are presented in the final section.

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2. Theory

The Hamiltonian of a system consisting of a donor electron situated within the confining geometry of a Q2D or Q1D or Q0D system interacting with the LO phonons and an externally applied field is given by

$$H = -\frac{\hbar^2}{2m^*}\nabla^2 - \frac{e^2}{4\pi K_0\epsilon_0 r} + V(r) + \sum_q \hbar\omega_q a_q^+ a_q + H_{\text{e-ph}} + \frac{e}{2m^*}(\boldsymbol{B}\cdot\boldsymbol{L}) + \frac{e^2A^2}{2m^*} \qquad (1)$$

where we have assumed that the donor is kept at the middle of the well (taken at the origin) and have ignored spin effects. K_0 is the permittivity of free space, while ω_q is the LO phonon frequency, and $\boldsymbol{B}$ and $\boldsymbol{L}$ are the magnetic induction and the angular momentum respectively. $\boldsymbol{A} = (\boldsymbol{B}\times\boldsymbol{r})/2$ is the vector potential. We take, in the spirit of the Frohlich Hamiltonian, $\hbar\omega_q$ as a constant ($\hbar\omega_0$) omitting dispersion of the LO phonons. In (1)

$$H_{\text{e-ph}} = \sum_q Q_q(a_q + a_{-q}^+)\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \qquad (2)$$

where

$$Q_q = (4\pi\alpha/v)^{1/2}(1/q)\hbar\omega_0(\hbar/2m^*\omega_0)^{1/2}$$

$$\alpha = (e^2/4\pi K_0\hbar)(1/\epsilon_0 - 1/\epsilon_\infty)(m^*/2\hbar\omega_0)^{1/2}.$$

In (1) and (2) a_q and a_q^+ are the phonon annihilation and creation operators respectively; m^* is the band mass; ϵ_0 and ϵ_∞ are the static and high-frequency dielectric constants. α is the Frohlich coupling constant. Lattice deformation about the donor ion is taken care of by using

$$U = \exp\left(\sum_q d_q(a_q - a_q^+)\right)$$

where $d_q = Q_q\langle\phi_e|\mathrm{e}^{\pm\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}|\phi_e\rangle$. The wave function is chosen to be $\psi = \phi_e U|0\rangle$ (Ercelebi and Tomak 1985, Elangovan and Navaneethakrishnan 1992a).

2.1. Quantum well

$$V(x,y,z) = \begin{cases} 0 & \text{for } |Z| < L/2,\ |x| < \infty \text{ and } |y| < \infty \\ \infty & \text{otherwise.} \end{cases}$$

We apply the magnetic field along the Z-axis. We take

$$\phi_e = N_1\exp[-(x^2+y^2)/8a^2]\exp(-z^2/8b^2)\cos(\pi z/L)$$

to be a trial wave function with a and b as the variational parameters. N_1 is the normalization constant which is evaluated to be $N_1 = [8\pi a^2 I_2]^{-1/2}$. The ground-state energy is given by

$$\langle H\rangle = R_1 + R_2 + R_3 + R_4 + R_5$$

where

$$R_1 = \left\langle -\frac{\hbar^2}{2m^*}\nabla^2 \right\rangle = \frac{\hbar^2}{2m^*}\left[\frac{1}{4a^2} + \frac{1}{16b^4}\frac{I_6}{I_2} + \frac{\pi^2}{L^2}\frac{I_4}{I_2} + \frac{\pi}{4Lb^2}\frac{I_8}{I_2} - \frac{\pi^2}{L^2}\right]$$

$$R_2 = \left\langle -\frac{e^2}{4\pi K_0\epsilon_0 r} \right\rangle = -\frac{e^2}{16\pi^2 K_0\epsilon_0 a^2}\frac{I_9}{I_2}$$

$$R_3 = \left\langle \frac{e}{2m^*}\boldsymbol{B}\cdot\boldsymbol{L} \right\rangle = 0$$

$$R_4 = \left\langle \frac{e^2A^2}{2m^*} \right\rangle = \frac{e^2B^2a^2}{2m^*}$$

$$R_5 = \langle H_{\text{e-ph}} \rangle = -\frac{1}{\hbar\omega_0}\sum_q d_q^2.$$

The ionization energy is obtained from $E_{\text{ion}} = E_1 + E_{\text{L}} - \langle H\rangle_{\min}$, where $E_1 = \hbar^2\pi^2/2m^*L^2$. The ground-state Landau level is given by $E_{\text{L}} = \hbar\omega_{\text{c}}/2$ with the cyclotron frequency $\omega_{\text{c}} = eB/m^*$.

The I_n are integrals as given in section 2.3 below.

2.2. *Quantum well wire*

The Hamiltonian of the system in the presence of an external magnetic field including the electron–lattice coupling is the same as that given by (1) with

$$V(x,y,z) = \begin{cases} 0 & \text{for } |x| < L/2,\ |y| < L/2 \text{ and } |z| < \infty \\ \infty & \text{otherwise.} \end{cases}$$

We consider a wire of square cross section. The magnetic field is applied to the xy-plane, i.e. along the [110] axis. The trial wavefunction is chosen as

$$\phi_{\text{e}} = N_2 \exp[-(x^2+y^2)/8b^2]\exp(-Z^2/8a^2)\cos(\pi x/L)\cos(\pi y/L)$$

where a and b are the variational parameters. The normalization constant N_2 is given by $N_2 = (8\sqrt{\pi}aI_2^2)^{-1/2}$.

The ground-state energy is $\langle H\rangle = S_1 + S_2 + S_3 + S_4 + S_5$ where

$$S_1 = \left\langle -\frac{\hbar^2}{2m^*}\nabla^2 \right\rangle = \frac{\hbar^2}{2m^*}\left[\frac{1}{8b^4}\frac{I_6}{I_2} + \frac{1}{8a^2} + \frac{2\pi^2}{L^2}\frac{I_4}{I_2} + \frac{\pi}{2b^2L}\frac{I_8}{I_2} - \frac{2\pi^2}{L^2}\right]$$

$$S_2 = \left\langle -\frac{e^2}{4\pi K_0\epsilon_0 r} \right\rangle = -\frac{e^2}{8\pi^{3/2}K_0\epsilon_0 a}\frac{I_{10}}{I_2^2}$$

$$S_3 = \left\langle \frac{e}{2m^*}\boldsymbol{B}\cdot\boldsymbol{L} \right\rangle = 0$$

$$S_4 = \left\langle \frac{e^2A^2}{2m^*} \right\rangle = \frac{e^2B^2}{8m^*}\left[2a^2 + \frac{I_6}{I_2}\right)$$

and

$$S_5 = \langle H_{\text{e-ph}} \rangle = -\frac{1}{\hbar\omega_0}\sum_q d_q^2.$$

The ionization energy follows from $E_{\text{ion}} = E_2 + E_{\text{L}} - \langle H\rangle_{\min}$, where $E_2 = \hbar^2\pi^2/m^*L^2$.

2.3. Quantum box

The Hamiltonian of the system is again given by (1) with

$$V(x, y, z) = \begin{cases} 0 & \text{for } |x| < L/2,\ |y| < L/2 \text{ and } |z| < L/2 \\ \infty & \text{otherwise.} \end{cases}$$

We consider the case of a cubic box. The magnetic field is applied along the Z-axis. The trial wavefunction is chosen as

$$\phi_e = N_3 \exp[-(x^2 + y^2)/8a^2] \exp(-Z^2/8b^2) \cos(\pi x/L) \cos(\pi y/L) \cos(\pi z/L)$$

where a and b are the variational parameters. The normalization constant is given by $N_3 = (8 I_1 I_2 I_3)^{-1/2}$.

The ground-state energy is $\langle H \rangle = T_1 + T_2 + T_3 + T_4 + T_5$ where

$$T_1 = \left\langle -\frac{\hbar^2}{2m^*} \nabla^2 \right\rangle$$

$$= \frac{\hbar^2}{2m^*} \left[\frac{1}{8a^4} \frac{I_5}{I_1} + \frac{1}{16b^4} \frac{I_6}{I_2} + \frac{\pi^2}{L^2} \left(\frac{2I_3}{I_1} + \frac{I_4}{I_2} \right) + \frac{\pi_x}{4L} \left(\frac{2}{a^2} \frac{I_7}{I_1} + \frac{1}{b^2} \frac{I_8}{I_2} \right) - \frac{3\pi^2}{L^2} \right]$$

$$T_2 = \left\langle -\frac{e^2}{4\pi K_0 \epsilon_0 r} \right\rangle = -\frac{e^2}{4\pi K_0 \epsilon_0} \frac{I_{11}}{I_1^2 I_2}$$

$$T_3 = \left\langle \frac{e}{2m^*} B \cdot L \right\rangle = 0$$

$$T_4 = \left\langle \frac{e^2 A^2}{2m^*} \right\rangle = \frac{e^2 B^2}{4m^*} \frac{I_5}{I_1}$$

and

$$T_5 = -\frac{1}{\hbar\omega_0} \sum_q d_q^2.$$

The ionization energy follows from $E_{\text{ion}} = E_3 + E_{\text{L}} - \langle H \rangle_{\text{min}}$, where $E_3 = 3\hbar^2\pi^2/2m^* L^2$. The integrals I_1 to I_{11} are

$$I_1 = \int_0^{L/2} \exp(-x^2/4a^2) \cos^2(\pi x/L) \, dx$$

$$I_3 = \int_0^{L/2} \exp(-x^2/4a^2) \, dx$$

$$I_5 = \int_0^{L/2} \exp(-x^2/4a^2) \cos^2((\pi x/L) x^2 \, dx$$

$$I_7 = \int_0^{L/2} \exp(-x^2/4a^2) \sin(2\pi x/L) x \, dx$$

$$I_9 = \int_{x=-\infty}^{\infty}\int_{y=-\infty}^{\infty}\int_{z=0}^{L/2} \exp[-(x^2+y^2)/4a^2]\exp(-z^2/4b^2)\cos^2(\pi z/L)\frac{1}{r}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$$

$$I_{10} = \int_{x=0}^{L/2}\int_{y=0}^{L/2}\int_{z=-\infty}^{\infty} \exp(-(x^2+y^2)/4b^2)$$
$$\times \exp(-z^2/4a^2)\cos^2(\pi x/L)\cos^2(\pi y/L)\frac{1}{r}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$$

$$I_{11} = \int_{x=0}^{L/2}\int_{y=0}^{L/2}\int_{z=0}^{L/2} \exp(-(x^2+y^2)/4a^2)$$
$$\times \exp(-z^2/4b^2)\cos^2(\pi x/L)\cos^2(\pi y/L)\cos^2(\pi z/L)\frac{1}{r}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z.$$

I_2, I_4, I_6 and I_8 are I_1, I_3, I_5 and I_7, respectively, in each of which b replaces a in the integrand.

In each case, $\langle H\rangle_{\min}$ was obtained variationally and the E_{ion} computed numerically. Our results are presented in figures 1–3 and in table 1.

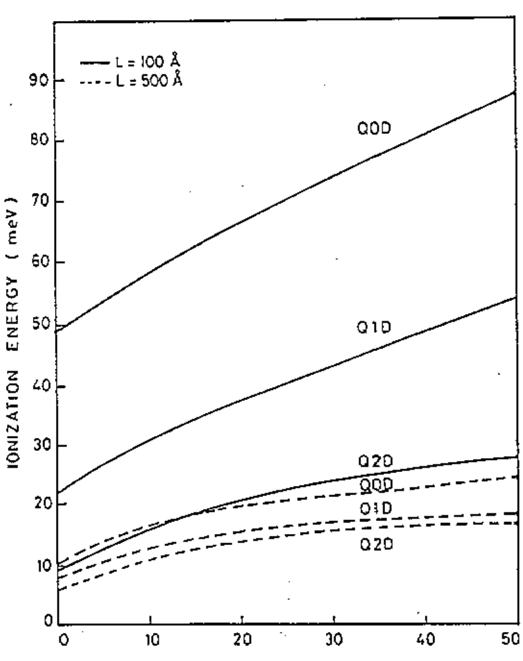

Figure 1. Donor ionization energy versus magnetic field for two different well widths.

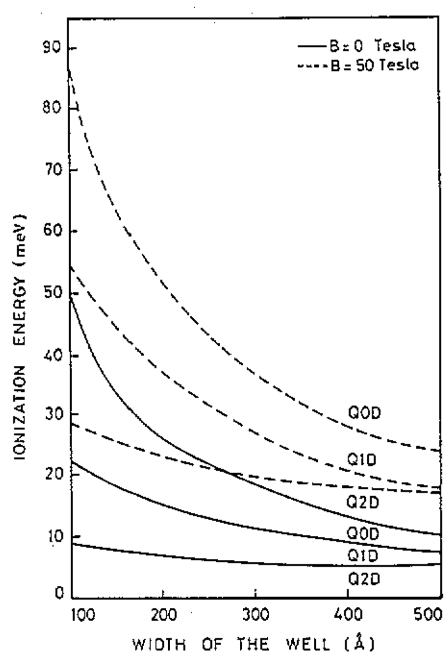

Figure 2. Variation of donor ionization energy with well width for $B = 0$ and $B = 50$ Tesla.

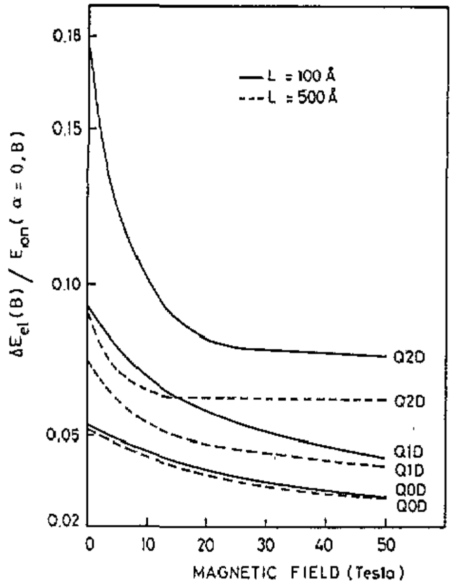

Figure 3. Variation of the polaronic shift with magnetic field in LDSSs.

Table 1. Donor ionization energies in low-dimensional GaAs/$Ga_{1-x}Al_xAs$ quantum wells in a magnetic field. γ is given by $\gamma = \hbar\omega_c/2R^*$ (ω_c is the cyclotron frequency and R^* is the effective Rydberg in GaAs). For Q1D and Q0D systems the results are given in figures 1 and 2; no experimental work or similar calculations are available (when $\gamma \neq 0$) for comparison.

	E_{ion} (meV)			
L	Q2D		Q1D	Q0D
(10^{-10} m)	$\gamma = 0$	$\gamma = 4$	$\gamma = 0$	$\gamma = 0$
	9.1	18.4	21.9	49.0
100	12.0[e]	20.9[f]	26.3[c]	49.6[a]
	12.8[f]		23.3[d]	56.6[b]
	7.9	16.0	14.5	25.0
200	9.5[e]	17.8[f]	16.5[c]	25.6[a]
	11.1[f]		16.9[d]	
	6.3	13.2	9.2	13.1
400	7.4[e]	14.6[f]	10.6[c]	13.8[a]
	7.3[f]		11.1[d]	
	5.8		8.0	10.8
500	6.9[e]		9.3[c]	
			9.9[d]	

[a] Elangovan and Navaneethakrishnan (1992a).
[b] Zhu *et al* (1990) (a spherical dot is considered in this work).
[c] Csavinsky and Oyoko (1991) (in this work a wire of cylindrical cross section is considered).
[d] El-Said and Tomak (1992).
[e] Sukumar and Navaneethakrishnan (1990a).
[f] Green and Bajaj (1985).

3. Results and discussion

The variation of the ionization energy with the magnetic field, when the electron lattice coupling is not taken into account, is given in figure 1. We see that the ionization energy increases when the magnetic field is increased for a given well width in all the three cases (Q0D, Q1D and Q2D). Also, E_{ion} increases when the spatial dimension of the system is reduced for a given field and for a given well width.

The variation of the ionization energy with well width is given in figure 2. It follows that the ionization energy decreases when the well width is increased for a given system (Q2D or Q1D or Q0D) and for a given magnetic field.

The ionization energies for Q2D, Q1D and Q0D systems for various well widths and for different magnetic fields are presented in table 1. Our values agree well with existing work. For Q1D and Q0D systems, the results are not available in the literature for high magnetic fields.

The change in the ionization energy due to the electron–lattice coupling is given by $\Delta E_{e-l}(B) = E_{ion}(\alpha \neq 0, B) - E_{ion}(\alpha = 0, B)$. However, we compute the values of $\Delta E_{e-l}(B)/E_{ion}(\alpha = 0, B)$ as an estimate of the polaronic shift and present them in figure 3. It is observed that the polaronic shift decreases when the magnetic field is increased in all the three systems. This decrease is more prominent in the Q2D than in the Q0D system. It also follows that the polaronic shift does not vary appreciably for a system with a larger well width. In a Q0D system, the variation is nearly the same irrespective of the value of the well width. Ercelebi and Tomak (1985) also observed that the polaronic effect decreased when the well width was increased for the case $B = 0$ in a Q2D system. Our results show that this trend continues even for cases $B \neq 0$.

An enhancement of the electron–lattice coupling in a strong magnetic field has been noticed by Peeters and Devreese (1982) for a free polaron in 3D in the longitudinal direction. Ercelebi and Saqqa (1988) observed an increase in the polaronic shift ΔE_{e-l} in a magnetic field in 2D. For GaAs Ercelebi and Saqqa obtain a value of 4.249 meV when $B = 10$ Tesla. For the same field we obtain (in the case of a Q2D system) 1.593 meV for the polaronic shift $|\Delta E_{e-l}|$, when the well width is 100 Å. Since the binding energy increases when the well width decreases our results ($L \to 0$) are in qualitative agreement with the results of Ercelebi and Saqqa.

It is interesting to note that the electron–lattice coupling softens in the transverse direction in a magnetic field both in 3D (Peeters and Devreese 1982, Balasubramanian and Navaneethakrishnan 1984) and in 2D (Peeters and Devreese 1983). In large magnetic fields, in the transverse direction, the characteristic frequency associated with the localization of the particle is the cyclotron frequency. The Coulomb potential is a weak perturbation in this limit. In such a case $\hbar\omega_c > \hbar\omega_{LO}$ and hence whatever coupling existed prior to the application of the field softens due to the adiabatic effect.

At present there is considerable interest in the study of polaronic effects arising due to (i) electron–bulk phonon coupling (3D), (ii) electron–interfacial phonon coupling (Zhong-Jun Shen *et al* 1990, Degani and Farias 1990), (iii) electron–slab phonon coupling (arising due to the shift in the oscillator energies due to confinement) and (iv) electron–half-space phonon coupling (due to phonons in barrier regions) (Guo-quiang Hai *et al* 1990). The electron–half-space phonon coupling does not exist in an infinite-barrier quantum well problem as there is no penetration of the wavefunction into the barrier region. Below we summarize the results of Guo-quiang Hai *et al* (1990) for the first three cases. For very thin wells (< 20 Å) the interfacial phonons dominate over the 3D phonons in the polaronic shift. The contribution from interfacial phonons decreases with an increase in well width and becomes insignificant when compared to the contribution from 3D phonons for fairly thick wells (~ 500 Å). The contribution from the slab phonons starts from a very small value for thin wells and rises to the value of the 3D phonons for thick wells. The cumulative effect of the interfacial phonons and confined slab phonons is significant only for thin wells. However, for larger well widths they add up to the 3D value. To our knowledge the effect of an external magnetic field on these contributions to the polaronic shift is not known. We believe that the same behaviour of these effects continues even in the presence of a magnetic field with a reduction in each of these contributions. Hence, as demonstrated by Guo-quiang Hai *et al* (1990) (in zero magnetic field, in a quantum well), the bulk phonon effects seem to be sufficient for reasonably thick wells (> 100 Å), with large barriers in the GaAs/$Ga_{1-x}Al_xAs$ systems.

To summarize we have found that the polaronic effect is important in low-dimensional semiconductor systems and should be included in all the estimates of the donor binding energies in these systems.

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