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Donor electron in a quantum well under the influence of an electric field

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Abstract. The ionization energies and the polarizabilities of a donor in an isolated well of a quasi two dimensional (Q2D) $GaAs/Ga_{1-x}Al_xAs$ heterostructure have been obtained for different well widths including electron-lattice coupling. A wave function that properly reduces to the hydrogenic function in the limiting case has been used. For fields of the order of 10^5 V/m, the ionization energies decrease slightly with electric fields for all well widths (10 nm to 50 nm) studied. Also for a given electric field, as the well width increases, the ionization energy decreases. For fields of the order of 10^7 V/m and for smaller well widths (< 10 nm), the ionization energy generally increases with electric field. The results also show that for electric fields of this order, no donor bound state associated with the lowest subband is possible for well widths greater than 20 nm. The polarizabilities estimated using the expression for the dipole operator show that as the well width increases, the polarizability values also increase and do not show any abnormal behaviour.

Keywords. Quantum well; Q2D system; donor energy; polarizability; electron-lattice coupling.

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1. Introduction

Among the low dimensional systems, $GaAs/Ga_{1-x}Al_xAs$ superlattice system has been subjected to vigorous experimental and theoretical analysis. The interest in these Q2D and Q1D systems stem from the fact that these systems exhibit several novel phenomena (Berggren 1988; Ando *et al* 1982). Donor states in these Q2D and Q1D systems have also been studied theoretically (Bastard 1981; Brown and Spector 1986) and experimentally (Delalande 1987; Meseguer *et al* 1987). Donor states under external perturbations like electric (Brum *et al* 1985) and magnetic fields (Greene and Bajaj 1985) have also been pursued with great interest. It has also been shown that no bound states are possible in a quantum well of a 2QD system with a finite barrier, separating the GaAs well and the GaAlAs regions under a strong electric field applied along the superlatice growth axis (Bastard *et al* 1983). Recently, the present authors worked out the polarizabilities of a quantum confined charge carrier in such a quantum well (Sukumar and Navaneethakrishnan 1989). The pressure dependence of the diamagnetic susceptibility of a donor has also been worked out recently (Sukumar and Navaneethakrishnan 1990). In the present work, we would like to report the results of our investigations on the ionization energies and the polarizabilities of a donor in a quantum well. The present work differs from the other calculations on the donor binding energies in the sense that we have used a wave function that correctly reduces to the hydrogenic form, in the limit $L \rightarrow \infty$ ($L-$ is the well width) and in the absence of the electric field. Also, for the first time we report the values of donor polarizabilities for an on-centre impurity. We also show that for electric field $\simeq 10^7$ V/m, the donor states can no longer be associated with the ground state subband. In these estimates we have included the effect of the electron-lattice coupling following the lines of Sukumar and Navaneethakrishnan (1989) and Xu Wang *et al* (1988).

2. Theory

The Hamiltonian for a system consisting of an electron in an infinite well moving under the influence of a donor at the middle of the well (taken as the origin), and an externally applied electric field along the z-direction (perpendicular to the walls) is given by

$$H = \frac{P^2}{2m^*} - \frac{e^2}{\varepsilon_0 r} + eFz + \sum_k \hbar_w a_k^+ a_k + \sum_k \frac{1}{k}(V_k \exp(i\bar{k}\cdot\bar{r})a_k + \mathrm{h\cdot c}) + V_w(z), \tag{1}$$

where a_k^+ (a_k) is the phonon creation (destruction) operator, ω is the zone-centre L.O phonon frequency, F is the externally applied electric field, $V_w(z)$ represents the infinite well and ε_0 is the static dielectric constant of GaAs. The fifth term in the above Hamiltonian is the Fröhlich electron-phonon interaction term with V_k given by

$$V_k = i\hbar\omega(\hbar/2m^*\omega)^{\frac{1}{4}}(4\pi\alpha/V)^{\frac{1}{2}},$$

where α is the electron lattice coupling constant.

In the previous work, wave functions which do not reduce to hydrogenic ground state wave function in the limit $L\to\infty$ and $F\to 0$ have been used as indicated in § 1. In the present work we use a wave function

$$\psi = N\exp(-\alpha_1 r)(1+\lambda F z)\cos\frac{\pi z}{L}, \tag{2}$$

where N is the normalization constant. This can be easily seen to reduce to hydrogenic 1s function in the proper limit. We have evaluated the ground state energy using this wave function. After going through the canonical transformations as given by Xu Wang *et al* (1988) we obtain for $\langle H\rangle$

$$E(\alpha_1,\lambda) = E_0 - \alpha\hbar\omega + \frac{\alpha\hbar^2}{12m^*}q_z^2 - \frac{\hbar^3}{32\omega m^{*2}}q_z^4,$$

where

$$E_0 = \frac{h^2}{2m^*}\left[\alpha_1^2 - \frac{\pi^2}{L^2} + 2N^2\lambda^2F^2\pi(I_1+I_2) + \frac{4N^2\pi^3}{L^2}(I_1+\lambda^2F^2I_3) + \frac{4N^2\pi^2\alpha_1}{L}\left(I_4+\lambda^2F^2I_5 - \frac{\lambda^2F^2I_6}{\alpha_1 L}\right) - 8N^2\lambda^2F^2\pi\alpha_1 I_7\right] - \frac{e^2N^2\pi}{\varepsilon_0}\left[\frac{(I_8+I_9)}{\alpha_1} + 4\lambda^2F^2I_7\right] + 8eN^2F^2\pi\lambda I_{10}$$

and

$$q_z = -8N^2\pi\alpha_1\lambda F I_7 - \frac{4N^2\pi^2\lambda F I_6}{L} + 2N^2\pi\lambda F(I_1 + I_2)$$

with

$$N^2 = [2\pi(I_1 + I_2) + 4\pi\lambda^2 F^2 I_{10}]^{-1}$$

$$I_1 = \int_0^\infty \int_0^{L/2} f(\rho, z)\rho \mathrm{d}\rho\, \mathrm{d}z; \quad I_2 = \int_0^\infty \int_0^{L/2} f(\rho, z)\cos\frac{2\pi z}{L}\rho \mathrm{d}\rho\, \mathrm{d}z$$

$$I_3 = \int_0^\infty \int_0^{L/2} f(\rho, z) z^2 \rho \mathrm{d}\rho\, \mathrm{d}z;$$

$$I_4 = \int_0^\infty \int_0^{L/2} f(\rho, z)(\rho^2 + z^2)^{-\frac{1}{2}} z \sin\frac{2\pi z}{L}\rho \mathrm{d}\rho\, \mathrm{d}z$$

$$I_5 = \int_0^\infty \int_0^{L/2} f(\rho, z)(\rho^2 + z^2)^{-\frac{1}{2}} z^3 \sin\frac{2\pi z}{L}\rho \mathrm{d}\rho\, \mathrm{d}z$$

$$I_6 = \int_0^\infty \int_0^{L/2} f(\rho, z) z \sin\frac{2\pi z}{L}\rho \mathrm{d}\rho\, \mathrm{d}z$$

$$I_7 = = \int_0^\infty \int_0^{L/2} f(\rho, z)(\rho^2 + z^2)^{-\frac{1}{2}} z^2 \cos^2\frac{\pi z}{L}\rho \mathrm{d}\rho\, \mathrm{d}z$$

$$I_8 = \int_0^{L/2} \exp(-2\alpha_1 z)\mathrm{d}z; \quad I_9 = \int_0^{L/2} \exp(-2\alpha_1 z)\cos\frac{2\pi z}{L}\mathrm{d}z$$

and

$$I_{10} = \int_0^\infty \int_0^{L/2} f(\rho, z) z^2 \cos^2\frac{\pi z}{L}\rho \mathrm{d}\rho\, \mathrm{d}z.$$

In the above integrals f is given by

$$f(\rho, z) = \exp(-2\alpha_1(\rho^2 + z^2)^{\frac{1}{2}}).$$

All these integrals can be evaluated in closed form.

The ionization energy is defined as

$$E_{\text{ion}} = E_{\text{sub}}(F) - E_{\min}(\alpha_1, \lambda), \tag{3}$$

where $E_{\text{sub}}(F)$ stands for the subband energy in an electric field. These values for different electric fields have been worked out in our earlier paper (Sukumar and Navaneethakrishnan 1989). $E_{\min}(\alpha_1, \lambda)$ is the minimum value of $E(\alpha_1, \lambda)$ obtained numerically. In the actual calculations, the donor ionization energies were obtained variationally, when $F = 0$, for different L. These variationally estimated values of α_1 were used in the subsequent calculations when $F \neq 0$. Values of $E_{\min}(\alpha_1, \lambda)$ were obtained for different L values by varying λ. The ionization energies have been calculated for different electric fields and well widths using (3).

To calculate the donor polarizability (α_p), we have used the expression for the dipole moment

$$P = \langle -ez \rangle_{F \neq 0} - \langle -ez \rangle_{F=0} \tag{4}$$

and $P = \alpha_p F$. From symmetry, it follows that the second term in (4) vanishes. The final expression for α_p is

$$\alpha_p = 8N^2 e\pi\lambda I_{10} \tag{5}$$

where I_{10} is given earlier.

3. Results and discussion

The donor ionization energies obtained using (3) for electric fields of $\sim 10^5$ V/m are given in table 1. For smaller electric fields the shift in the ionization energies, from the field free values, were not appreciable. The variation of the subband energies for different electric fields and well widths are given in table 2. The donor polarizabilities for different well widths are presented in table 3.

Table 1. Donor ionization energies (meV) for different electric fields.

L (nm)	F(10^5 V/m) 0	1	2	3	4
10	12·06 (12·06)	11·66 (13·80)	11·66 (18·49)	11·66 (23·29)	11·66 (26·98)
20	9·49 (9·49)	9·40 (9·30)	9·40 (−3·74)	9·41 (−24·81)	9·42 (−50·73)
40	7·37 (7·37)	7·35 (−49·36)	7·31 (−136·15)	7·24 (−232·03)	7·14 (−333·04)
50	6·86 (6·86)	6·80 (−88·09)	6·63 (−215·60)	6·37 (−352·25)	6·05 (−494·20)

The quantities within parentheses refer to E_{ion} for electric fields in 10^7 V/m.

Table 2. Subband energies for different electric fields.

L (nm)	F(10^5 V/m) 0	1	2	3	4
10	53·72 (53·72)	53·29 (51·44)	53·29 (46·03)	53·29 (37·49)	53·29 (26·25)
20	11·56 (11·56)	11·45 (−11·22)	11·44 (−55·89)	11·42 (−109·31)	11·40 (−167·77)
40	1·01 (01·01)	0·94 (−108·49)	0·80 (−252·72)	0·57 (−406·12)	0·26 (−564·65)
50	−0·25* (−0·25)	−0·38 (−158·09)	−0·71 (−352·34)	−1·22 (−555·78)	−1·88 (−764·52)

The quantities within parentheses refer to E_{sub} for electric fields 10^7 V/m.

*The negative value for $F = 0$ arises due to $\alpha\hbar\omega \approx 2{\cdot}5$ meV while $E_{\text{sub}} = 2{\cdot}25$ meV.

Table 3. Donor polarizabilities (10^7 Å^3) as a function of well width.

L (nm)	$F = 10^5$ V/m 1	2	3	4	Mean
10	0·012	0·012	0·012	0·012	0·012
20	0·124	0·124	0·123	0·123	0·123
40	0·945	0·927	0·901	0·865	0·909
50	1·567	1·509	1·423	1·325	1·456

An important result of this paper is that when the strength of the electric field is increased to 10^7 V/m, for well widths larger than 20 nm, we have found that E_{ion} is negative (see, Table 1). It is well known that for a well of finite strength and for larger electric fields one has only quasi bound or unbound states (Bastard *et al* 1983). Surely such a situation does not arise in the present case since we have restricted our calculations to wells of infinite strength. A zero ionization energy would mean that the donor state is in the continuum of the $n = 1$ subband. A negative value for the ionization energy means that the ground state subband moves downwards faster than the donor ground state for such a large electric field. However, a transition from the ground state of the donor to the $n = 2$ (first excited) subband in the quantum well is still possible which will make E_{ion} positive, provided this subband does not descend rapidly with electric field. This indeed is the case as can be easily demonstrated using the results of Ahn and Chuang (1987), where it is shown that the $n = 2$ subband shows a slight increase upwards for small fields and slow decrease for larger fields. This conclusion, viz., the donor states are no longer associated with the ground state subband for electric fields $\gtrsim 10^7$ V/m appears difficult to be verified experimentally, as the barrier heights in reality are finite. An infinite well model is generally employed as it reduces the amount of numerical work. It is also well-known that the results of the infinite well model agree very well with the results of a finite barrier for thick wells ($\gtrsim 50$ nm) (Greene and Bajaj 1983). For $L < a^*$ (the effective Böhr radius), the applicability of the effective-mass theory is questionable.

It is true that in such thick wells the intersubband separation is small. Still, if the conduction band discontinuty is $\sim 85\%$ of the band-gap difference in the superlattice, for reasonably strong electric fields, one may still observe an anomalous behaviour in the I–R absorption associated with a donor.

It appears, from (5), that α_p depends on F through λ. It is also true that the F values chosen are large. In spite of this, we have obtained the values of α_p which are fairly independent of F (see, table 3). It follows that for smaller well widths the electron behaves like a particle possessing larger inertia due to the boundary conditions, viz., $\psi = 0$ at $|z| = L/2$. Hence non-linearities do not seem to set in even for such a high field in an infinite quantum well. It can be seen that as L increases the donor polarizability also increases. For comparision, α_p for $L = \infty$ is given by, $4{\cdot}5\ a_0^{*3}$ in the effective-mass approximation, where $a_0^* = 195{\cdot}52$ a.u. for GaAs and α_p, $5{\cdot}01 \times 10^6$ Å^3. From table 3, it follows that the polarizability values are one order less for 10 nm and one order higher for 50 nm when compared to the $L = \infty$ value. For $L = \infty$, our results indicate $\alpha_p > 5 \times 10^6$ Å^3. This discrepancy arises due to the wave function, given in (3), which contains only a first order term in the electric field. The hydrogenic value is obtained using an exact wave function which contains a second order term in the electric field also (Schiff 1968).

We find that the contribution from the electron-lattice coupling, to the ionization energies, is $\approx 2{\cdot}5$ meV for all well widths. In an electric field of 4×10^7 Vm^{-1}, the contribution from the $(e\text{–}l)$ coupling to the ionization energies are 2·40, 2·48, 2·49 and 2·50 meV for $L = 10, 20, 40$ and 50 nm respectively. Hence, it follows that the polaronic effects are important. In an earlier paper, Ercelebi and Tomak (1985) showed that the contribution from the $(e\text{–}l)$ coupling decreases with the increase of well width in the absence of electric field. It is known that as $L \to \infty$, the $(e\text{–}l)$ contribution should reach $\alpha\hbar\omega_{\mathrm{L.O}} \simeq 2{\cdot}57$ meV for GaAs (Elangovan and Navaneethakrishnan 1982). This behaviour is not observed in the work of Ercelebi and Tomak (1985). Our results, on the other hand, seem to be of the correct order and show the proper trend as L increases to the bulk case.

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