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HYDROGENIC DONOR IN A QUANTUM WELL WITH AN ELECTRIC FIELD *

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ABSTRACT

Variational calculations of the binding energy of a hydrogenic donor in a quantum well formed by GaAs and $Ga_{1-x}Al_xAs$ with a constant electric field are performed for different electric fields and well widths. A critical electric field is defined and its variation with well width is presented.

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I. INTRODUCTION

There have been several theoretical investigations on the shallow donors in a quantum well formed by a layer of GaAs between $Ga_{1-x}Al_xAs$ barriers [1]. This system is of considerable interest from the technological point of view and also it serves as a relatively simple system for studying many physical effects. Experimental results on the binding of donors in quantum well structures based on far-infra-red magnetospectroscopy have been reported recently [2]. Bastard et al. [3] have performed variational calculations on the quantum well in an electric field and obtained the Stark shift and the electric field induced spatial shift of the particle wave function. Brum and Bastard [4] have reported their results on the electric field induced dissociation of excitons.

In the present work we report the results of our calculations on the effect of an electric field on the binding energy of a hydrogenic donor in the GaAs-$Ga_{1-x}Al_xAs$ quantum well. In Sec.II we give the theoretical model and the results and conclusions are presented in Sec.III.

II. THEORY

The Hamiltonian for a hydrogenic donor at the centre of a quantum well subjected to an electric field F perpendicular to the interface (this direction is taken as the Z-axis) is given by

$$H = -\nabla^2 + V_w(z) + \gamma z - \frac{2}{r} , \qquad (1)$$

where the units of length and energy are the effective Bohr radius a_B $(= \epsilon_0 \hbar^2/m^* e^2)$ and the effective Rydberg R $(= m^* e^4/2\epsilon_0^2 \hbar^2)$, m^* being the effective mass of the electron and ϵ_0 the static dielectric constant of GaAs. With the material parameters for GaAs, $a_B = 98.7$ Å and $R = 5.83$ meV. γ in Eq.(1) is a measure of the electric field strength and is equal to $e\, a_B F/R$. $V_W(Z)$ is the potential energy due to the quantum well and is taken to be of the form

$$V_W(Z) = \begin{cases} 0 & |z| < \frac{1}{2} \\ V_0 & \text{outside the well} \end{cases} \qquad (2)$$

For calculating the ground state energy of a donor variationally, we use a trial wave function given by

$$\Psi(\rho,\phi,z) = N\psi_0(z)\,e^{-a\rho} \quad , \tag{3}$$

where N is the normalization constant and $\psi_0(Z)$ is given by

$$\psi_0(z) = \begin{cases} A\exp(\beta-b)z & ; \quad z < -\frac{L}{2} \\ B\cos\alpha z\,\exp(-bz) & ; \quad |z| < \frac{L}{2} \\ C\exp[-(\beta+b)z] & ; \quad z > \frac{L}{2} \end{cases} \tag{4}$$

With b = 0, Eq.(4) gives the exact eigenstate of the Hamiltonian (1) without the electric field term and the impurity potential. The constants A, B, C, and α are obtained using the continuity of ψ_0 and its first derivative at $Z = \pm L/2$ and the normalization. The lowest sub-band energy is obtained by solving the transcendental equation

$$\sqrt{\frac{E_{sb}}{V_0}} = \cos\left(\sqrt{E_{sb}}\,\frac{L}{2}\right) \tag{5}$$

The value of b in Eq.(4) is fixed by a variational calculation with the impurity potential removed from the Hamiltonian in Eq.(1). Calculations are done for different electric field and well width. Having fixed b, the expectation value of H in Eq.(1) is minimized with respect to the parameter a in Eq.(3). The donor binding energy E_B is defined as

$$E_B = E_{Sb}(F) - \langle H \rangle_{minimum} \quad . \tag{6}$$

III. RESULTS AND CONCLUSIONS

The calculated sub-band energies as functions of both the electric field and width of the well are shown in Fig.1. As can be seen from this figure, the sub-band energy moves towards the bottom of the well as the electric field increases. The actual amount of lowering (ΔE_{Sb}) depends sensitively upon the well width. For the particular composition under study (x = 0.3) the shift becomes insensitive to the field as the well width is

near 0.3 and at a critical well width of 0.1 again ΔE_{Sb} becomes drastic with an accompanying lowering of the critical electric field as can be seen from Fig.2. The above behaviour shows that the sub-band lowering depends on its location before the field is applied (see inset in Fig.1). The critical electric field F_c is defined as the field for which there is no minimum for the expectation value of H or the field for which the above minimum value is zero where the bottom of the well is located. This critical field increases as the well width increases, reaches a maximum and then decreases as L is still further increased. The region over which the critical field is less sensitive to the variation of L will depend on the well depth V_0. Fig.3 shows the variation of ΔE_{Sb} with L for different electric fields.

The electric field dependent donor binding energies are shown in Fig.4 for different well widths. In general the binding energy E_B decreases with increase of electric field. This variation is however insensitive to the electric field for L = 0.3. For L = 0.1 there is an initial slight increase of E_B which then decreases with increase of the field. This is a result of the variational calculation for the details of the difference between the sub-band movement and that of the donor ground state. As the well width is lowered the decrease of E_B is more pronounced with a more sensitive dependence on the field. The binding energy E_B as a function of the well width for two typical electric fields is shown in Fig.5.

The above conclusions are well revealed by the behaviour of the wave functions which are shown in Figs.6 and 7. Fig.6 shows a noticeable shift in the wave function for L = 1.00, while Fig.7 shows a very small shift for L = 0.36.

Low temperature photoluminescence measurements reported by Mendez et al. [5] reveal impurity effects and give estimates of the critical field F_c at which the impurity originated line disappears. The actual value for F_c inferred from these measurements is not in detailed agreement with our results. This is to be expected because our calculations assume an isolated quantum well while the experiments are on multiple quantum wells where the tunnelling effects are important.

All the above calculations are repeated assuming an energy-dependent effective mass for taking into account the non-parabolicity of the band. The results are shown as dotted lines in Figs.2 and 4. Non-parabolicity effects increase the critical electric field with no noticeable consequence as L becomes larger. The donor binding energy shows an increase for non-parabolic case, the difference becoming drastic as L becomes smaller. This is in agreement with the results of Chaudhudri and Bajaj [6] for donor binding energies in the absence of the electric field.

The predictions of the present work can be tested experimentally on the lines of the work of Mendez et al. [5] who have employed Schottky barrier configuration in their heterostructure.

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NOTE ADDED: At the time of submitting the paper, we came across the following two papers: (i) "Electric field dependence of the binding energy of shallow donors in GaAs-$Ga_{1-x}Al_xAs$ quantum wells" by J.A. Brum, C. Priester and G. Allan, Phys. Rev. B32, 2378 (1985); (ii) " Measurements of electric-field-induced energy-level shifts in GaAs single-quantum-wells using electro-reflectance" by C. Alibert, S. Gaillard, J.A. Brum, G. Bastard, P. Frijlink and M. Erman, Sol. State Comm. 53, 457 (1985).

In (i) theoretical results are presented for impurity binding energy vs electric field for a QW of width 100 Å and 200 Å and with $x = 0.38$ for impurity positions at $-\frac{L}{2}$, $-\frac{L}{4}$, 0, $\frac{L}{4}$ and $\frac{L}{2}$. Impurity binding energy vs QW thickness is also presented for electric fields 0, 100, 150 and 200 kv/cm. Our calculations are for the case of the impurity at the centre of the well and with $x = 0.30$. The nature of variation of the impurity binding energy with the electric field for L = 100 Å is similar in both works. Our work is in greater detail for small well widths and has discussions on the critical electric field.

The insensitiveness of the subband shift for small well widths discussed in our work is revealed by the experimental results of (ii), (especially the electroreflectance spectrum for a QW of width 37 Å and electric fields 10 and 200 kv/cm).

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FIGURE CAPTIONS

Fig.1 Variation of ΔE_{sb} with electric field F. The arrow indicates the critical field for L = 0.10.

Inset Quantum well in an electric field: 1 shows the sub-band for large L and 2 for small L when the field is zero.

Fig.2 Critical electric field F_c as a function of L.
Solid curve: results for parabolic band,
dotted curve: results for non-parabolic case.

Fig.3 Variation of ΔE_{sb} with well width L. Curves 1, 2 and 3 are for the electric field 25,50 and 100 kV/cm. respectively.

Fig.4 Donor binding energy E_B as a function of electric field F. Dotted lines are for the non-parabolic case.

Fig.5 Donor binding energy E_B as a function of well width L. Curves 1 and 2 are for electric fields 0 and 100 kV/cm. respectively.

Fig.6 Variation of the amplitude of wave function with position for L = 1.00. Curve 1 is for F = 0 and curve 2 is for F = 100 kv/cm.

Fig.7 Same as Fig.6 except L = 0.36.

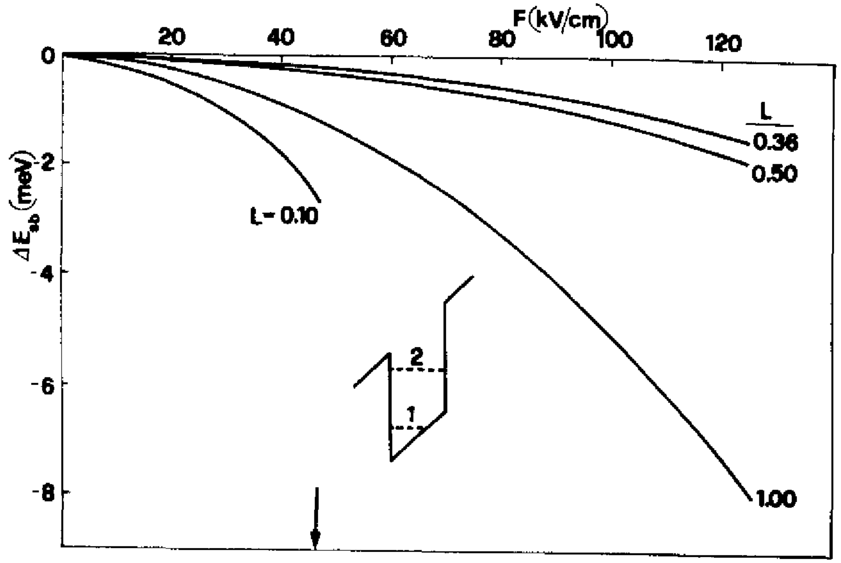


Fig.1

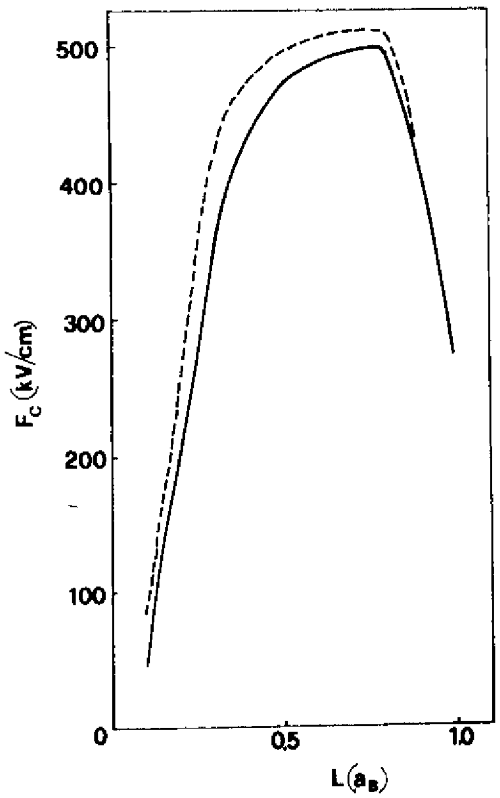

500
400
300
200
100
0
0.5
1.0
F_C (kV/cm)
$L(a_B)$

Fig.2

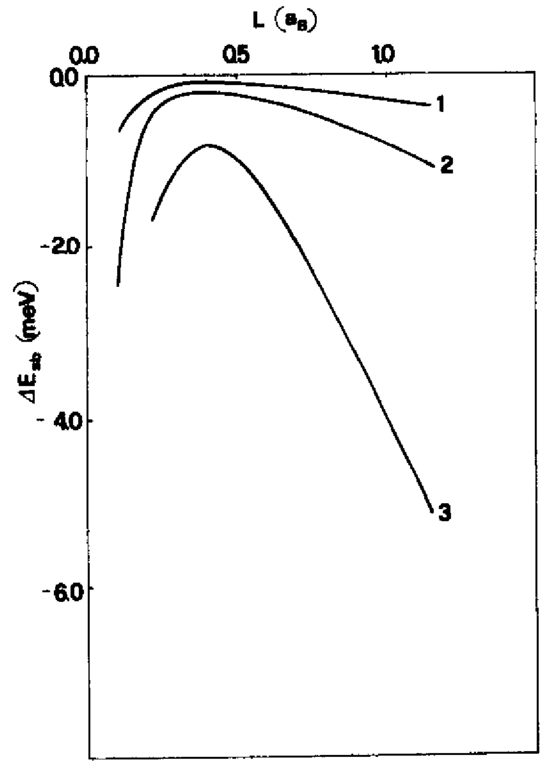
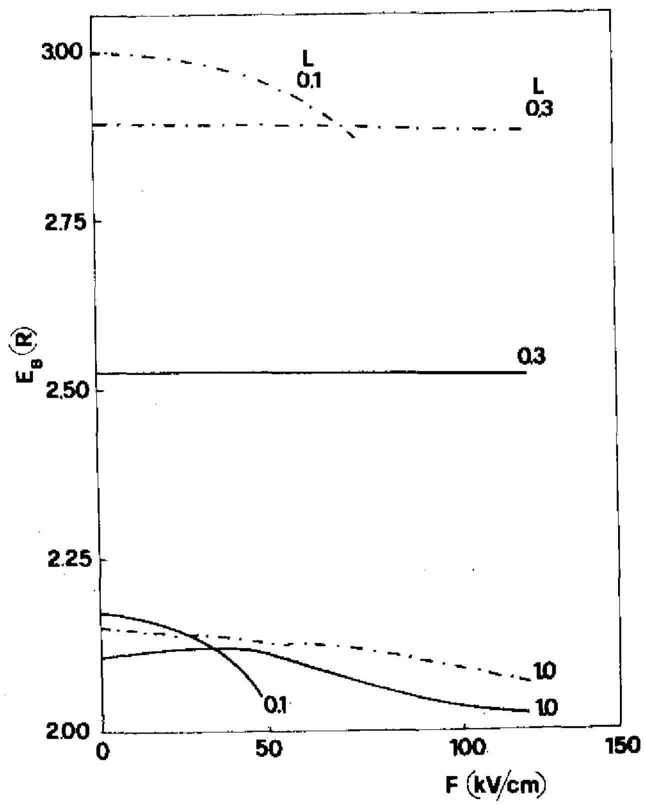
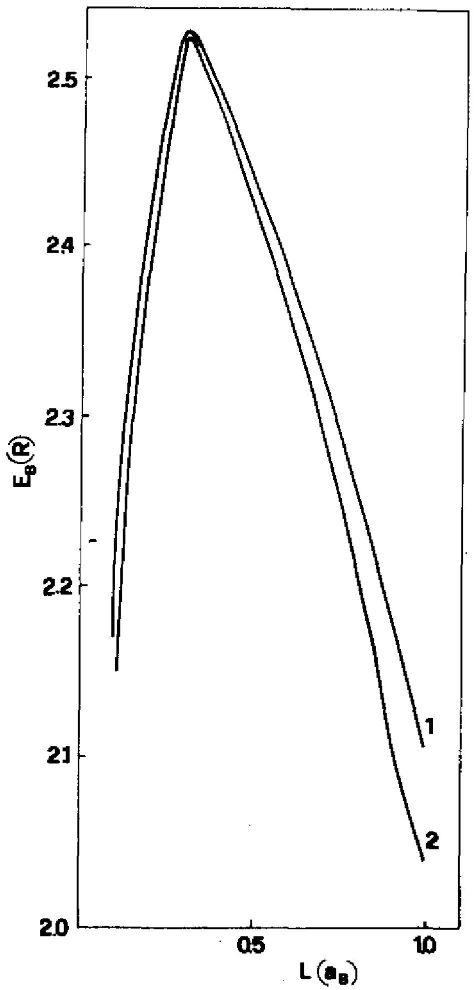

L (a_B)
0.0
0.5
1.0
0.0
-2.0
-4.0
-6.0
ΔE_{sb} (meV)
1
2
3

Fig.3



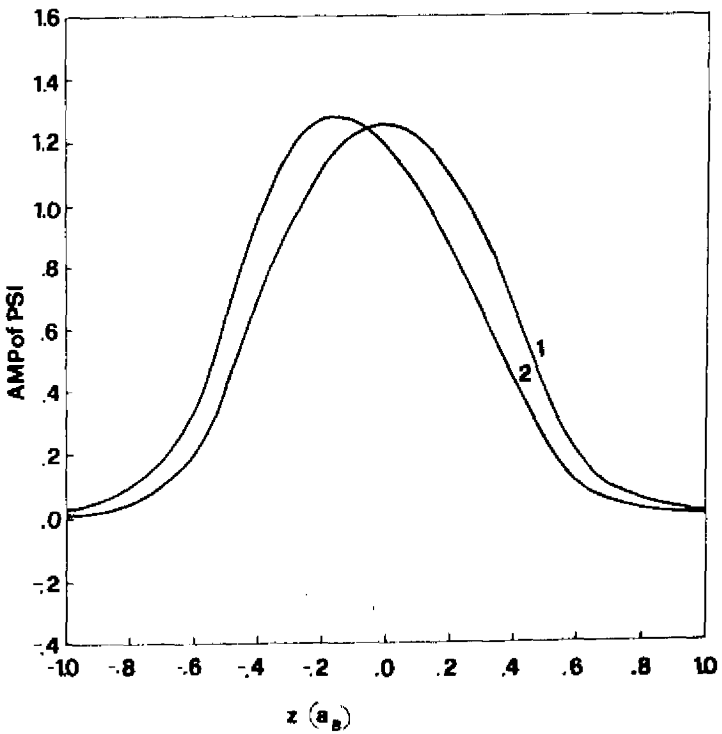
3.00
2.75
2.50
2.25
2.00
L
0.1
L
0.3
0.3
1.0
0.1
1.0
0
50
100
150
F (kV/cm)

Fig.4



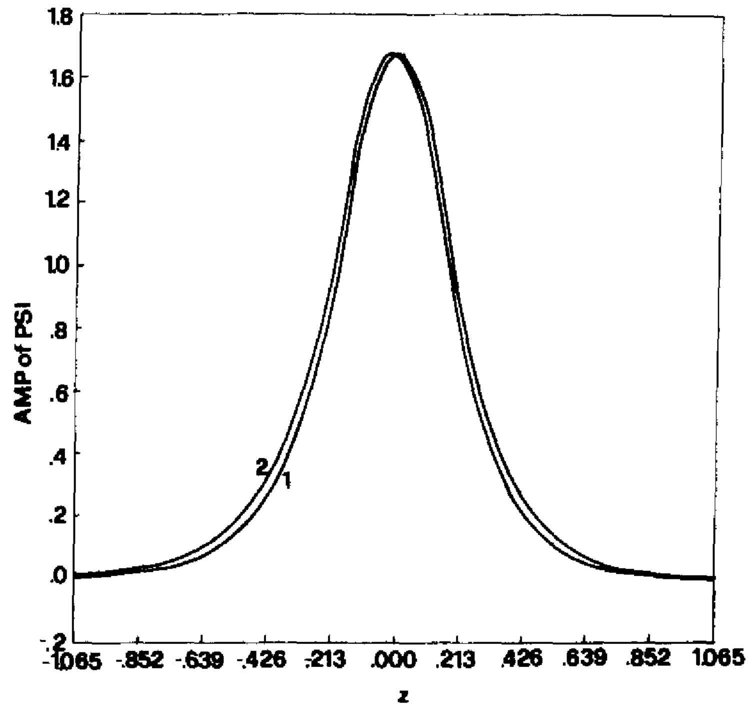
2.5
2.4
2.3
2.2
2.1
2.0
1
2
0.5
1.0

Fig.5



1.6
1.4
1.2
1.0
.8
.6
.4
.2
.0
-.2
-.4
AMP of PSI
1
2
-1.0 -.8 -.6 -.4 -.2 .0 .2 .4 .6 .8 1.0
z (a_B)

Fig.6



1.8
1.6
1.4
1.2
1.0
.8
.6
.4
.2
.0
-.2
AMP of PSI
2
1
-1.065 -.852 -.639 -.426 -.213 .000 .213 .426 .639 .852 1.065
z

Fig.7