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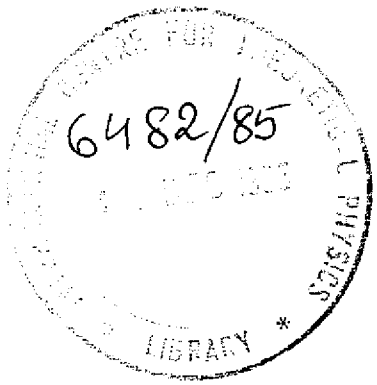

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RESONANT IMPURITY STATES IN A QUANTUM WELL †

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ABSTRACT

The position of a resonant state relative to a localized donor state and the width of the resonant state are calculated for a hydrogenic donor in a GaAs-$Ga_{1-x}Al_xAs$ quantum well as a function of the width of the well. The results are compared with experiments and earlier theoretical estimates.

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1. INTRODUCTION

Hydrogenic donors in a semiconductor quantum well have been studied extensively during the past few years [1]. With highly controllable growth techniques, experimental studies on the properties of the shallow donors in semiconductor quantum well structures have now become possible. For example, Jarosik et al. [2] have reported the far-infrared magnetospectroscopic measurements on shallow donors in GaAs-$Al_xGa_{1-x}As$ multiple quantum well structures. Perry et al. [3] have carried out resonant Raman scattering experiments on GaAs(Si doped)-$Al_xGa_{1-x}As$ quantum well structures and observed narrow, resonant donor states. Earlier, Priester et al. [4] have calculated the position and width of resonant states assuming an infinitely deep quantum well. For a quantum well of finite depth, it is known, at least for the discrete donor states, that the spreading of the donor wavefunction outside the well for small well widths considerably alters the results of the infinite well case. The samples used in the experimental work of Ref.3 are sufficiently thick (238 Å and 460 A) and the experimental resonant energy positions could be compared with the calculations of Priester et al. It will be of interest to calculate the resonant states as a function of well width for a finite well depth.

In the present work, we report our results of variational calculations of the position and width of resonant states in a GaAs quantum well of finite depth for different well widths.

II. THEORY

We consider a donor atom at the centre of a symmetrical quantum well described by the potential energy function

$$V_B(z) = 0 \quad , \quad |z| < \frac{L}{2} \, , \qquad (1)$$
$$= V_0 \quad , \quad |z| > \frac{L}{2} \, .$$

The Hamiltonian for the donor electron is given as

$$H = H_0 - \frac{e^2}{\epsilon_0 r} \quad , \tag{2}$$

where

$$H_0 = \frac{p^2}{2m^*} + V_B(z) \quad . \tag{3}$$

m^* in Eq.(3) is the electron effective mass and ϵ_0 in Eq.(2) is the static dielectric constant of GaAs. The eigenstates of H_0 are

$$\psi_{k_x,k_y,\alpha}(\vec{r}) = \frac{1}{\sqrt{S}} \exp[i(k_x x + k_y y)] f_\alpha(z) \quad , \tag{4}$$

where S is the layer surface area and

$$\begin{aligned} f_\alpha(z) &= A \exp(\beta z) \quad , \quad z < -\frac{L}{2} \quad , \\ &= B \cos \alpha z \quad , \quad |z| < \frac{L}{2} \quad , \\ &= C \exp(-\beta z) \quad , \quad z > \frac{L}{2} \quad . \end{aligned} \tag{5}$$

for even parity states. The continuity of $f_\alpha(z)$ and its derivative at $z = \pm L/2$ and the normalization condition determines the constants A, B and C and the allowed values for α. β in Eq.(5) is related to α and the depth of the well V_0. For odd parity states A is replaced by -A and $\cos\alpha z$ by $\sin\alpha z$. We shall use the effective Bohr radius $a_B = \epsilon_0 \hbar^2/m^* e^2$ as the unit of length and the effective Rydberg $R = m^* e^4/2\epsilon_0^2\hbar^2$ as the unit of energy. The eigenvalues of H_0 are

$$E = (k_x^2 + k_y^2) + \alpha^2 \quad , \tag{6}$$

where α is obtained as solutions of the equation

$$\begin{aligned} \pm \frac{\alpha}{\sqrt{V_0}} &= \cos\left(\frac{\alpha L}{2}\right) \quad , \quad \text{(even parity)} \quad , \\ &= \sin\left(\frac{\alpha L}{2}\right) \quad , \quad \text{(odd parity)} \quad . \end{aligned} \tag{7}$$

For the even parity states the argument of cosine is either in the first or third quadrant. Similarly, for the odd parity states $(\alpha L/2)$ should be in the second or fourth quadrant.

With the impurity potential present, we take as a trial function for the donor ground state

$$\psi_\alpha(\rho, \phi, z) = N \exp(-a_\alpha \rho) f_\alpha(z) \quad , \tag{8}$$

where the variational parameter a_α is obtained by minimizing the expectation value of H. One thus obtains the ground state of hydrogenic donors associated with any subband.

We wish to calculate a state above the first subband (in the continuum of the first subband) and is resonant with the ground state of a donor associated with the third subband. This resonant state is conveniently obtained if one gets the energy around which the partial density of states has a peak. The partial density of states is related to the imaginary part of Green's function for the resolvent operator $(E' - H)^{-1}$, where H is the Hamiltonian in Eq.(2). If we write E_i as the impurity ground state energy the diagonal part of Green's function is given by [4]

$$G = \left[E - E_i - P\sum_k \frac{|V_{ik}|^2}{E - E_k} + i\pi \sum_k |V_{ik}|^2 \delta(E - E_k)\right]^{-1} , \tag{9}$$

where V_{ik} is the matrix element of the impurity potential between the localized impurity ground state (wave function in Eq.(8)) and the band state (wave function in Eq.(4)). The position of the resonant level and its width are given, respectively, by

$$E_R = E_i + P\sum_k \frac{|V_{ik}|^2}{(E_R - E_k)} \quad , \tag{10}$$

and

$$\Gamma = \pi \sum_k |V_{ik}|^2 \delta(E_R - E_k) \cdot \tag{11}$$

The summation may be replaced by an integration with respect to energy. Substituting for the matrix elements, E_R is obtained as the solution of the equation

$$E - E_i - 16a^2 P \int_{E_{Sb1}}^{\infty} dE' \frac{1}{E - E'} F(E') = 0 \ , \tag{12}$$

where

$$F(E') = \left[\int_0^{\infty} d\rho\, \rho\, e^{-a\rho} \cos\sqrt{E'}\rho\, g(\rho)\right]^2 + \left[\int_0^{\infty} d\rho\, \rho\, e^{-a\rho} \sin\sqrt{E'}\rho\, g(\rho)\right]^2 . \tag{13}$$

$g(\rho)$ in Eq.(13) is given by

$$g(\rho) = \int_0^{L/2} dz\, B_1 B_3 \cos\alpha_1 z \cos\alpha_3 z \frac{1}{\sqrt{\rho^2 + z^2}} + \int_{L/2}^{\infty} dz\, A_1 A_3 \exp[-(\beta_1 + \beta_3)z] \frac{1}{\sqrt{\rho^2 + z^2}} \cdot \tag{14}$$

The width of the resonant state becomes

$$\Gamma = 16a^2 F(E_R) \quad . \tag{15}$$

The numerical results are presented in the next section.

III. RESULTS AND DISCUSSIONS

The binding energy of a donor ground state associated with the third subband (even parity) as a function of well width is presented in Fig.1. This figure also shows the separation of the resonant level from the impurity level, again as a function of well width. As the well width decreases the separation increases and then starts decreasing. Thus qualitatively we observe similar results for the resonant state and the localized ground state when a finite well is considered. The "turning over" is however not sharp for the resonant states.

In order to make direct contact with the experiments we have presented in Table 1 our results for the two wells of widths 238 Å and 460 Å. Since the Al content in the two experimental samples were different, this has also been taken into account in the present calculations. Transition energies are in reasonable agreement with the experimental results.

Table 2 shows the variation of the width of the resonant state as a function of well width. The widths are of the same order of magnitude as the separation of the resonant state from the localized state. This feature is similar to the results in Ref.4. The numerical values of Ref.4, however, are quite different from the results presented in our work.

One can repeat the calculations for the odd parity states. Experimentally, transitions involving the first and second subbands have been observed [3]. We expect qualitatively the same features for this case also with regard to variations with well widths.

In summary, we have calculated the position and width of resonant donor states involving the first and third subband for a GaAs quantum well with finite depth.

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TABLE 1

Comparison of the calculated values with experimental results

L	x	$E_R - E_i$ (meV)	$E_{i1} \rightarrow E^*_{Sb3}$ (meV)		$E_{i1} \rightarrow E_R$ (meV)	
			Th.	Exp.	Th.	Exp.
2.41	0.23	0.070	70.37	-	63.31	∿ 58
		(0.064)	(66.64)		(59.76)	
4.66	0.24	0.026	25.36	23.4	20.23	21.6
		(0.034)	(24.84)		(19.76)	

* E_{i1} is the impurity ground state associated with the first subband and E_{Sb3} is the third subband energy. Quantities in brackets are estimates based on the 'Miller rule'[5] for getting V_0. The other values are based on the 'Dingle rule' [6].

TABLE 2

Variation of width of the resonant state (Γ) with well width (L) for V_0 = 29.2

L (a_B)	Γ (R)
1.20	0.001125
1.50	0.006058
1.60	0.006957
2.00	0.009335
2.20	0.010602
2.41	0.003439
3.50	0.017649
4.66	0.024460

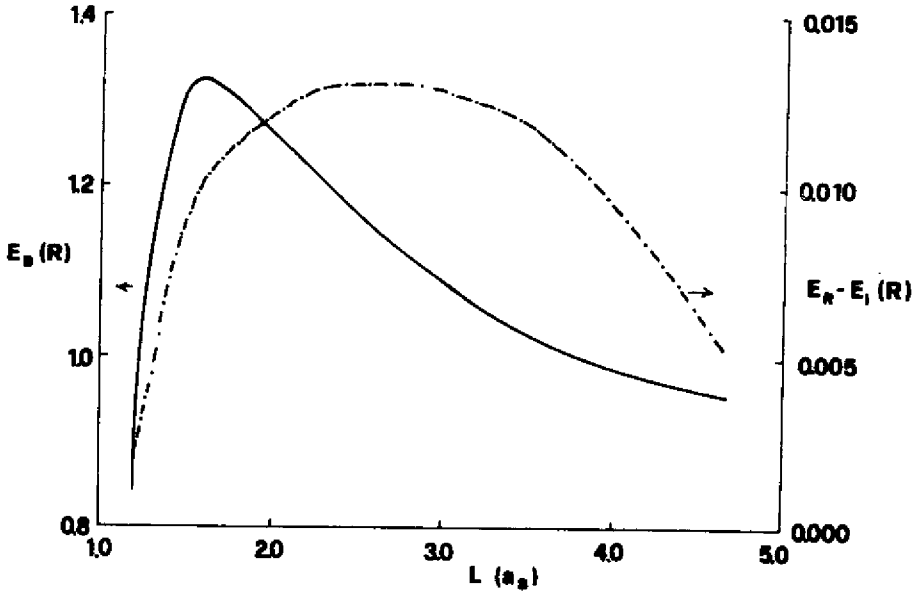

Fig.1 ——— Variation of donor binding energy (E_B) with well width (L) for a composition x = 0.24.

-·-·-·-·- Variation of the separation of the resonant state from the localized state ($E_R - E_i$) as a function of the well width (L) for a composition x = 0.24.