Polarizabilities of shallow donors in quantum wells

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Polarizabilities of shallow donors in GaAs/$Al_x Ga_{1-x}$As quantum wells are calculated with use of the Hasse variational method within the effective-mass approximation. The magnetic field dependence of polarizabilities is also studied.

I. INTRODUCTION

In recent years, there has been considerable theoretical and experimental interest in shallow donors in GaAs/$Al_x Ga_{1-x}$As quantum-well (QW) structures.[1-9] Far-infrared-magnetospectroscopy experiments have provided detailed results, for QW's with the magnetic field along the growth direction, which are in good agreement with variational calculations.[5] Good agreement is also obtained for low magnetic fields in the case of an applied magnetic field in the plane of the quantum wells.[8]

To the best of our knowledge, the polarizabilities of shallow donors in QW's are not yet reported. The earlier calculations of polarizabilities concentrated on the rather complicated case of bulk Si, where complications arise mainly from the many-valley structure.[10,11]

In this work, we extend the Hasse variational approach[12] used for bulk impurities to the case of those in QW structures.

II. DONOR POLARIZABILITIES

In the presence of weak applied electric and magnetic fields in the same z direction, the growth direction of the QW, the Hamiltonian for the donor electron becomes

$$H=-\nabla^2-\frac{2}{r}+V_B(z)+\eta z+\gamma L_z+\tfrac{1}{4}\gamma^2\rho^2 , \qquad (1)$$

where $V_B(z)$ is the infinite barrier potential which confines the carrier in the QW for $|z|\leq L/2$.

Here, we use the effective Bohr radius $a^*=\hbar^2\kappa_0/m^*e^2$, the effective Rydberg $R^*=m^*e^4/2\hbar^2\kappa_0^2$, and $\gamma=\hbar\omega_c/2\mathcal{R}^*$ with $\omega_c=eB/m^*c$ as the units of length, energy, and magnetic field, respectively. κ_0 is the static dielectric constant of GaAs. $\gamma=1$ is the magnetic field at which the diamagnetic energy is equal in magnitude to the Coulomb energy. The electric field term is $\eta z=|e|a^*Fz/\mathcal{R}^*$, where η is a measure of the electric field F. Here, the electric field is assumed to be applied along the z direction.

The polarizability α is defined by

$$E(B,\eta)=E(B,0)-\tfrac{1}{2}\alpha\eta^2 , \qquad (2)$$

i.e.,

$$\alpha=2\lim_{n\to 0}\frac{E(B,0)-E(B,\eta)}{\eta^2} . \qquad (3)$$

Following the Hasse variational method,[11] with the trial wave function proper for an infinite-barrier QW,

$$\psi=N\cos(k_1 z)\exp[-\beta(\rho^2+z^2)^{1/2}](1+\lambda\hat{\epsilon}\cdot\mathbf{r}) , \qquad (4)$$

where $\hat{\epsilon}=\mathbf{F}/F$, $k_1=\pi/L$, and N is a normalization constant, we have derived an expression for the polarizabili-

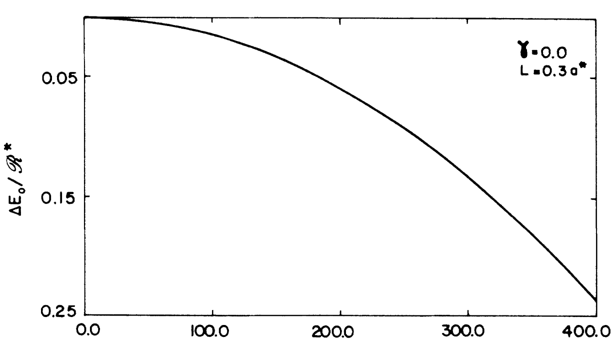

FIG. 1. The variation of impurity subband energy ΔE_0 as a function of electric field F.

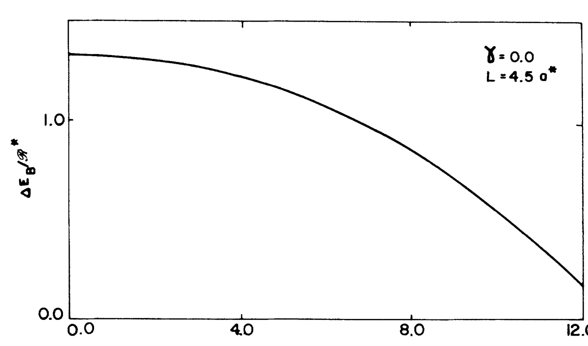

FIG. 2. The variation of impurity binding energy ΔE_B as a function of electric field F.

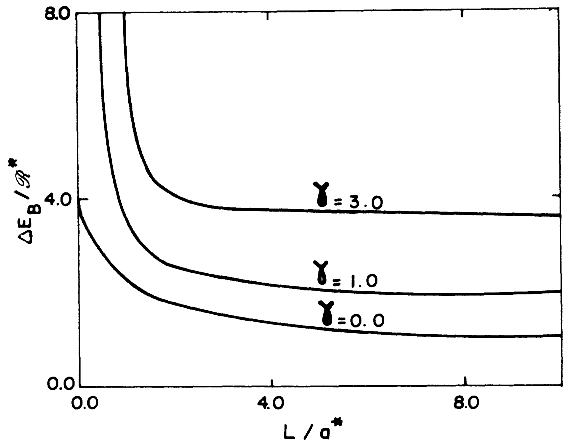

FIG. 3. The variation of impurity binding energy ΔE_B as a function of well width L and magnetic field γ.

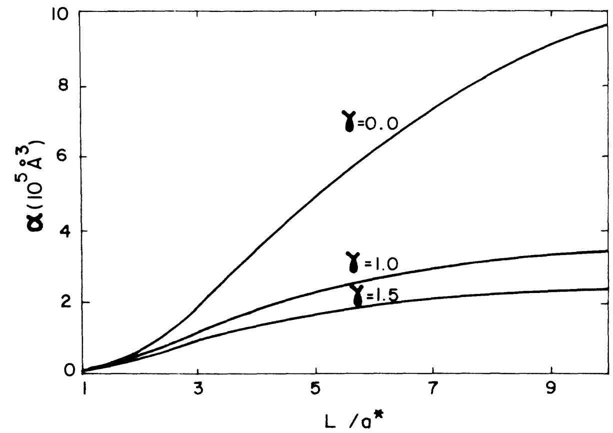

FIG. 4. The impurity polarizability values α as a function of well width L and magnetic field γ.

ty. In Eq. (4), λ is used as the variation parameter.

With the trial wave function given by Eq. (4), the donor-electron-energy expectation becomes

$$\langle E \rangle = \frac{T_1 + \eta T_3 \lambda + T_2 \lambda^2}{N_1 + N_2 \lambda^2} , \tag{5}$$

where

$$T_1 = \langle \psi_0 | (-\nabla^2 - 2/r) | \psi_0 \rangle , \tag{6}$$

$$T_2 = \langle \hat{\epsilon}\cdot\mathbf{r}\psi_0 | (-\nabla^2 - 2/r) | \hat{\epsilon}\cdot\mathbf{r}\psi_0 \rangle , \tag{7}$$

$$T_3 = \langle \hat{\epsilon}\cdot\mathbf{r}\psi_0 | z | \psi_0 \rangle , \tag{8}$$

$$N_1 = \langle \psi_0 | \psi_0 \rangle , \tag{9}$$

$$N_2 = \langle \hat{\epsilon}\cdot\mathbf{r}\psi_0 | \hat{\epsilon}\cdot\mathbf{r}\psi_0 \rangle , \tag{10}$$

with

$$\psi_0 = N \cos(k_1 z) \exp[-\beta(\rho^2 + z^2)^{1/2}] . \tag{11}$$

The value of λ that minimizes the energy expression $\langle E \rangle$ is obtained as

$$\lambda = -\frac{N_2 T_1 - N_1 T_2}{N_2 T_3 \eta} \left[1 - \left\{ 1 + \frac{N_1 N_2 T_3^2 \eta^2}{(N_2 T_1 - N_1 T_2)^2} \right\}^{1/2} \right] . \tag{12}$$

Substituting this value of λ into Eq. (5) and expanding $\langle E \rangle$ binomially in powers of ϵ, one gets for polarizability

$$\alpha = \frac{T_3^2}{2(N_2 T_1 - N_1 T_2)} . \tag{13}$$

III. RESULTS AND CONCLUSIONS

Polarizability values with and without the magnetic field are calculated using the following input parameters: the effective mass $m^* = 0.067 m_e$, and the static dielectric constant $\kappa_0 = 12.5$ suitable for quantum wells made out of GaAs. The effective Rydberg $\mathcal{R}^* = 5.83$ meV and the effective Bohr radius $a^* = 98.7$ Å define the relevant energy and length scales.

TABLE I. Polarizability values (in units of 10^5 Å^3) with and without magnetic field as a function of well width (in units of effective Bohr radius $a^* = 98.7$ Å.

L/a^*	$\gamma = 0.0$ (10^5 Å^3)	$\gamma = 1.0$ (10^5 Å^3)	$\gamma = 1.5$ (10^5 Å^3)
1.0	0.058	0.057	0.057
2.0	0.656	0.536	0.464
3.0	1.896	1.196	0.936
4.0	3.392	1.768	1.336
5.0	4.880	2.248	1.656
6.0	6.210	2.624	1.892
7.0	7.320	2.904	2.064
8.0	8.280	3.108	2.184
9.0	9.040	3.260	2.272
10.0	9.640	3.372	2.336

To study first the effect of electric field on the impurity binding energy $E_B^0=(\pi/L)^2-\langle H\rangle_{\min}$, we calculate E_B^0 variationally without the electric- and magnetic-field terms and with the wave function given by Eq. (4) taking $\lambda=0$ and considering β as a variational parameter. This corresponds to the Bastard case.[1] We then repeat the calculation with full ψ as in Eq. (4) to calculate E_B including the electric-field term in Eq. (1). For the latter calculation, we need to consider the shift ΔE_0 of the subband energy as a result of applied electric field. ΔE_0 is calculated using second-order perturbation theory as it is done by Bastard *et al.*[4] The calculated E_0 values are shown in Fig. 1. The difference $\Delta E_B=E_B-E_B^0$ is a measure of the effect of electric field on the donor binding energy. ΔE_B values are shown in Fig. 2 for a well width of $L=4.5a^*$. As expected, the electric field reduces the donor binding energy.

To study next the effect of the magnetic field, the electric field term in the Hamiltonian and λ term in the trial wave function given by Eq. (4) are omitted. The donor binding energy E_B is then calculated, taking into account the shift in subband energy, as a function of well width L and the magnetic field. The results are shown in Fig. 3, and these are in accord with earlier calculations.[1]

The numerical values for polarizability α are given in Table I for $\gamma=0.0$, 1.0, and 1.5, where $\gamma=1$ corresponds to a magnetic field of 67.4 kG. The calculated polarizability values have reasonable magnitudes and correctly reflect the effect of a magnetic field which confines the electron more and reduces the polarizability. The numerical values for extremely narrow QW's cannot be accurate as the effective-mass formalism may not be applicable for this case. (See Fig. 4.)

There is considerable room for improvement in the present calculation. Firstly, the form of the variational wave function, Eq. (4), should be modified to take into account the presence of the magnetic field better. This will also improve the calculation of the subband energy shift as a function of magnetic field. The screening effects could be taken into account better by using a position-dependent dielectric function $\kappa_0(r)$ instead of the constant κ_0, which unfortunately further complicates the calculation.

One of the most important limiting assumptions of the present work is the infinite barrier, which prevents the impurity electron wave function from extending over to the neighboring $Al_xGa_{1-x}As$ regions. The calculation should be repeated for the finite-barrier model to get quantitatively dependable results. One should also keep in mind that the magnetic fields in the z direction are least effective in compressing the wave function in that direction, resulting in a wave function more in contact with the walls of the well. Nevertheless, the simpler infinite-barrier model employed in the present work is expected to give a qualitatively correct picture of all the important features of the problem.

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