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LETTER TO THE EDITOR

D^0 and D^- off centre in strong magnetic fields and quantum wells

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Abstract. Variational calculations are performed for the ground and first excited states of D^0 off centre and the lowest singlet and triplet states of D^- off centre in quantum wells in a magnetic field. It is found that the off-centre effect on the binding energies increases with increasing magnetic field. The binding energy of the triplet state can be larger than that of the corresponding singlet one if the magnetic field is strong enough.

There have been many investigations of the electronic structures and properties of neutral shallow donors D^0 in GaAs–$Ga_{1-x}Al_xAs$ quantum wells (QWs) with and without doping in strong magnetic fields. Recently, negative donors D^-, i.e. neutral donors that bind an additional electron, have already been observed (Huant *et al* 1990) and identified (Mueller *et al* 1992) in multiple QWs. The effective-mass model has been applied to D^- centres in a magnetic field in two-, quasi-two-, and three-dimensional (2D, Q2D, and 3D) cases (Natori and Kamimura 1978, Larsen 1979a, b, Phelps and Bajaj 1983, Louie and Pang 1992, Zhu 1992, Larsen and McCann 1992a, b, Sandler and Proetto 1992). All of the theoretical and experimental studies have shown that the binding energy of the lowest singlet state is much larger than that of the triplet one, that the magnetic field can introduce more bound states, and that the binding energies of D^- centres in a magnetic field are strongly dependent on the confined dimensionality, i.e., the dimensions and strength of the magnetic field. However, no information seems to be available concerning the properties of D^- off centre in QWs in a strong magnetic field. In this letter, we report a variational calculation of the lowest singlet and triplet states and study the field effect on the binding energies of D^- off centre in QWs, which is in sharp contrast to that mentioned above.

Within the framework of an effective-mass approximation, the Hamiltonian of a D^0 off centre in GaAs–$Ga_{1-x}Al_xAs$ QWs in a magnetic field γ perpendicular to the interface can be written as

$$H(\rho, \phi, z) = -\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) - \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2} - \frac{\partial^2}{\partial z^2} - \frac{2}{[\rho^2 + (z - z_0)^2]^{1/2}} + V(z) + \frac{\gamma^2}{4}\rho^2 + \gamma L_z \tag{1}$$

with

$$V(z) = \begin{cases} V_0 & \text{if } |z| \geqslant L/2 \\ 0 & \text{if } |z| < L/2 \end{cases} \tag{2}$$

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where V_0 is the barrier height and can be obtained from a fixed ratio of the band-gap discontinuity, γL_z is the Zeeman term, L the well width, and z_0 the z component of cylindrical polar coordinates of the donor ion. The polarization and image charge effects have been ignored as is reasonable for GaAs–$Ga_{1-x}Al_xAs$ quantum-well systems. It should be pointed out that we have ignored the Zeeman spin energy, which does not affect the binding energies. In this letter, effective atomic units are used so that all energies are measured in units of the effective Rydberg Ry* and all distances are measured in units of effective Bohr radius a^*.

The corresponding Hamiltonian of a D^- off centre in the QWs is as follows:

$$H = H(\rho_1, \phi_1, z_1) + H(\rho_2, \phi_2, z_2) + \frac{2}{[\rho_{12}^2 + (z_1 - z_2)^2]^{1/2}} \tag{3}$$

where $\rho_{12} = |\rho_1 - \rho_2|$.

(1) can be rewritten as

$$H(\rho, \phi, z) = H_0(\lambda, \alpha, \rho, \phi, z) + H'(\lambda, \alpha) \tag{4}$$

with

$$H_0(\lambda, \alpha, \rho, \phi, z) = -\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) - \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2} - \frac{2\lambda}{\rho + \alpha} - \frac{\partial^2}{\partial z^2} + V(z) + \frac{\gamma^2}{4}\rho^2 + \gamma L_z \tag{5}$$

and

$$H'(\lambda, \alpha) = \frac{2\lambda}{\rho + \alpha} - \frac{2}{[\rho^2 + (z - z_0)^2]^{1/2}}. \tag{6}$$

Exact solutions of H_0 with well defined magnetic quantum number m can be obtained (Zhu *et al* 1990). Taking the eigenfunctions of the ground ($m = 0$) and first excited ($m = 1$) states of H_0 as trial functions with variational parameters α and λ, the energies $E(D^0, 0)$ and $E(D^0, 1)$ of ground and first excited states can be obtained by a variational calculation and, then, the binding energies $E_B(D^0, 0)$ and $E_B(D^0, 1)$ of D^0 off centre in QWs in a magnetic field γ are respectively given by

$$E_B(D^0, 0) = E(e, 0) - E(D^0, 0) \tag{7}$$

and

$$E_B(D^0, 1) = E(e, 0) - E(D^0, 1) \tag{8}$$

where $E(e, 0)$ is the ground-state energy of an electron in the QWs in the magnetic field γ.

With the use of the forms of (5) and (6), (3) can be rewritten as

$$H = \tilde{H}(\lambda_1, \lambda_2, \alpha_1, \alpha_2) + H_{in}(\lambda_1, \lambda_2, \alpha_1, \alpha_2) \tag{9}$$

with

$$\tilde{H}(\lambda_1, \lambda_2, \alpha_1, \alpha_2) = H_0(\lambda_1, \alpha_1, \rho_1, \phi_1, z_1) + H_0(\lambda_2, \alpha_2, \rho_2, \phi_2, z_2) \tag{10}$$

and

$$H_{\text{in}} = H'(\lambda_1, \alpha_1) + H'(\lambda_2, \alpha_2) + \frac{2}{[\rho_{12}^2 + (z_1 - z_2)^2]^{1/2}}. \tag{11}$$

Using the exact eigenfunctions of the ground ($m = 0$) and first excited ($m = 1$) states of $H_0(\lambda, \alpha_1, \rho_1, \phi_1, z_1)$ and $H_0(\lambda_2, \alpha_2, \rho_2, \phi_2, z_2)$, the Chandrasekhar-type trial functions with well defined total magnetic quantum number $M = m_1 + m_2$ can be obtained. The trial function Ψ_0 of the lowest singlet s ($M = 0$) state is given by

$$\Psi_0 = A(1 + c\rho_{12})\psi(z_1)[\psi_0(\alpha_1, \lambda_1, \rho_1)\psi_0(\alpha_2, \lambda_2, \rho_2) + \psi_0(\alpha_1, \lambda_1, \rho_2)\psi_0(\alpha_2, \lambda_2, \rho_1)] \tag{12}$$

while the trial functions Ψ_1^+ and Ψ_1^- of singlet and triplet p ($M = 1$) states are given by

$$\Psi_1^{\pm} = B(1 + c\rho_{12})\psi(z_1)\psi(z_2)[\psi_0(\alpha_1, \lambda_1, \rho_1)\psi_1(\alpha_2, \lambda_2, \rho_2)e^{-i\phi_2} \pm \psi_0(\alpha_1, \lambda_1, \rho_2)\psi_1(\alpha 2, \lambda_2, \rho_1)e^{-i\phi_1}]. \tag{13}$$

Here $\psi(z)\psi_0(\alpha, \lambda, \rho)$ and $\psi(z)\psi_1(\alpha, \lambda, \rho)e^{-i\phi}$ are the eigenfunctions of the ground and first excited states of $H_0(\alpha, \lambda, \rho, \phi, z)$, respectively; λ_1, λ_2, α_1, α_2, and c are variational parameters. A and B are the normalization constants. Then, the variational energy $E(D^-, 0)$ of the singlet s state is as follows:

$$E(D^-, 0) = \min_{\lambda_1 \lambda_2 \alpha_1 \alpha_2 c} \langle \Psi_0 | H | \Psi_0 \rangle \tag{14}$$

and the variational energies $E^+(D^-, 1)$ and $E^-(D^-, 1)$ of singlet and triplet p states are as follows:

$$E^{\pm}(D^-, 1) = \min_{\lambda_1 \lambda_2 \alpha_1 \alpha_2 c} \langle \Psi_1^{\pm} | H | \Psi_1^{\pm} \rangle. \tag{15}$$

Once $E(D^-, 0)$ and $E^{\pm}(D^-, 1)$ are obtained, the binding energies $E_B(D^-, 0)$ and $E_B(D^-, 1)$ of singlet s and triplet p states and the singlet–triplet splitting energies ΔE_{13} of p states are given by

$$E_B(D^-, 0) = E(D^0, 0) + E_0(e, 0) - E(D^-, 0) \tag{16}$$

$$E_B(D^-, 1) = E(D^0, 0) + E_0(e, 0) - E^-(D^-, 1) \tag{17}$$

and

$$\Delta E_{13} = E^+(D^-, 1) - E^-(D^-, 1) \tag{18}$$

respectively.

In order to know whether the trial functions used here are suitable or excellent for the calculation of D^- states in quantum wells in a magnetic field and check the calculation method, we have calculated the binding energies $E_B(D^0, 0)$ and $E_B(D^-, 0)$ of D^0 and D^- centres ($z_0 = 0$) in GaAs–$Ga_{0.25}Al_{0.75}As$ QWs with a well width 200 Å (about $2a^*$), and compared the results with those obtained by a diffusion quantum Monte Carlo method (Louie and Pang 1992). As shown in table 1, our results are slightly less than but close to

Table 1. Binding energies of D^- and D^0 centres in $Ga_{0.75}Al_{0.25}As$ QWs with well width 200 Å. The energies are in effective Rydberg Ry* of GaAs; 1 Ry* = 5.806 meV. The Monte Carlo error bars are estimated at two units of the last digit in the data (Louie and Pang 1992).

	γ	Present results	Monte Carlo results
D^-	0	0.214	0.23
	1	0.641	0.65
	3	0.910	0.94
D^0	0	1.701	1.74
	1	2.441	2.52
	3	3.242	3.36

theirs and the differences are comparable to the statistical fluctuations of the Monte Carlo calculation. Therefore, it would be expected that using the trial functions and the calculation method, reasonable results can be obtained for the singlet and triplet states of D^- off centre in QWs in a magnetic field.

The ground ($m = 0$) and first excited ($m = 1$) states of D^0 off centre in QWs of $V_0 = 80$ Ry* with $L = 2a^*$ have been calculated for $z_0 = 0.5$, 0.625, and $0.75a^*$, respectively. In figure 1, the binding energies $E_B(D^0, m)$ have been plotted as a function of γ. It is readily seen that all of $E_B(D^0, m)$ increase with increasing γ and the values are larger for smaller z_0 than for larger z_0. However, the variation with z_0 is much larger for ground states than for the first excited states. This is easy to understand if we note that the $\psi_1(\alpha, \lambda, \rho)$ of excited states are more extended than the $\psi_0(\alpha, \lambda, \rho)$ of ground states and, then, z_0 has a strong effect on the Coulomb creation energies of D^0 ground states.

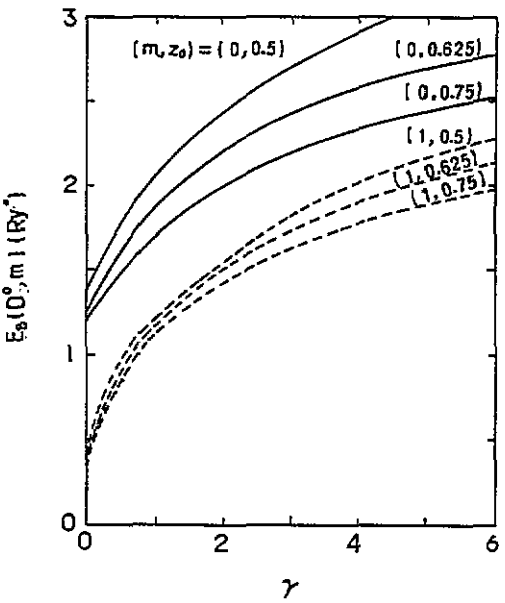

Figure 1. Binding energies $E_B(D^0, m)$ of s ($m = 0$) and p ($m = 1$) states of D^0 off centre in QWs of $L = 2a^*$ with $V_0 = 80$ Ry* are shown as a function of γ for $z_0/a^* = 0.5$, 0.625, and 0.75, respectively.

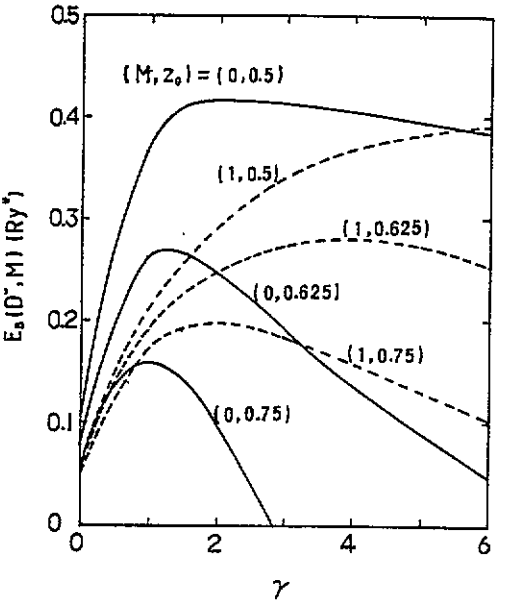

Figure 2. Binding energies $E_B(D^-, M)$ of singlet s ($M = 0$) and triplet p ($M = 1$) states of D^- off centre in QWs of $L = 2a^*$ with $V_0 = 80$ Ry* are shown as a function of γ for $z_0/a^* = 0.5$, 0.625, and 0.75, respectively.

Using the trial functions of (12) and (13), the singlet and triplet states of D^- off centre in the QWs have been calculated for the same z_0, i.e., 0.5, 0.625, and $0.75a^*$, respectively. In figure 2, the binding energies $E_B(D^-, M)$ have been shown as a function of γ. It is interesting to point out that the variations with γ are quite different for the singlet s ($M = 0$) and triplet p ($M = 1$) states and for different z_0. As seen in the figure, with increasing γ the binding energy $E_B(D^-, 1)$ of $z_0 = 0.5a^*$ increases continually while the $E_B(D^-, 0)$ increases rapidly until a maximum value and, then, decreases slowly. There is an intersection of the two curves at $\gamma = \gamma_c = 5.5$. This means that the triplet states of D^- off centre in QWs can be bound more strongly than the singlet ones due to an applied strong magnetic field.

With increasing z_0, the transformational point γ_c decreases as shown in the figure. The γ_c is respectively equal to 2.0 and 0.7 for $z_0 = 0.625$ and $0.75a^*$. It is worthwhile to note that there are maxima for both $E_B(D^-, 0)$ and $E_B(D^-, 1)$ as z_0 is larger and that there is no bound D^- state of $z_0 = 0.75a^*$ as $\gamma > 9.2$. This means that for a fixed z_0, an applied magnetic field can not only increase but also decrease the binding energies of D^- off centre in QWs and that the effect of a magnetic field on D^- states with $z_0 \neq 0$ in QWs is in sharp contrast to that on D^- ones with $z_0 = 0$ in QWs. A very strong magnetic field can dissociate a D^- off centre in a QW into an electron and D^0 off centre in the QW. It is also found that the singlet–triplet splitting energies ΔE_{13} of p ($M = 1$) states increase with increasing γ and are almost independent of z_0 in the presence of strong fields.

What has been mentioned above can be understood on the basis of the following. In QWs, z_0 has much less effect on the single-electron Coulomb and exchange integrals of $-2/[\rho^2 + (z - z_0)^2]^{1/2}$ for more extended orbitals than for more localized ones. Therefore, both $E_B(D^-, 0)$ and $E_B(D^-, 1)$ are much more sensitive to z_0 in strong magnetic fields than in weak ones and the effect of z_0 on $E_B(D^-, 0)$ is larger than that on $E_B(D^-, 1)$.

Furthermore, z_0 has only a small effect on ΔE_{13} in strong fields because the two-electron Coulomb and exchange integrals are less affected.

In summary, we have for the first time reported calculation results of binding energies D^0 and D^- off centre in GaAs–$Ga_{1-x}Al_xAs$ QWs of $L = 2a^*$ in a magnetic field. For $z_0 = 0$, our results are in good agreement with those obtained by the Monte Carlo method. The results for $z_0 \neq 0$ have clearly demonstrated the off-centre effect. This is larger for the states with localized orbitals than for those with extended ones and increases with increasing γ and z_0. However, the variation of $E_B(D^-, 0)$ and $E_B(D^-, 1)$ is quite different from that of $E_B(D^0, 0)$ and $E_B(D^0, 1)$. It is predicted that the $E_B(D^-, 1)$ can be larger than $E_B(D^-, 0)$ and a D^- off centre in a QW can be dissociated into an electron and a D^0 off centre in the QW due to a strong magnetic field. This prediction could be confirmed experimentally in the future.

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