Energy levels of D^0 and D^- in graded quantum-well structures of GaAs/$Ga_{1-x}Al_xAs$ under magnetic fields

Jia-Lin Zhu
*Chinese Center of Advanced Science and Technology (World Laboratory), P.O. Box 8730, Beijing 100080, China and Department of Physics, Tsinghua University, Beijing 100084, China**

D. L. Lin
Department of Physics, State University of New York at Buffalo, Buffalo, New York 14260-1500

Y. Kawazoe
Institute for Materials Research, Tohoku University, Sendai 980, Japan
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Energy levels of D^0 and D^- confined in graded quantum wells of GaAs/$Ga_{1-x}Al_xAs$ structures under magnetic fields are investigated in detail by the variational method. Binding energies as well as the $1s \rightarrow 2p^-$ transition energy for D^0 and D^- in a square well calculated from the same trial wave functions are shown to be in good agreement with existing Monte Carlo calculations and with experimental data. An interesting quantum shape effect is revealed by studying the ratio of D^- transition energy to its binding energy. A detailed study of D^0 and D^- states in graded quantum wells shows that (a) D^- binding energies first increase with the magnetic field and then decrease when the field increases further, (b) for a given well gradient, the singlet s-like state binding energy peaks at a much lower field strength than the triplet p-like states, producing the energy level crossing phenomenon, and (c) D^- will be dissociated into a D^0 and an electron when either the field or the gradient increases. [S0163-1829(96)06548-4]

I. INTRODUCTION

Stimulated by the interest in fundamental research and technological applications, a great variety of low-dimensional semiconductor microstructures have been fabricated and investigated in recent years. The properties of impurities doped by various doping schemes are of particular importance in the design of devices. Energy levels of a neutral hydrogenic donor or D^0 in GaAs/$Ga_{1-x}Al_xAs$ quantum wells and transitions between $1s$ and np levels under arbitrary magnetic fields have been investigated for $n=2,3,4$.[1] The negatively charged donor D^-, a bound state of an electron and D^0, has also been identified in multiple-quantum-well structures recently.[2,3] Since then a large amount of work, both theoretical and experimental, has been carried out.[2–17] It is found that for D^- situated at the square quantum-well (SQW) center, the binding energy for the lowest singlet state is much larger than that for the lowest triplet state,[3,6] and that the number of bound states increases under the applied magnetic field.[3,9] As is well known, the binding energy of D^0 increases with increasing magnetic fields. The same behavior of D^- binding energy is easily understood. The ratio σ of D^0 and D^- binding energies approaches a constant and freezes in the high-field limit.[17] A recent study[18] reveals that in high fields σ depends strongly on the dimensionality. Numerical calculations show that $\sigma \sim 0.055$ for three dimensions (3D), ~ 0.1 for 2D, ~ 0.2 for 1D, and ~ 0.3 for 0D, depending upon the detailed shape of confinement potentials. Since strong magnetic fields serve the purpose of confinement for charge carriers, σ increases from ~ 0.055 with the increasing magnetic field and approaches ~ 0.2 in the strong field limit in 3D. In a narrow SQW, the increasing magnetic field in the growth direction changes σ from ~ 0.1 to ~ 0.3.

Although extensive studies on various aspects of impurity states in multiple-quantum-well systems and superlattices of different combinations have been made in the past, they are mainly concerned with impurities in a square quantum well. An observation[19] of a transient electrical polarization phenomenon in sawtooth superlattices of GaAs/$Ga_{1-x}Al_xAs$ in 1983 has attracted much attention to the electronic structure and related phenomena of graded-gap microstructures with their possible device applications in mind.[20–25] It is expected that the break of reflection symmetry in such structures can give rise to a number of interesting new phenomena. In particular, it has been found that the electron-phonon scattering rate in an asymmetric quantum well differs remarkably from that in symmetric wells due to the applied field and changed phonon modes, which is useful in devices.[25]

The electronic structures in graded quantum-well (GQW) systems with or without the external electric field have been investigated in great detail. For example, in order to achieve high on-off ratio and low operation voltage, a GQW structure has been proposed,[20–22] in which both the conduction- and valence-band edges in the well vary linearly along the growth direction. In this paper, we investigate the effects of the broken reflection symmetry on the energy levels of D^0 and D^- confined in a quantum well, and attempt to calculate energy level schemes in GQW structures with and without the magnetic field.

The organization of this paper is as follows. In Sec. II we describe the Hamiltonian of the problem. The procedure of calculation is briefly outlined in Sec. III. Energy levels of D^0 and D^- in a SQW are obtained in Sec. IV as a function of

the well width for given magnetic fields, and compared numerically with existing results from the Monte Carlo calculation[5] as well as with experimental measurements.[16] In Sec. V the ground-state energy as well as the $1s$-$2p^-$ transition energy are calculated for D^0 and D^- in GQW's in arbitrary magnetic fields. Results for a few particular field strengths are presented as a function of the field strength for various spatial gradients of the GQW. A few concluding remarks are also discussed in this section.

II. THEORY

Consider a donor in a GaAs quantum well of GaAs/$Ga_{1-x}Al_x$As structure with a magnetic field B applied in the growth direction. If the impurity is situated at z_0 from the center of the well, the Hamiltonian can be put in the form

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

where the 3D position vector $\mathbf{r}=(\boldsymbol{\rho},z)$, the effective Rydberg $\mathrm{Ry}^*=e^2/2\epsilon a^*$, and the effective Bohr radius $a^*=\epsilon\hbar^2/m^*e^2$ are taken to be the energy and length units, respectively. The magnetic field is measured in the unit $\gamma=e\hbar B/2m^*c\mathrm{Ry}^*=\hbar\omega_c/2\ \mathrm{Ry}^*$ with the cyclotron frequency ω_c. It is noted that in obtaining Eq. (1), we have ignored the polarization and image charge effects, as well as the Zeeman spin energy which has no influence on the binding energy. The confinement potential is taken to be

$$V(z)=\begin{cases}V_0 & \text{for } |z|\geq L/2\\ R(L/2+z) & \text{for } |z|<L/2,\end{cases} \tag{2}$$

where R is the constant gradient of the potential well. The GQW becomes a regular SQW when $R=0$. V_0 and R can be determined by a fixed ratio of the band-gap discontinuity which depends on the aluminum concentration in the sample.

The Hamiltonian for a D^- center at z_0 in the QW is given by

$$H=H(\rho_1,\varphi_1,z_1)+H(\rho_2,\varphi_2,z_2)+\frac{2}{[\rho_{12}^2+(z_1-z_2)^2]^{1/2}}, \tag{3}$$

where $\rho_{12}=|\boldsymbol{\rho}_1-\boldsymbol{\rho}_2|$. To solve the problem, we start with Eq. (1), which can be rewritten as

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

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

$$H'(\lambda,a)=\frac{2\lambda}{\rho+a}-\frac{2}{[\rho^2+(z-z_0)^2]^{1/2}}, \tag{4c}$$

where we have introduced two parameters λ and a to be determined by the variational principle. Because of the cylindrical symmetry, exact solutions of H_0 with the well-defined magnetic quantum number m can be obtained by a series expansion method similar to the quantum dot problem.[26] If the ground state of H_0 is s-like ($m=0$) and the first excited state is p^--like ($m=-1$), the corresponding eigenfunctions can be written as $\psi(z)\psi_0(a,\lambda,\rho)$ and $\psi(z)\psi_1(a,\lambda,\rho)e^{-i\varphi}$. The energy levels and hence the $1s\rightarrow 2p^-$ transition energy for $H(\rho,\varphi,z)$ can be found by a variational calculation.

Let $E(D^0,m)$ denote the energy level of D^0 in the state m, then the binding energy in this state is given by

$$E_B(D^0,m)=E(e,0)-E(D^0,m), \tag{5a}$$

where $E(e,0)$ stands for the ground state of an electron in a quantum well in the magnetic field of strength γ. The $1s\rightarrow 2p^-$ transition energy is given by

$$\Delta E(D^0)=E(D^0,1)-E(D^0,0). \tag{5b}$$

In a similar fashion, we rewrite (3) for D^- as

$$H=H_0(\lambda_1,a_1,\lambda_2,a_2)+H_{\mathrm{int}}(\lambda_1,a_1,\lambda_2,a_2), \tag{6a}$$

$$H_0(\lambda_1,\lambda_2,a_1,a_2)=H_0(\lambda_1,a_1\rho_1,\varphi_1,z_1)+H_0(\lambda_2,a_2,\rho_2,\varphi_2,z_2), \tag{6b}$$

$$H_{\mathrm{int}}=H'(\lambda_1,a_1)+H'(\lambda_2,a_2)+\frac{2}{[\rho^2+(z_1-z_2)^2]^{1/2}}. \tag{6c}$$

Using the exact D^0 eigenfunctions given above, we can easily construct the trial functions Ψ_M of Chandrasekhar type[27] with the well-defined total magnetic quantum number $M=m_1+m_2$. Thus we have the trial functions

$$\Psi_0=A_0(1+c\rho_{12})\psi(z_1)\psi(z_2)[\psi_0(\lambda_1,a_1\rho_1)\psi_0(\lambda_2a_2,\rho_2)+\psi_0(\lambda_1,a_1,\rho_2)\psi_0(\lambda_2,a_2,\rho_1)] \tag{7a}$$

for the lowest singlet s-like state, and

$$\Psi_1^{\pm}=A_1(1+c\rho_{12})\psi(z_1)\psi(z_2)\times[\psi_0(\lambda_1,a_1,\rho_1)\psi_1(\lambda_2,a_2,\rho_2)e^{-i\rho_2}\pm\psi_0(\lambda_1,a_1,\rho_2)\psi_1(\lambda_2,a_2,\rho_1)e^{-i\rho_1}] \tag{7b}$$

for the singlet $(+)$ and triplet $(-)$ p^--like states. We have introduced one more variational parameter c in Eqs. (7). A_1 and A_2 are normalization constants.

III. METHOD OF CALCULATION

We are now in a position to calculate the D^- energy eigenvalues $E(D^-,0)$, $E^+(D^-,1)$ and $E^-(D^-,1)$ for the singlet s-like, and singlet and triplet p-like states, respectively. Since the D^0 states in quantum wells under arbitrary magnetic fields have been well investigated, both experimentally and theoretically,[1,3,5,15] we can check our calculations with existing results as a test of our choice of trial wave functions. It turns out that the above trial wave functions yield very good results compared to the Monte Carlo calculations[3] as we shall see later.

To describe the method of calculation, it is most conve-

nient to illustrate the procedure by considering a specific case. Let us calculate the eigenenergy

$$\langle\Psi_1^-|H|\Psi_1^-\rangle=\langle\Psi_1^-|H(\lambda_1,a_1,\lambda_2,a_2)|\Psi_1^-\rangle + \langle\Psi_1^-|H(\lambda_1,a_1)+H(\lambda_2,a_2)|\Psi_1^-\rangle + \left\langle\Psi_1^-\left|\frac{2}{[\rho_{12}^2+(z_1-z_2)^2]^{1/2}}\right|\Psi_1^-\right\rangle. \quad (8)$$

The first two terms of the energy eigenvalue can be evaluated in a straightforward manner by making use of the expansion

$$\frac{1}{\rho_{12}}=\sum_{m=-\infty}^{\infty}\frac{|m-1|!!}{|2m|!!}\frac{\rho_<^m}{\rho_>^{m+1}}F(m+\tfrac{1}{2},\tfrac{1}{2},m+1,\rho_<^2/\rho_>^2)\times e^{im(\varphi_1-\varphi_2)}, \quad (9)$$

where $F(a,b,c,x)$ is the hypergeometric function, $\rho_<=\min\{\rho_1,\rho_2\}$, and $\rho_>=\max\{\rho_1,\rho_2\}$. The last term of (8) involves five-dimensional integrals of the type

$$F_{MN}=\int\frac{\Lambda(\lambda_1,a_1,\rho_1,\lambda_2,a_2,\rho_2)e^{iM\varphi}\rho_{12}^N\psi^2(z_1)\psi^2(z_2)}{[\rho_{12}^2+(z_1-z_2)^2]^{1/2}}\times dz_1dz_2d\rho_1d\rho_2d\varphi, \quad (10)$$

where $M=\pm1$, $N=0,1,2$, and φ stands for the angle between the position vectors of the two electrons. The function Λ represents the integrand in the Coulomb and exchange integrals. More explicitly, we have

$$\Lambda(\lambda_1,a,\rho_1,\lambda_2,a_2,\rho_2)=\psi_0^2(\lambda_1,a_1,\rho_1)\times\psi_1^2(\lambda_2,a_2,\rho_2)\rho_1\rho_2 \quad (11a)$$

for Coulomb integrals and

$$\Lambda(\lambda_1,a_1,\rho_1,\lambda_2,a_2,\rho_2)=\psi_0(\lambda_1,a_1,\rho_1)\psi_1(\lambda_2,a_2,\rho_2)\times\psi_0(\lambda_1,a_1,\rho_2)\times\psi(\lambda_2,a_2,\rho_1)\rho_1\rho_2 \quad (11b)$$

for exchange integrals.

In order to evaluate these multidimensional integrals, we need an effective numerical method with high accuracy. This is accomplished by introducing the functions

$$I(\rho_{12})=\int\int\frac{\psi^2(z_1)\psi^2(z_2)}{[\rho_{12}^2+(z_1-z_2)^2]^{1/2}}dz_1dz_2, \quad (12a)$$

$$G_{MN}(\rho_1,\rho_2)=\int\rho_{12}^N I(\rho_{12})e^{iM\varphi}d\varphi. \quad (12b)$$

Both functions can be found by evaluating the integrals numerically for a given set of parameters including the gradient R, the well width L, and the barrier height V_0 which is determined by the relative aluminum concentration in the well and barrier of the system. With these functions stored numerically in the computer, Eq. (10) becomes essentially a two-dimensional integral,

$$F_{MN}=\int\Lambda(\lambda_1,a_1,\rho_1,\lambda_2,a_2,\rho_2)G_{MN}(\rho_1,\rho_2)d\rho_1d\rho_2 \quad (13)$$

and can be carried out without difficulty.

After $E(D^-,0)$ and $E^-(D^-,1)$ are found, the binding energy of the singlet s-like state follows directly as

$$E_B(D^-,0)=E(D^0,0)+E(e,0)-E(D^-,0). \quad (14a)$$

Similarly, the binding energy of a triplet p^--like state is

$$E_B(D^-,1)=E(D^0,0)+E(e,0)-E^-(D^-,1). \quad (14b)$$

To determine the transition energies, we note that in addition to the spin conservation, the dipole-excited D^- transitions in Faraday geometry obey the selection rule $\Delta M=\pm1$. The D^- transitions of $\Delta M=+1$ and -1 are analogous to $1s\rightarrow2p^+$ and $1s\rightarrow2p^-$ D^0 transitions, respectively.[6,16] Since the p^+- and p^--like states are separated exactly by the cyclotron energy 2γ for parabolic conduction bands, the $1s\rightarrow2p^+$ D^- transition energy is

$$\Delta E^+(D^-)=\Delta E(D^-)+2\gamma, \quad (15a)$$

where

$$\Delta E(D^-)=E^+(D^-,1)-E(D^-,0) \quad (15b)$$

is the $1s\rightarrow2p^-$ D^- transition energy.

TABLE I. Comparison of D^0 and D^- binding energies with Monte Carlo results. Energy is expressed in the unit Ry*.

Impurity	γ	L (Å)	This work	Monte Carlo[a]
D^0	0	100	2.096	2.09
		200	1.701	1.74
	1	100	2.894	2.92
		200	2.441	2.52
	3	100	3.858	3.89
		200	3.242	3.36
D^-	0	100	0.252	0.29
		200	0.214	0.23
	1	100	0.736	0.77
		200	0.641	0.65
	3	100	1.082	1.13
		200	0.910	0.94

[a]The error bars of the Monte Carlo calculation are estimated at two units of the last digit in the data as shown in Ref. 5.

IV. D^0 AND D^- STATES IN A SQW

To verify the validity of the trial wave functions as well as the accuracy of the calculation we first compute the binding energies $E_B(D^0,0)$ and $E_B(D^-,0)$ for D^0 and D^- at the well center of GaAs/$Ga_{0.25}Al_{0.75}As$ structure with well widths 200 and 100 Å. The parameters we use are Ry*=5.8 meV, a^*=100 Å, and $\gamma=1$ corresponds to $B=6.75$ T. Our results are posted in Table I along with the diffusion quantum Monte Carlo results[4,5] for various magnetic fields. It is clear that the present work yields consistently smaller binding. However, the differences are comparable to the statistical fluctuations of the Monte Carlo calculation. Thus the trial

TABLE II. Comparison of $1s \rightarrow 2p^-$ transition energies in SQW's with experimental data. The unit for energy is cm^{-1}.

Transition energy	B (T)	Well/barrier widths L (Å)	Theory	Experiment[a]
$\Delta E(D^0)$		95	75.0	75
	10	144	65.6	66
		194	58.0	59
$\Delta E_b(D^0)$		95/190	9.5	10
	10	144/190	7.3	7
		194/190	6.2	6
$\Delta E(D^-)$		95	47.9	48
	10	144	43.4	44
		194	40.2	40
		95	37.8	38
	5	144	35.0	35
		194	32.1	33

[a]Data are taken from Ref. 16.

wave functions we have assumed are reasonable and the numerical work is sufficiently accurate.

D^0 and D^- cyclotron resonance energies have been measured in GaAs/$Ga_{1-x}Al_x$As SQW's of different widths. Experimental magneto-optical transition energy is found to increase with decreasing well width, in good agreement with the variational quantum Monte Carlo results.[16] We compare our results with those of Ref. 16 in Table II, in which $1s \rightarrow 2p^-$ transition energies $\Delta E(D^-)$ and $\Delta E(D^0)$ at the center of SQW's, and $\Delta E_b(D^0)$ at the barrier center[28] computed for various cases are listed along with available experimental data.[16] That very good agreement is obtained in all cases once more confirms the validity of the present treatment.

To further study the dependence of the D^- transition energy on the well width and applied magnetic fields, we compute the ratio $\eta = \Delta E(D^-)/E_B(D^-,0)$ along with $\Delta E(D^-)$ in SQW's of GaAs/$Ga_{0.25}Al_{0.75}$As systems for various well widths and magnetic fields. Table III lists $1s \rightarrow 2p^-$ transition energies calculated for D^- at the well center for $L=0$, 100, and 200 Å in fields $\gamma=0,1,3,5,10$. The fact that $\eta > 1.0$ for all cases implies that the p^-- (p^+-) like excited state lies above the Landau level $N=0$ ($N=1$) and hence is not bound. In general, one finds that the transition energy increases with the increasing field strength when the width is fixed, but decreases with the increasing well width for a given field. The ratio η decreases with the increasing L for a given field. On the other hand, the variation of η with the field depends strongly on the well width. It is monotonically increasing function of γ in the 2D case ($L=0$), but peaks at certain γ value depending on the well width. An interesting quantum shape effect may be noted from the data and is perhaps worth further investigation. As the confinement in the xy plane due to the magnetic field is of the order of the quantum-well confinement in z direction, we find that the ratio η is close to 1. Hence η may be regarded as a shape-dependent parameter characterizing the confinement. The higher symmetry the system has, the closer is its value to unity. It is expected that η is closest to 1 in a spherical dot.

V. D^0 AND D^- STATES IN A GQW

We now consider graded quantum wells of $Ga_{1-y}Al_yAs/Ga_{1-x}Al_xAs/Ga_{1-y}Al_yAs$ structures. To be more specific, we take $V_0=40$ Ry*, $L=2\alpha^*$, and $R=$Ry*/$a^*=0,5,10$. The aluminum concentration $y=30\%$ in the barrier, while x in the well changes linearly along the growth direction from 0 to 7.5% and from 0 to 15% for $R=5$ and 10, respectively.

In Fig. 1, we plot the binding energies $E_B(D^0,m)$ as a function of γ for $m=0$ and 1 in GQW's with $R=0,5,10$. It is observed that in general, the binding energies increase with the field but decrease with increasing R. It is also noted that the binding energy change is slower in the excited state ($m=1$) than in the ground state ($m=0$) when $\gamma > 1$. This is not difficult to understand, because the excited-state wave function is more extended than that of the ground state, resulting in a much stronger effect of R on the Coulomb energy in the ground state as we shall discuss later.

TABLE III. Variation of $\Delta E(D^-)$ and η in a SQW with the well width and external fields.

L (Å)	γ	$\Delta E(D^-)$ (Ry*)	η
0	0	0.454	1.00
	1	1.251	1.13
	3	2.196	1.25
	5	2.879	1.32
	10	4.030	1.38
100	0	0.252	1.00
	1	0.888	1.21
	3	1.369	1.27
	5	1.628	1.24
200	0	0.214	1.00
	1	0.735	1.15
	3	1.047	1.15
	5	1.220	1.11
	10	1.396	1.05

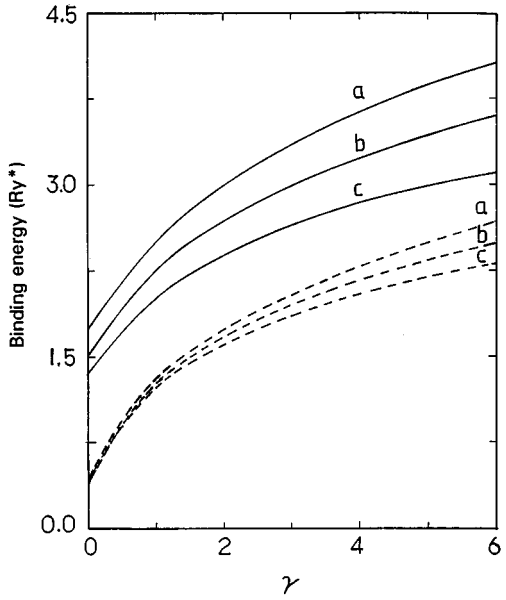

FIG. 1. Variation of the binding energy $E_B(D^0,m)$ for states $m=0$ (solid lines) and $m=1$ (dashed lines) with the magnetic field γ in GQW's of depth $V_0=40$ Ry*, width $L=2a^*$, and gradient (a) $R=0$, (b) $R=5$, and (c) $R=10$ Ry*/a^*.

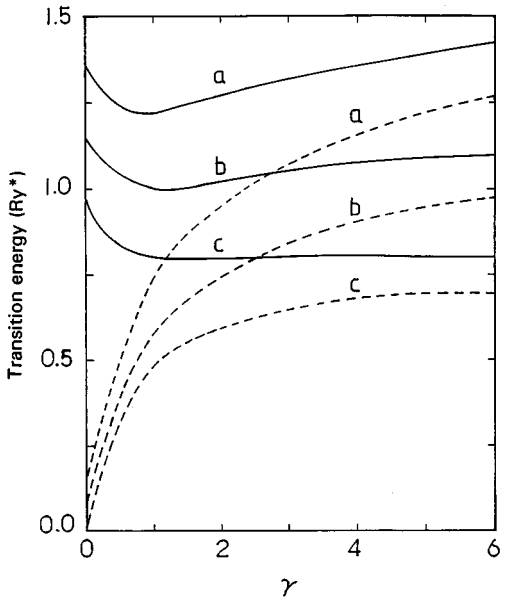

FIG. 3. Variation of the $1s\rightarrow 2p^-$ transition energy for D^0 (solid line) and D^- (dashed line) with the magnetic field γ in GQW's of depth $V_0=40$ Ry*, width $L=2a^*$, and gradient (a) $R=0$, (b) $R=5$, and (c) $R=10$ Ry*/a^*.

D^- states in the same GQW system are also calculated on the trial wave functions given by Eqs. (7). Figure 2 depicts the binding energies $E_B(D^-,M)$ as a function of γ for different gradients R. Here we find that the binding energy variation with the field for the singlet s-like ($M=0$) state is quite different from triplet p-like ($M=1$) states when R increases. Curves marked by a represent the case of zero gradient ($R=0$) and indicate that the binding energy increases monotonically with the magnetic field in SQW's. The situation changes for $R\neq 0$, as is shown by curves b and c for which the binding energies increase with the magnetic field to a peak and then decrease when γ increases further. The field strength that yields the largest binding is a decreasing function of R. The most interesting feature of this study is perhaps the level crossing phenomenon in GQW's. For $R=10$, it is clearly seen that the crossing occurs at $\gamma_c=1.65$. This means that the s-like state becomes less bound than the p-like states when the field is $\gamma_c>1.65$. The corresponding field for $R=5$ is $\gamma_c=7.5$. Furthermore, we find that all the D^- states in a GQW may become unbound when the magnetic field is sufficiently strong. In Fig. 2, this occurs for the s-like state at $\gamma=4.85$ for $R=10$. Thus a strong magnetic field can dissociate a D^- into an electron and a D^0 in GQW's.

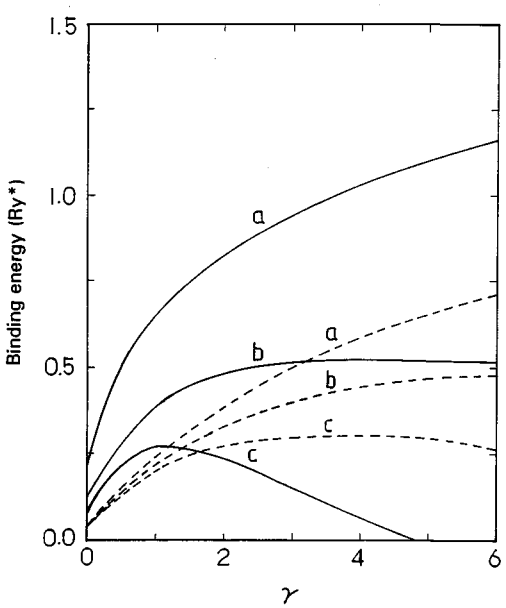

FIG. 2. Same as in Fig. 1 except for D^- singlet (solid line) and triplet (dashed line) states.

The phenomena observed in Fig. 2 may be understood qualitatively as follows. For a donor D^0 or D^- located at the well center, the reflection symmetry break due to a nonzero R shifts the wave function towards the deeper side of the well. Since the Coulomb and exchange integrals are determined by the mean value of $[\rho^2+z^2]^{-1/2}$, and since the s-like orbital is more localized than the p-like orbital, it is easy to understand that for a fixed γ the binding energy for the s orbital is more sensitive to R than that of the p orbital because the magnetic field reduces the mean size ρ and the gradient R changes the mean z value. Hence the D^0 binding for a given R always increases with increasing γ, but for a fixed γ decreases with increasing R. On the other hand, the mean distance between the two electrons in D^- decreases with increasing R, the repulsive energy therefore results in a decreased D^- binding and eventually leads to the dissociation. This effect is enhanced as the magnetic field increases.

The transition energies $\Delta E(D^0)$ and $\Delta E(D^-)$ are plotted in Fig. 3 as a function of γ again for $R=0,5,10$. The magnetic field dependence of the transition energy for D^0 and D^- in the low-field region are qualitatively different from one another. This is not surprising and can be seen from Figs. 1 and 2. The rate at which $E_B(D^0,1)$ increases with γ is much faster than $E_B(D^0,0)$ at the beginning until $\gamma\sim 1$, and

then the trend starts to reverse gradually. On the other hand, $E(D^-,0)$ increases much faster with γ at the beginning and starts tapering off after $\gamma \geq 1$. Moreover, it is also clearly seen from this figure that for a given R in sufficiently strong fields ($\gamma > 1$), $\Delta E(D^-)$ depends much more sensitively on γ than $\Delta E(D^0)$ and the two transition energies approach each other slowly as the field increases further. For a fixed γ, we find that the difference between the two transition energies decreases slowly with increasing R. This implies that the greater the gradient, the more difficult to distinguish the two transitions in experiments, but there is still a difference of about 0.15 Ry* for the worst case ($R=10$ Ry*/a*, $\gamma=6$) in the plot. It is most interesting to note from Fig. 2 that for $R \neq 0$, the singlet D^- binding energy decreases with increasing γ. This means that the D^- state energy increases with the magnetic field in GQW's, so that eventually it becomes unbound for a γ value depending on R. This peculiar feature is in sharp contrast to what can be found in the literature,[2–18] and provides us with an unambiguous way to identify the D^- transitions in GQW's. It is subjected to experimental verification in the future.

Finally, it should be interesting to point out that the $1s \rightarrow 2p^-$ transition energy $\Delta E_b(D^0)$ of a D^0 impurity situated in the barrier ($z_0 > L/2$) may not be easily distinguished from the corresponding D^- transition in the well. This situation may also exist even when $R \neq 0$. On the other hand, $\Delta E_b(D^0)$ is usually much smaller than the corresponding $\Delta E(D^0)$ in the well in weak fields. Some particular cases are given in Table II. This is easily understood because the electron in the well is on the average far from its parent donor in the barrier. In practice, the transitions $\Delta E(D^-)$ and $\Delta E_b(D^0)$ are often discriminated by doping in the barrier farther away from the interface. When the field increases, however, $\Delta E(D^-)$ and $\Delta E(D^0)$ gradually become comparable. Therefore D^0 and D^- transition lines in the well can easily be distinguished from the transition line of D^0 in the barrier by observing the field dependence of the transition energy.[29]

In conclusion, we have found from our study of D^0 and D^- states in GQW's that the reflection symmetry break has profound effects on the electronic structures and optical properties. The most remarkable change is the occurrence of the level crossing phenomenon among D^- states. While the magnetic field raises impurity binding energies monotonically in a square well, this is not always the case in GQW's. As we have seen in Fig. 2, the binding energy of D^- states is raised only to a peak by the magnetic field and then decreases when the field keeps increasing. That the s-like level reaches its peak at much lower field than the p-like level results in the level crossing which never occurs in SQW's. This field dependence of the binding energy also implies that all D^- states in GQW's eventually become unbound for sufficiently strong fields. Furthermore, we note that the concept of the freezing effect of σ is no longer valid in GQW's because the D^- binding energy may decrease as a consequence of the symmetry break.

*Permanent address.

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