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The bound states of D^- centres in a quantum well in the presence of an applied high magnetic field

Hong-ye Chen[1], **Xiao-jun Kong**[2,3], **Dai-zhao Han**[1] **and Man Shen**[2]

[1] Mechanical Engineering College, Shijiazhuang, Hebei Province (050003), People's Republic of China
[2] College of Physics, Hebei Normal University, Shijiazhuang, Hebei Province (050016), People's Republic of China

E-mail: kongxj@mailhebtu.edu.cn

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Abstract
The binding energies of the ground and some low-lying excited states of a D^- centre in a GaAs/GaAlAs quantum well have been calculated as a function of the presence of an applied magnetic field and well width respectively. In comparison with exact two-dimensional results, which show only four bound states, a larger number of D^- bound states appear in a quantum well. Moreover, the critical magnetic field values at which the excited states change from unbound to bound are obtained, and the reasons of the binding energy as function of magnetic field and well width are discussed. Our results are in good agreement with those in the literature.

1. Introduction

There has been an increasing interest in the investigation of two-dimensional and quasi-two-dimensional systems such as quantum wells and superlattices since three-dimensional examples of the D^- centre were first discovered in material semiconductors [1–3]. The D^- centre was found in multi-layer quantum wells by Huant *et al* [4], and identified by Muller *et al* [5], Subsequently, the ground state energies of the 2D D^- centre were calculated by Phelps and Bajaj *et al* [6]. From this point on, the study of D^- centres, both experimental and theoretical, expanded extensively.

A negative-donor centre (D^-) in a semiconductor is formed by a neutral centre (D^0) trapping an extra electron. Their properties depend delicately on a balance between the electron–electron interaction and the interaction of the two electrons with the charge to which they are bound. So there are some new phenomena in the D^- state compared with the D^0 centre. With an applied magnetic field, the D^- centre has strong effects on the optical and transition properties of semiconductor devices. Many novel effects, such as the quantum Hall effect in

[3] Author to whom any correspondence should be addressed.

quantum wells, Mott phase transitions [7, 8] and electron localizations, are intimately related to the D^0 centre and the D^- centre. In addition, a D^- centre is the simplest three-body system, thus the exact solution of the D^- centre problem would help us understand the e–e correlation effects in low-dimensional systems.

D^- centres in 2D and 3D have already been studied [1–4, 9–14, 24] in an applied magnetic field. Experimentally, cyclotron resonance and magneto-optical conduction etc [15, 16] have been used to measure the D^- centre energy levels in GaAs quantum wells. We think the bound state number of the D^- centre should be a function of the thickness of the well, for the following reasons: there are only four bound states existing in a 2D system no matter how strong the magnetic field is, but infinitely many bound states in 3D materials. The QW is a structure situated between two and three dimensions. On the other hand, both theory and experiment have also indicated that the ground and excited state energies are strongly affected by the magnetic fields, so in the presence of an external magnetic field the number of the D^- centre's bound states is determined by both the spatial dimension and the intensity of the magnetic field.

The variational approach [14, 17, 18] is usually used for calculating D^- centre properties in quantum wells, but the results depend closely on the trial wavefunction. In this paper, we obtained the results by numerically calculating the secular equation. The basic function we have used is the product of the Landau level wavefunction and the free electron wavefunction in the well. Using this wavefunction, we have calculated the binding energies of the ground and several low-lying excited states of a D^- centre in a quantum well. We have performed calculations of the critical magnetic field values at which the D^- states converted from unbound to bound in wells of various thickness size, and the distribution of the D^- states as a function of the well width and the critical magnetic field has also been obtained.

2. Theoretical framework

The Hamiltonian of D^- centres in a QW and magnetic field, $\vec{B} = \nabla \times \vec{A}$, perpendicular to the well structures is

$$H = H_{\mathrm{e}1} + H_{\mathrm{e}2} - v(\vec{r}) + v_{\mathrm{w}}, \tag{1}$$

where $v(\vec{r}) = v_1 + v_2 - v_{12}$ is the Coulomb potential of the two electrons, and v_{w} is the barrier of the quantum well. Using atomic units (energies in units of $R_y = \frac{e^2}{2\varepsilon a_{\mathrm{B}}^*}$, lengths in unit of $a_{\mathrm{B}}^* = \frac{\varepsilon\hbar^2}{m_{\mathrm{e}}^* e^2}$) the Hamiltonian of the single electron is

$$H_{\mathrm{e}} = -\nabla^2 + \tfrac{1}{4}\gamma^2\rho^2 + \gamma L_z, \tag{2}$$

$\gamma = \frac{\hbar\omega_{\mathrm{c}}}{2R_y}$ is the dimensionless magnetic-field intensity.

The wavefunction of the D^- centre is expressed as

$$\psi^{\pm} = \sum_{\{lnm\}} \frac{1}{\sqrt{2}} \alpha_{\{lnm\}} \{|l_1 n_1 m_1\rangle_1 |l_2 n_2 m_2\rangle_2 \pm |l_2 n_2 m_2\rangle_1 |l_1 n_1 m_1\rangle_2\} \tag{3}$$

and we use the following basic function, in which the Coulomb potential could be diagonalized:

$$|lnm\rangle = \chi_l(z)\phi_{nm}(\rho)\mathrm{e}^{\mathrm{i}(n-m)\varphi}, \qquad l = 1, 2, 3, \ldots, \quad m = 0, 1, 2, \ldots, \quad n = 0, 1, 2, \ldots. \tag{4}$$

In equation (3), '±' represents symmetric and antisymmetric states respectively; the symbol $\{lnm\}$ represents all possible sets of the quantum numbers $\{l_1 n_1 m_1\}$ and $\{l_2 n_2 m_2\}$, and $|l_1 n_1 m_1\rangle_1 |l_2 n_2 m_2\rangle_2$ is the product of the wavefunctions of electron one and electron two.

The total angular momentum $M = (n_1 - m_1) + (n_2 - m_2)$ is conserved. In equation (4), $\chi_l(z)$ is the wavefunction of a free electron in the well,

$$\chi_l(z) = \begin{cases} A\cos(-kd/2)\mathrm{e}^{\alpha d/2}\mathrm{e}^{\alpha z} & (-\infty, -d/2) \\ A\cos(kz) & (-d/2, d/2) \\ A\cos(kd/2)\mathrm{e}^{\alpha d/2}\mathrm{e}^{-\alpha z} & (d/2, +\infty) \end{cases} \tag{5}$$

$\chi_l(z)$ can also be odd parity when l is a even number. The constants k and α are the wavevector in the well and the decay factor in the barrier respectively, and depend on the well width d and quantum number l. They are determined by solving the Schrödinger equation numerically. A is the normalization constant, and is given by

$$A = \left\{\frac{d}{2} + \frac{1}{2k}\sin(kd) + \frac{1}{\alpha}\cos^2(kd/2)\right\}^{-1/2}.$$

In equation (4), $\phi_{nm}(\rho)\mathrm{e}^{\mathrm{i}(n-m)\varphi}$ is an in-plane Landau level wavefunction. Its radial part

$$\phi_{nm}(\rho) = (-1)^{i_<}\frac{\mathrm{e}^{-\rho^2/4l_c^2}}{\sqrt{2\pi l_c^2}}\sqrt{\frac{i_<!}{i_>!}}\left(\frac{\rho}{\sqrt{2l_c^2}}\right)^{i_>-i_<} L_{i_<}^{i_>-i_<}\left(\frac{\rho^2}{2l_c^2}\right). \tag{6}$$

Here the electron total angular momentum $M = n - m = 0, \pm 1, \pm 2\ldots$, and $l_c = \left(\frac{\hbar c}{eB}\right)^{1/2}$. The function L is a Laguerre polynomial, and the notation $i_>$ and $i_<$ represents the greater or lesser of n and m respectively. It can be shown that with this definition $\phi_{nm}(\rho)\mathrm{e}^{\mathrm{i}(n-m)\varphi}$ is normalized.

The energy of the electron can be written as $E_{nl} = (n + \frac{1}{2})\hbar\omega_c + E_l$ with quantum numbers l, n and m, where E_l is the energy of the electron when it occupies the lth level. The Coulomb potential is diagonal with this set of states.

Only when the system energy is less than the ground energy of D^0 centre plus the lowest energy of a free electron, i.e. the D$^-$ centre cannot be decomposed into a D^0 centre and a free electron, can a bound D$^-$ centre exist.

The binding energy of the D$^-$ centre is defined as

$$E_B = E_{D^0} + E_e - E_{D^-} \tag{7}$$

in which E_{D^0} is the ground state energy of the D^0 centre in the quantum well with an applied magnetic field; E_e is the ground state energy of the electron with the same magnetic field and E_{D^-} is the system energy of the D$^-$ centre.

The Coulomb potential between two electrons is

$$v_{12}(r) = \frac{2}{\sqrt{(\vec{\rho}_1 - \vec{\rho}_2)^2 + (z_1 - z_2)^2}}.$$

For matrix elements of the Coulomb potential

$$_2\langle l_2 n_2 m_2|_1\langle l_1 n_1 m_1|v_{12}(\vec{\rho}, z)|l_1 n_1 m_1\rangle_1|l_2 n_2 m_2\rangle_2, \tag{8}$$

the integral along the Z axis can be calculated. We define

$$\begin{aligned} v_{l_1 l_2 l_1' l_2'}(\vec{\rho}_1 - \vec{\rho}_2) &\equiv \frac{2}{(2\pi)^2}\int\int q\,\mathrm{d}q\,\mathrm{d}\varphi\,\tilde{v}_{l_1 l_2 l_1' l_2'}(q)\mathrm{e}^{-\mathrm{i}\vec{q}\cdot(\vec{\rho}_1 - \vec{\rho}_2)} \\ &= \langle l_2|\langle l_1|v(\vec{\rho}_1 - \vec{\rho}_2, z_1 - z_2)|l_1'\rangle|l_2'\rangle. \end{aligned} \tag{9}$$

Then expression (8) can be written as

$$\frac{2}{(2\pi)^2}\int\int q\,\mathrm{d}q\,\mathrm{d}\varphi\,\tilde{v}_{l_1 l_2 l_1' l_2'}(q)\cdot {}_2\langle n_2 m_2|\mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{\rho}_2}|n_2' m_2'\rangle_2\,{}_1\langle n_1 m_1|\mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{\rho}_1}|n_1' m_1'\rangle_1. \tag{10}$$

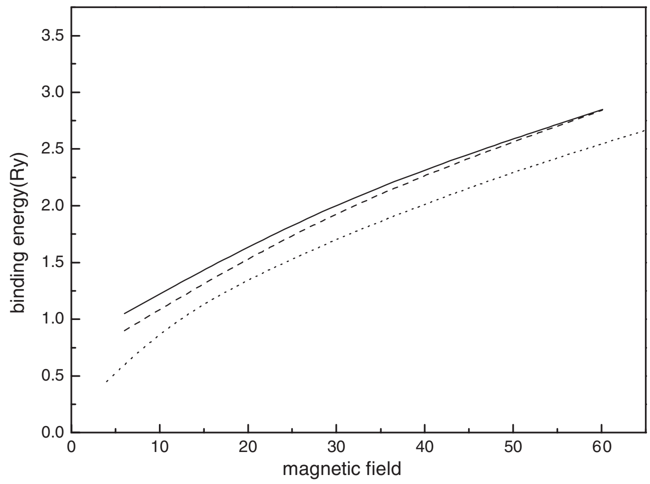

Figure 1. Binding energy of the $M = -1$ state of D^- in the 2D case; the solid line is our results; the dashed line is the results of [9] and the dotted line is [24].

From references [20, 21], we have

$$\langle nm|e^{-i\vec{q}\cdot\vec{\rho}}|n'm'\rangle = e^{-q^2l_c^2/2}G_{n'n}(ql_c)G_{m'm}(ql_c)e^{i(n'-n+m-m')\varphi}, \tag{11}$$

where

$$G_{s's}(ql_c) = \sqrt{\frac{s_<!}{s_>!}}\left(-\frac{iql_c}{\sqrt{2}}\right)^{s_>-s_<} L_{s_<}^{s_>-s_<}(q^2l_c^2/2). \tag{12}$$

The definition of the notations $s_>$ and $s_<$ is consistent with the notations $i_>$ and $i_<$ given above. The integral of φ can be calculated because the total angular momentum is conserved. We obtain

$$\langle v_{12}\rangle = \frac{2}{2\pi}\int q\,dq\,\tilde{v}_{l_1l_2l_1'l_2'}(q)e^{-q^2l_c^2}G_{n_1'n_1}(ql_c)G_{m_1'm_1}(ql_c)G_{n_2'n_2}(-ql_c) \\ \times G_{m_2'm_2}(-ql_c)\cdot\delta_{n_1-m_1+n_2-m_2,n_1'-m_1'+n_2'-m_2'}. \tag{13}$$

In an exactly two-dimensional system, $\tilde{v}_{l_1l_2l_1'l_2'}(q) = \frac{2\pi}{q}$; and in a quantum well $\tilde{v}_{l_1l_2l_1'l_2'}(q) = \frac{2\pi}{q}\cdot F_{l_1l_2l_1'l_2'}(q)$, in which $F_{l_1l_2l_1'l_2'}(q)$ [19] is the form factor, defined as

$$F_{l_1l_2l_1'l_2'}(q) = \int\int dz_1\,dz_2\,\chi_{l_1}(z_1)\chi^*_{l_1'}(z_1)\chi_{l_2}(z_2)\chi^*_{l_2'}(z_2)e^{-q|z_1-z_2|}. \tag{14}$$

An explicit form for $F_{l_1l_2l_1'l_2'}(q)$ can be obtained in a quantum well. For an infinitely deep well, making the lowest subband approximation, the form factor is [22]

$$F_{1111}(q) = \frac{2}{qd} + \frac{qd}{q^2d^2+4\pi^2} - 2(1-e^{-qd})\left(\frac{1}{qd} - \frac{qd}{q^2d^2+4\pi^2}\right)^2. \tag{15}$$

Thus, the matrix element of the Coulomb potential of electron interactions can be obtained. The calculation of the matrix element of the Coulomb potential between electron and donor centre is simpler, and can be obtained analogously.

The system energies of the ground and the excited states of a two-dimensional D^- centre in an intense magnetic field were calculated, and the energies of the $M = -1$ state were compared with the results of [9] and [24] (figure 1). We found our results agree well with [9] in high magnetic field limit, and have the same trend compared with [24]. So, it can be proved that the method we used is a suitable one, especially in the high field limit.

In calculating, only the first sublevel is considered. In fact, the second and higher sublevels in the well may affect the binding properties of D$^-$ centre's states in a thick enough well. We regret that we did not account for their effect. The reason that this shortcoming exists may be that our first calculation is for the narrowest well, e.g. 5, 10 and 20 Å etc. We hope someone, including ourselves, could consider this problem.

3. Results and discussion

In the case of GaAs–Ga$_{1-x}$AsAl$_x$, we use the following material data: the doped density of Al is $x = 0.33$; the conduction bound offset is 224 meV, and the dielectric constant ε is 12.5. In addition, the electron effective mass is 0.0665 m_0 in the well and $(0.0665 + 0.083x)\, m_0$ [23] in the barrier, in which m_0 is the mass of the free electron, and the strength of the magnetic field can be denoted by the dimensionless quantity γ. Throughout the calculations, the difference of the electron effective mass in the well and in the barriers is taken into account, while the mismatch of the dielectric constant is ignored.

We have calculated the properties of the D$^-$ centres in different width wells and placed into high magnetic field. We can conclude that there exist more bound states of the D$^-$ centre. This situation is not different from the 2D case, in which only four bound states appear with a high magnetic field limit.

3.1. Infinitely deep quantum well

There appear five bound states when the width of the QW is 10 Å. When the fifth state appears, the value of the critical magnetic field γ_c in which the D$^-$ centre states would convert from unbound to bound is 185.4. For the $M = -3$ state γ_c is 36.4, which is obviously lower than that of $10^{5.8}$ in [11] in 2D. When the width of the QW increases to 20 Å, seven bound states have appeared and the values of their critical field are not larger than 90.2. In the same QW, for the $M = -3$ state γ_c is 17.3, and for the $M = -5$ state 89. When the width of the well is further increased, to 70 Å, there appear a total of eight bound states when $\gamma < 15$, and for a well size of 100 Åthere are seven excited states when $\gamma < 7.5$. The values of γ_c for the excited states are obviously lower than that in the 70 Å well.

The $M = 0$ state is always bound in an infinitely deep well.

As the size of the well increases, the binding energy of the $M = 0$ state decreases. This is because the shape of the $M = 0$ state's wavefunction is uniformly and symmetrically distributed in spherical form and is constrained to lie within the barriers of the QW; the narrower the quantum well width is, the more obviously is the wavefunction squeezed by the barrier, so the larger is the binding energy of the system. On the other hand, the binding energy increases as the magnetic field increases because the wavefunction of the electron changes from the free distribution with no magnetic field to a Landau level distribution which is limited by the magnetic field in the QW plane.

As we can see from figures 2 and 3, as the width of the QW increases, the binding energies of the $M = -1, -2, -3, \ldots$ states increase, while the critical magnetic fields of these states decrease with increasing well width in figure 4. This is because the wavefunction of these states is not spherically symmetric as in 3D but, instead, is oblate, for the reason that the constraints due to the QW destroy the symmetry along the magnetic field direction. As the width of the QW increases, the wavefunction's distribution becomes more localized in the QW plane. As a result, the system energy decreases, while the binding energy increases, and the γ_c gets smaller.

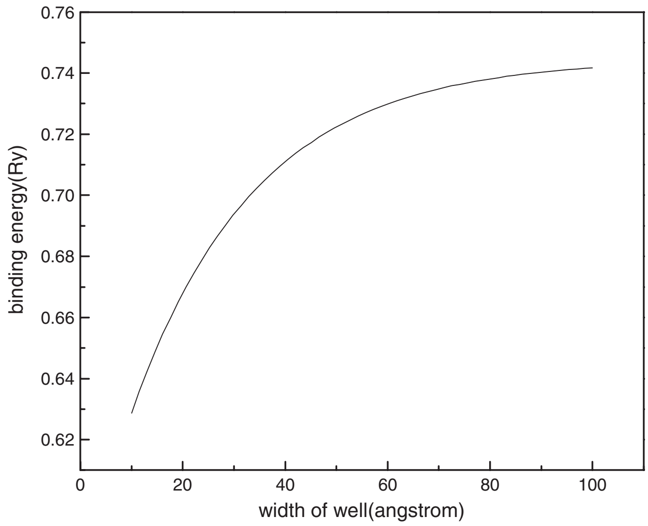

Figure 2. Binding energy of $M = -1$ state of D^- in an infinitely deep well with $\gamma = 6$ shown as a function of width of well.

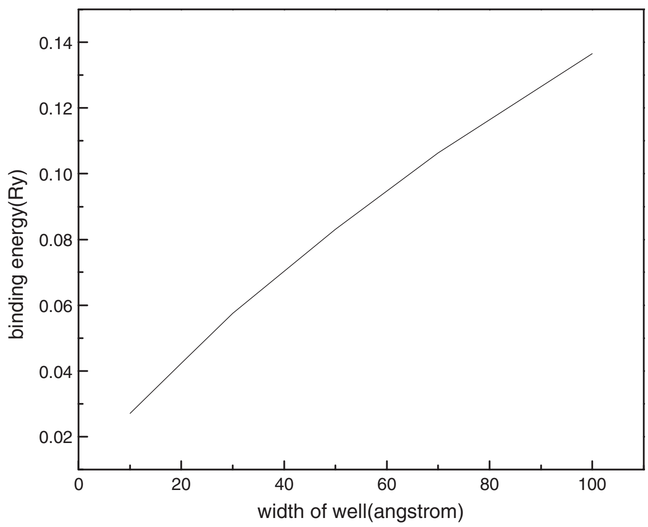

Figure 3. Binding energy of $M = -2$ state of D^- in an infinitely deep well with $\gamma = 6$ shown as a function of width of well.

In our results, the γ_c of some states is very intense, especially for some states which are situated at wider wells. For example, γ_c is 70.9 and 10.6 respectively for the $M = -7$ and -3 states in the 30 Å well. The critical magnetic field drawn from our calculation is so high that it is usually impossible to realize in experiment, but it can be predicated that as the width of the QW increases, the critical magnetic field will decrease, then the existence of the bound states can be observed.

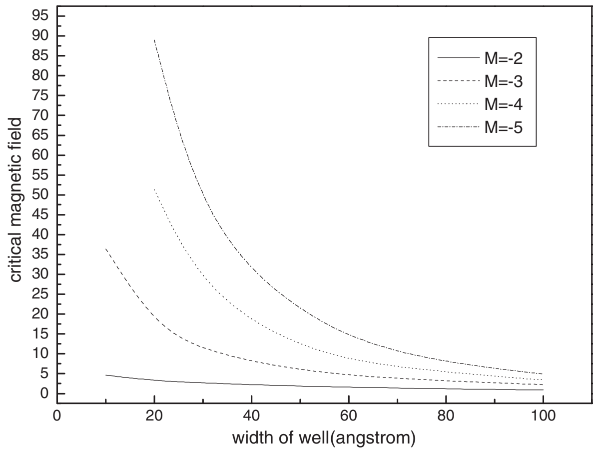

Figure 4. The critical magnets of $M = -2, -3, -4, -5$ states of D$^-$ in an infinitely deep well are shown as a function of the width of the well.

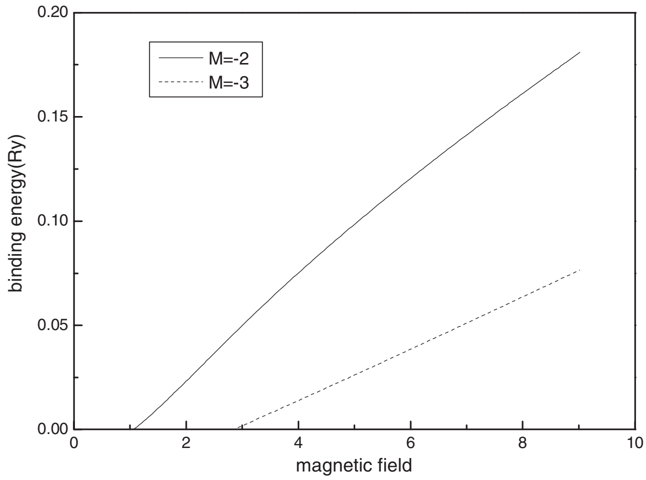

Figure 5. Binding energies of $M = -2, -3$ states of D$^-$ in a finitely deep well $d = 50$ Å as a function of magnetic field.

3.2. Finitely deep quantum well

The binding energies of all D$^-$ excited states are larger than those in the infinitely deep well. For example, when the width of the QW is 10 Å, γ_c for the fifth bound state is less than 30 (cf 184.9 in an infinitely deep well). For thin wells of 20 and 30 Å, there appear four bound states when γ is less than 7.5. Six bound states would appear when the width of the well increases to 50 Å. In a cell of width 70 Å, the eighth bound state appearing at γ_c is about 6.13, while in a cell of width 100 Å the critical field γ_c is 4.12 when the eighth bound state appears.

Again, the state with $M = 0$ is always bound in a finitely deep well, which is the same as the situation in an infinitely deep well. Besides, the binding energy of $M = 0$ state in a finitely deep well is lower than that in an infinitely deep well.

We can see from figure 5 that as the magnetic field increases the binding energies of each state also increase. The binding energies of the $M = -1, -2, -3, \ldots$ states are

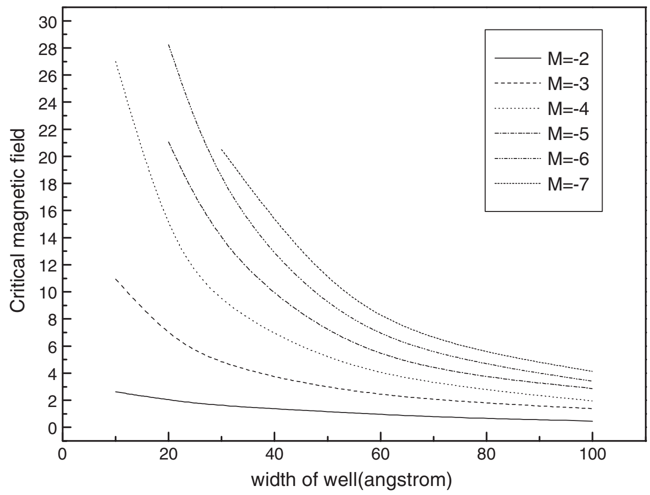

Figure 6. The critical magnetic fields of $M = -2, -3, -4, -5, -6, -7$ states of D^- in a finitely deep well are shown as a function of the width of the well.

correspondingly higher than in the infinitely deep well, which is different from the $M = 0$ state case. The conclusion that the values of these states' critical magnetic fields are comparatively low compared with the case in an infinitely deep well can be drawn from figure 6. All of these results are owing to the reason that the wavefunctions of the D^- centre in a finitely deep well could penetrate into the barriers and the limitation to the wavefunctions in a finitely deep well is not so strong as that in a infinitely deep well.

The binding energies of some states, e.g. $M = -2$ in a 50 Å finitely deep well, can be seen from figure 5 to increase linearly with the increasing magnetic field. We comment for this case that the magnetic field has become so intense that the electron–electron and electron–donor Coulomb interactions can be ignored because of their small size compared with the magnetic energy.

Although the γ_c of some excited states is very intense and its binding energy is comparatively smaller (e.g. $E_b = 0.195$ meV at $M = -4$, $d = 100$ Å, $\gamma = 7.52$), γ_c is expected to decrease as the well width increases, and this would suggest that the D^- centre can be more easily observed in wider wells when the thickness is large. From the above point on, we concluded that from 2D to 3D it is impossible to have a certain width QW in which there appear the wholly infinite bound states of a D^- centre. This means that the number of bound states is determined by both the intensity of the magnetic field and the width of the well together.

Because our aim is to find out the criterion under which the bound state appears, we have not taken into account the high magnetic field value obtained from theory.

All the excited states discussed above are spatially antisymmetric states, and only the $M = -1$ symmetric state is calculated. There does not exist a bound state when γ is 90.2 in the infinitely deep well, nor in the finitely deep well with $\gamma = 75.18$. For practicality, no further calculations were carried out for these states.

4. Conclusion

The appearance of a bound state is determined by both the well width and the intensity of the magnetic field. If the intensity of the magnetic field is constant, the number of bound states will become greater and greater as the width of the well increases gradually. There are more bound states for the D^- centre in a QW than the number that appeared in the exactly two-dimensional case [9, 10], which is not more than four. As the well width increases, the binding energy of the $M = 0$ state decreases while those of the others increase, and the $M = 0$ state is always bound.

In a finitely deep well, the binding energy of each excited state is larger and the critical magnetic field is lower than those in an infinitely deep well. Although some low-excited states ($M = -1, -2, \ldots - 7$) all appeared in an infinitely deep well, the magnetic field expected to be applied is too intense, and the binding energy is rather small. So, we suppose the method to get the bound states observed is to increase the width of the well or apply a more intense magnetic field or turn to both of them.

Our results indicate that the barriers have a squeezing effect on the wavefunctions of the D^- centre, and that the narrower the well is the more obvious the squeezing effect is. Hence, the binding energy of the state will change with the well width. The squeezing degree of the barriers on the wavefunction in a finitely deep well is lighter than that in an infinitely deep well. The wavefunction in a finitely deep well can penetrate into the barriers, which leads to the different binding properties of the D^- centre between an infinitely deep well and a finitely deep well.

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