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# Barrier $D^-$ quantum dots in magnetic fields

Wenfang Xie

Department of Physics, Guangzhou Normal University, Guangzhou 510405, People's Republic of China

E-mail: gzxiewf@public1.guangzhou.gd.cn

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**Abstract.** Using the method of few-body physics, the states of the barrier $D^-$ centre, which consists of a positive ion located on the $z$-axis at a distance from the two-dimensional quantum dot plane and two electrons in the dot plane bound by the ion, are investigated in a arbitrary strength of magnetic field. This configuration was called a barrier $D^-$ centre. Discontinuous ground-state transitions induced by an external magnetic field have been obtained. The dependence of the binding energy of the ground state of the barrier $D^-$ centre on the dot radius for a few values of the magnetic field strength is obtained.

## 1. Introduction

Recently, advances in nanofabrication technology have made it possible to manufacture quantum dots (QD's) containing one, two and more electrons, and these have been intensively investigated experimentally and theoretically. A QD is semiconductor nanostructure with a three-dimensional confinement of electrons [1]. They have been fabricated in different shapes; for example, a disk-like (cylindrical) shape [2] and a spherical shape [2, 3]. From a theoretical point of view, these few-body systems represent a challenging problem. The standard tools of the condensed-matter physicist, such as the many-body techniques relying on Hartree or Hartree–Fock approximations are often not sufficient, since the exchange and correlation energies can be far from negligible [4]. A fully quantum mechanical treatment is needed. An example is the problem of a strictly two-dimensional $D^-$ centre QD in the presence of a perpendicular magnetic field. This centre consists of a single positive ion and two electrons which are bound to the positive ion. It is analogous to a negative hydrogen ion $H^-$ [5]. $D^-$ centres are one of the simplest 'many-body' electronic systems, which cannot be solved exactly. They can be used as a test for the theoretical description of electron–electron interaction [6].

Since the existence of a $D^-$ in centre-doped $GaAs/Al_xGa_{1-x}As$ multiple quantum wells was first reported by Huant *et al* [7], many experimental [8–10] and theoretical [11–17] investigations for negative donors in quantum wells, quantum dots with and without magnetic fields, have been carried out.

A system in which two electrons confined to a parabolic QD are bound by a positive ion located on the $z$-axis at a distance $d$ from the dot plane is called a barrier $D^-$ centre QD. There has been interest in the subject lately. Rich electronic structures and optical properties, and a variety of structural phase transitions are predicted in such systems. Recently some authors

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[18] have studied the states of a strictly two-dimensional barrier $D^-$ centre at high magnetic fields.

In this paper, we will propose a procedure to diagonalize the Hamiltonian of the barrier $D^-$ centre in QD's with a parabolic lateral confining potential in an arbitrary strength of magnetic field by using the method of few-body physics. The low lying energy levels as well as the ground state electronic structure are calculated systematically as a function of magnetic fields of arbitrary strength. As a consequence of our calculations, it is found that the ground state transitions of the barrier $D^-$ centre occur as the magnetic fields increase. The dependence of the binding energy of the ground state of the $D^-$ centre on the dot radius for a few values of the magnetic field strength is obtained. We find that there exists a critical radius $R^c$, such that if the dot radius $R < R^c$ ($R > R^c$) the $D^-$ configuration is stable (unstable).

## 2. Theory

The Hamiltonian for the barrier $D^-$ centre QD in the effective-mass approximation when the magnetic field is applied perpendicular to the $x$–$y$ plane is given by

$$H = \sum_{i=1,2}\left[\frac{1}{2m_e^*}\left(\vec{p}_i + \frac{e}{c}\vec{A}_i\right)^2 + \frac{1}{2}m_e^*\omega_0^2 r_i^2\right] + V_1 + V_2 - g^*\mu_B B S_z \tag{1}$$

$$V_1 = -\frac{e^2}{\epsilon}\sum_{i=1,2}\frac{1}{\sqrt{r_i^2 + d^2}} \tag{2}$$

$$V_2 = \frac{e^2}{\epsilon r_{12}} \tag{3}$$

where $\vec{r}_i$ ($\vec{p}_i$) is the position vector (the momentum vector) of the $i$th electron originating from the centre of the dot, $m_e^*$ is the effective mass of an electron, $r_{12} = |\vec{r}_1 - \vec{r}_2|$ is the electron–electron separation, $\omega_0$ is the strength of the confinement, $g^*$ is the effective Lande factor, $\mu_B$ is the Bohr magneton, $S_z$ is the $z$-component of the total spin and $d$ is the distance between the fixed positive ion on the $z$-axis and the dot plane. In this work we have used the natural units of the material: the effective Bohr radius $a_B^* = \hbar^2\epsilon/m_e^*e^2$ as the length unit and the effective Rydberg $Ry^* = m_e^*e^4/\hbar^2\epsilon^2$ as the energy unit. With the symmetric gauge for magnetic field $\vec{A} = (B/2)(-y, x, 0)$, the Hamiltonian then reads

$$H = \sum_{i=1,2}\left(\frac{p_i^2}{2m_e^*} + \frac{1}{2}m_e^*\omega^2 r_i^2\right) + V_1 + V_2 + \frac{1}{2}\omega_c L - g^*\mu_B B S_z \tag{4}$$

where $\omega = \sqrt{\omega_0^2 + \omega_c^2/4}$, $\omega_c = eB/(m_e^*c)$ is the cyclotron frequency and $L$ is the total orbital angular momentum along in the $z$-direction.

Introducing the coordinates

$$\vec{r} = \vec{r}_{12} = \vec{r}_1 - \vec{r}_2 \qquad \vec{R} = (\vec{r}_1 + \vec{r}_2)/2 \tag{5}$$

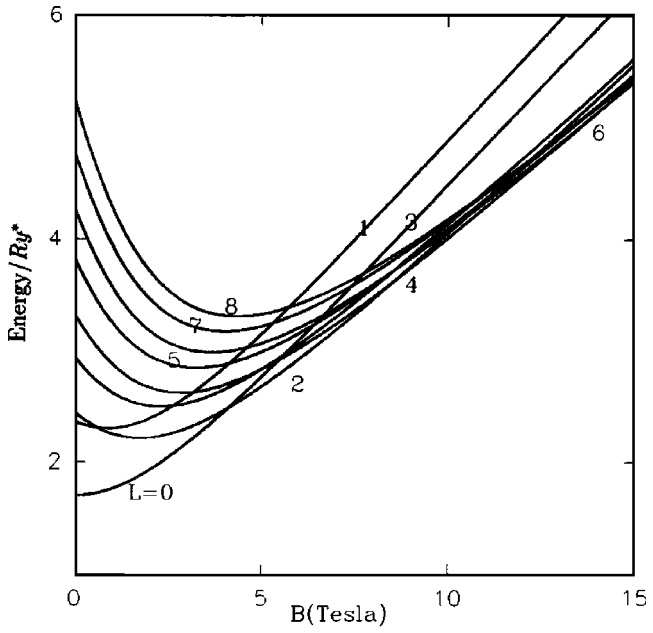
then equation (1) can be rewritten as

$$H = H_0 + V_1 + V_2 \tag{6}$$

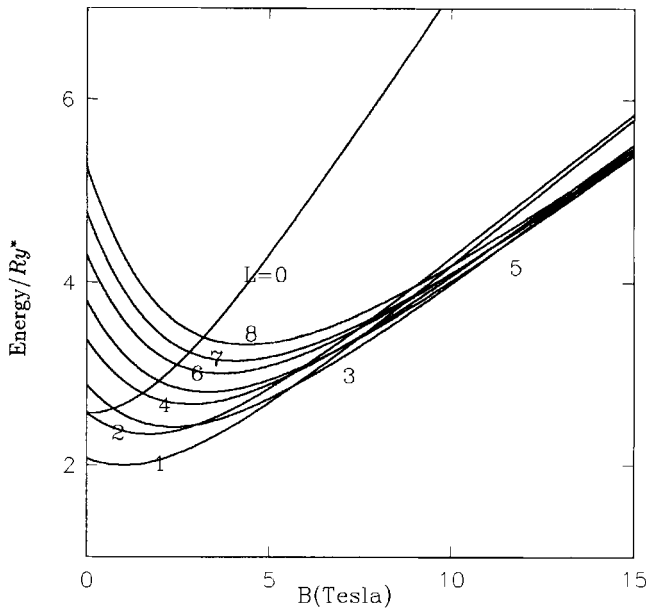
with

$$H_0 = \frac{P^2}{2M} + \frac{1}{2}M\omega^2 R^2 + \frac{p^2}{2\mu} + \frac{1}{2}\mu\omega^2 r^2 + \frac{1}{2}\omega_c L - g^*\mu_B B S_z \tag{7}$$

where $M = 2m_e^*$; and $\mu = m_e^*/2$.



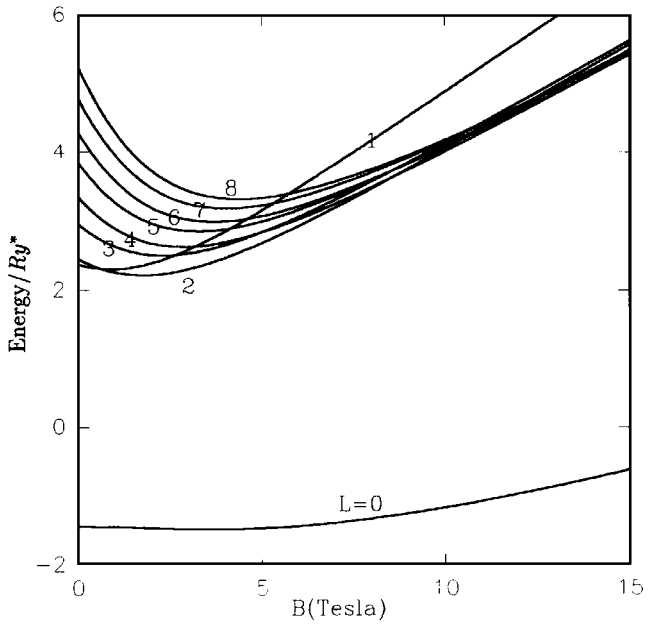

(a)



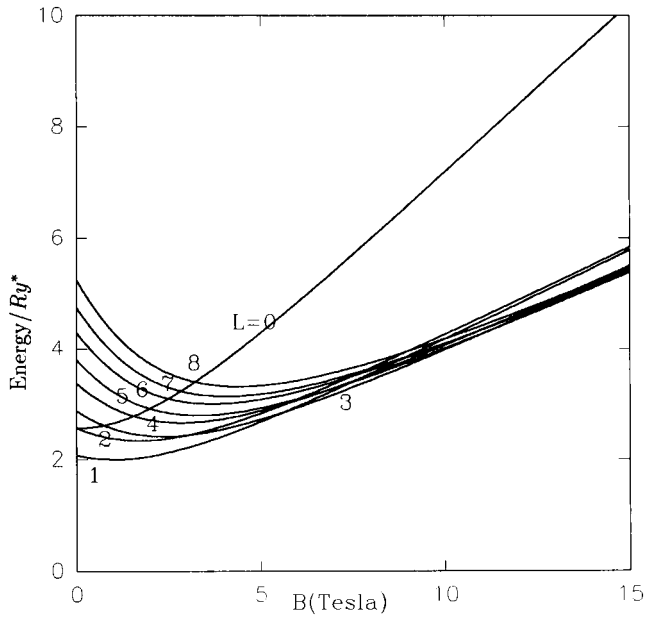

(b)

**Figure 1.** Variations of the energy levels (in units of $Ry^*$) of $L$ as a function of the magnetic field: (a) $S = 0$; (b) $S = 1$. The numbers in the figures label the angular momentum of the state. Parameters are taken appropriate for GaAs, $\hbar\omega_0 = 0.5Ry^*$, $d = 10$ nm.

The eigenstates of the barrier $D^-$ centre QD can be classified according to the total orbital angular momentum of the electrons along the $z$-direction and the permutation symmetry of the spatial wave functions upon interchange of electron coordinates (single and triplet,




(a)




(b)

**Figure 2.** The same as figures 1 except for $d = 0$.

corresponding to symmetric and antisymmetric space wave functions, respectively). To obtain the eigen-function and eigen-energies, we diagonalized $H$ in a model space spanned by the translationally invariant harmonic product bases

$$\Phi_{[K]} = \tilde{A}\{[\phi_{n_1\ell_1}(\vec{R})\phi_{n_2\ell_2}(\vec{r})]_L \chi_S\} \tag{8}$$

where $\chi_S = [\xi(1)\xi(2)]_S$, $\xi(i)$ is the spin state of the $i$th electron and the spins of two electrons are coupled to $S$, $\phi_{n\ell}(\vec{r})$ is a two-dimensional harmonic oscillator state with frequencies $\omega$ and an energy $(2n + |\ell| + 1)\hbar\omega$, and $\tilde{A}$ is the antisymmetrizer. $[K]$ denotes the whole set of quantum numbers $(n_1, \ell_1, n_2, \ell_2)$ in brevity, $\ell_1 + \ell_2 = L$ is the total orbital angular momentum. The angular momentum $L$ = odd if the spin $S = 1$, and $L$ = even if $S = 0$ such that the wave function is antisymmetried. The matrix elements of $H$ are then given by the following expressions:

$$\langle \Phi_{[K]}|H_0|\Phi_{[K']}\rangle = [2(n_1 + n_2) + |\ell_1| + |\ell_2| + 2 + \tfrac{1}{2}\omega_c L - g^*\mu_B B S_z]\hbar\omega\delta_{[K][K']} \tag{9}$$

$$\langle \Phi_{[K]}|V_1|\Phi_{[K']}\rangle = -2 \sum_{[K''],[K''']} B_{[K][K'']}B_{[K'][K''']}U^I_{n''_2 n'''_2}\delta_{n''_1 n'''_1}\delta_{\ell''_1 \ell'''_1}\delta_{\ell''_2 \ell'''_2} \tag{10}$$

$$\langle \Phi_{[K]}|V_2|\Phi_{[K']}\rangle = U^{II}_{n_2 n'_2}\delta_{n_1 n'_1}\delta_{\ell_1 \ell'_1}\delta_{\ell_2 \ell'_2} \tag{11}$$

with

$$U^I_{nn'} = \int_0^\infty R_{n\ell}(r)\frac{e^2}{\epsilon\sqrt{r^2 + d^2}}R_{n'\ell}(r)r\,\mathrm{d}r \tag{12}$$

$$U^{II}_{nn'} = \int_0^\infty R_{n\ell}(r)\frac{e^2}{\epsilon r}R_{n'\ell}(r)r\,\mathrm{d}r \tag{13}$$

$$B_{[K][K']} = \int \Phi_{[K]}(\vec{R}, \vec{r})\Phi_{[K']}(\vec{R}', \vec{r}')\,\mathrm{d}\vec{R}\,\mathrm{d}\vec{r} \tag{14}$$

where $R_{n\ell}(\vec{r})$ is the radial part of two-dimensional harmonic oscillator function and $B_{[K][K']}$ is the transformation bracket of two-dimensional harmonic product states with two different sets of coordinates, which allows us to reduce the otherwise multi-integral into a single-integral. Non-vanishing $B_{[K][K']}$ occurs only when both the states $\Phi_{[K]}(\vec{R}, \vec{r})$ and $\Phi_{[K']}(\vec{R}', \vec{r}')$ have exactly the same eigen-energy and eigen-angular momentum. The analytical expression for $B_{[K][K']}$ has already been derived in [19]. The set of canonical coordinates $(\vec{R}', \vec{r}')$ are defined by $\vec{r}' = \vec{r}_1$, $\vec{R} = \vec{r}_2$. The dimension of the model space is constrained by $0 \leqslant N = 2(n_1 + n_2) + |\ell_1| + |\ell_2| \leqslant 24$. If $N$ is increased by 2, the ratio of the difference in energy is less than 0.001%.

## 3. Numerical results

Using $m_e^* = 0.067m_e$ ($m_e$ is the free-electron mass), $\hbar\omega_0 = 0.5Ry^*$, $d = 10$ nm and $\epsilon = 12.4$ for GaAs QD's, we calculated the energy spectrum of low lying states with $L \leqslant 8$. In figure 1, we plot the energies of the barrier $D^-$ centre QD as a function of the external magnetic field $B$ separately for $S = 0$ and $S = 1$. It is clear that Coulomb attraction terms in the $D^-$ Hamiltonian decrease in strength as $d$ increases, whereas the electron–electron repulsion term is independent of $d$. Thus, at larger values of $d$, the repulsion becomes relatively more important, and the electrons can lower their energy most effectively by forming highly correlated states in which they are well separated in position. Hence, it is the competition between the single particle energy and the interaction energy that finally determines the total energy. The existence of the Zeeman term $\omega_c L/2$ (negative) makes it possible for states with larger $L$ to be even lower in energy than those with smaller $L$. As a result, the lowest state for a given spin configuration occurs at larger $L$ as the magnetic field increases. However, the transition is strictly restricted to occur between two even numbers of $L$ for $S = 0$ and two odd numbers of $L$ for $S = 1$, as in the case of a two-electron QD [20].

It is interesting to calculate the $d \to 0$ case because the qualitative nature of the lowest-lying $D^-$ states will change with decreasing values of $d$. Coulomb attraction terms in the

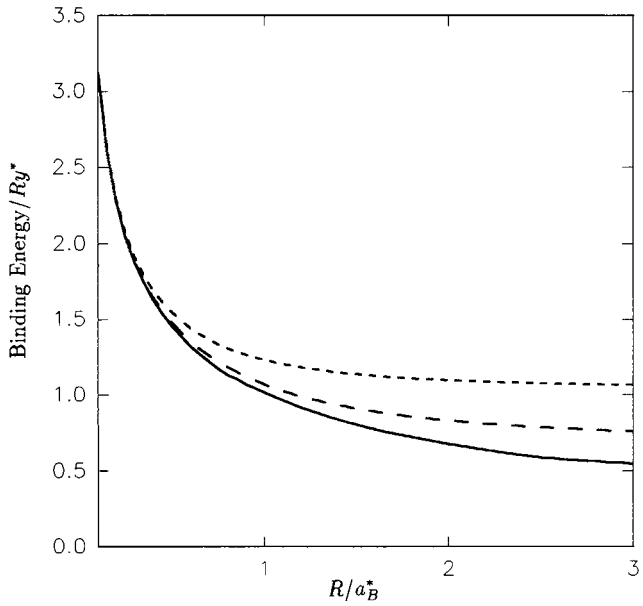



**Figure 3.** Dependence of the binding energy $E_B(\mathrm{D}^-)$ on the QD radius $R$ normalized by the effective Bohr radius $a_B^*$ with $d = 0$ is plotted.

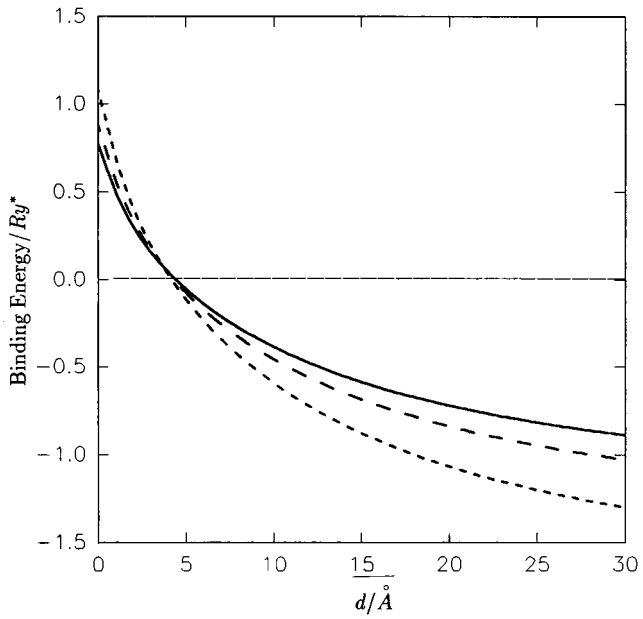



**Figure 4.** Dependence of the binding energy $E_B(\mathrm{D}^-)$ on the distance $d$ (in units of nm) from the QD plane with $\hbar\omega_0 = 1.0Ry^*$ is plotted.

$\mathrm{D}^-$ Hamiltonian decrease in strength as $d$ increases, whereas the electron–electron repulsion term is independent of $d$. Thus, at lower values of $d$, the attraction becomes relatively more important. Correlation between electrons is relatively weak in the bound $d = 0$ eigenstates.

The calculation shows that at $d \to 0$ the ground state transition cannot occur (see figure 2). The ground state of the $D^-$ centre QD is always the $^1S$ state, i.e., the state of $L = 0$ and $S = 0$.

We define the binding energy of the negative donor as

$$E_B(D^-) = E(D^0) + E_0 - E(D^-) \tag{15}$$

where $E(D^-)$ is the $D^-$ ground-state energy in the QD's and $E_0$ and $E(D^0)$ are, respectively, the lowest levels of an electron in the QD's without and with the Coulomb potential. The dependences of $E_B(D^-)$ on the dot radius $R$ with $d = 0$ for a few different values of magnetic fields are plotted in figure 3. The binding energy reduces as the dot radius is increased. However, the binding energy of the ground state of $D^-$ centre QD's in lower magnetic fields reduces with increasing the dot radius $R$ more rapidly than in higher magnetic fields. As shown in figure 3, the binding energies of $D^-$ centre QD's increase with increasing magnetic field $B$. Hence, the binding energies of $D^-$ centre QD's in a magnetic field are strongly dependent on the confined strength and the strength of the magnetic field.

It is clear that as $d$ increases from zero, the attractive interaction responsible for binding decreases. However, the binding energy of the $D^-$ centre in QD depends on the difference between the energy of the $D^-$ centre and that of the neutral donor ($D^0$) left behind when one electron is removed from the $D^-$ ion. Both the total (two-electron) binding of the $D^-$ ion and that of the $D^0$ decrease as $d$ increases. The pertinent question is which decreases fastest. In figure 4, we plot $E_B(D^-)$ versus $d$ for the magnetic fields $B = 0, 5, 10$ T with $\hbar\omega_0 = 1.0\ Ry^*$. It is readily seen that $E_B(D^-)$ decreases with increasing $d$, but it reaches a maximum at around $d \sim 1$ nm. When $d$ increases further, $E_B(D^-)$ drops to zero. This indicates that no bound state exists for the barrier $D^-$ QD at $d > 5$ Å.

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