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Binding Energies of D^- Centers Trapped by a Quantum Dot in a Magnetic Field*

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Abstract *A investigation of the properties of the bound states of D^- centers confined in a parabolic quantum dot has been performed for the case with the presence of a perpendicular magnetic field. Calculations are carried out by using the method of numerical diagonalization of Hamiltonian matrix within the effective-mass approximation. The binding energies of the ground and some bound-excited states are obtained as a function of the applied magnetic field strength. Detailed calculations of the binding energies for a number of low-lying states show that for field strength less than $B = 2.1$ T, the D^- center confined in a quantum dot possesses two bound states, for $2.1 \leq B < 2.4$ T, there exist three bound states, etc. Further relevant characteristics of the D^- center quantum dots in magnetic fields are provided.*

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A negative-donor (D^-) center in a semiconductor is formed by a neutral (D^0) center trapping an extra electron.[1] It is analogous to a negative hydrogen ion (H^-). The D^- center is one of the simplest many-body systems which cannot be solved exactly. This system is very interesting in the study of electron-electron interaction,[2] because we can expect that one of the electrons can screen the positive ion for the other one and this would not be affected by the Coulombic interaction. On the other hand, impurities in semiconductors influence both transport and optical properties so that topics like confined D^- centers in low-dimensional space have been extensively investigated. Since the existence of D^- centers in center-doped GaAs/Al_xGa_{1-x}As multiple quantum wells (QWs) was first reported by Huant, Najda, and Etienne[3] in 1990, many experimental[4–6] and theoretical[7–23] investigations for D^- centers in QWs, quantum dots (QDs) with and without magnetic fields have been carried out. Much of this work has concentrated on GaAs/GaAlAs structures; particularly on isolated nanostructures subjected to an external magnetic field directed perpendicular to the heteroplanes. The reason for this is that the magnetic field significantly increases the stability of D^- centers.

According to the Hill theorem,[24] the D^- centers in a bulk semiconductor possess only one bound state with the spin-singlet configuration. Due to relatively small binding energy of D^- centers in bulk semiconductors, they can only be observed at very low temperatures. This situation limits to some extent their practical importance in semiconductors. Recent progress in semiconductor technology has made possible the fabrication of individual QDs. Such microstructures confine electrons in all three space dimensions. Indeed, the quantum confinement leads to a significant increase in binding energy and a formation of bound excited states of D^- centers. On the other hand, the applied external magnetic field also leads to an increasing of binding energy and a formation of bound excited states of the D^- centers.[25] Hence, there is an increasing interest in the electronic structure and properties of D^- centers in semiconductors QDs under magnetic field.

Since QDs are created mainly through producing a lateral confinement restricting the motion of the electrons, which are initially confined in a very narrow QW, they usually have the shape of flat disks, with transverse dimensions considerably exceeding their thickness. The energy of single-electron excitations across the disk exceeds other characteristic energies in the system, and the confined electrons can be considered as two-dimensional. In most studies, a harmonic oscillator potential were used to describe the lateral confinement of electrons. In present work, we will focus on studying binding energy spectrum of the D^- centers in QDs with a parabolic lateral confining potential in magnetic fields by using the method of numerical diagonalization of Hamiltonian. This work can be considered as an extension of the study of our previous study[18,22,23] on the D^- centers in QDs.

In the effective-mass approximation, the Hamiltonian for the D^- center in a parabolic QD when the magnetic field is applied perpendicular to the x-y plane is given by

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

with

$$V_c = -\frac{e^2}{\epsilon}\sum_{i=1,2}\frac{1}{r_i} + \frac{e^2}{\epsilon r_{12}}\,, \tag{2}$$

where $\vec{r}_i$ ($\vec{p}_i$) is the position vector (the momentum vector) of the i-th electron originating from the center 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; ω_0 is the strength of the confinement, ϵ is the effective dielectric constant, g^* is the effective Lande factor, μ_B is the Bohr magneton and

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S_z is the z-component of the total spin. With the symmetric gauge for magnetic field $\vec{A} = (B/2)(-y, x, 0)$, the Hamiltonian then reads

$$H = \sum_{i=1,2} \Big(\frac{p_i^2}{2m_e^*} + \frac{1}{2} m_e^* \omega^2 r_i^2 \Big) + \frac{1}{2}\omega_c L_z + V_c - g^* \mu_B B S_z \,, \quad (3)$$

where $\omega^2 = \omega_0^2 + \omega_c^2/4$, $\omega_c = eB/cm_e^*$ is the cyclotron frequency, and L_z is the z -component of the total angular momentum. Throughout the present paper, we use the donor Rydberg $R_D = m_e^* e^4/2\hbar^2\epsilon^2$ as a unit of energy, and the donor Bohr radius $a_D = \hbar^2\epsilon/m_e^* e^2$ as a unit of length.

Introducing the coordinates

$$\vec{\xi}_1 = \vec{r}_1 - \vec{r}_2, \quad \vec{\xi}_2 = \frac{1}{2}(\vec{r}_1 + \vec{r}_2) \,, \quad (4)$$

then Eq. (3) can be rewritten as

$$H = H_0 + V_c \,, \quad (5)$$

with

$$H_0 = \frac{p_{\xi_1}^2}{2M} + \frac{1}{2} M\omega^2 \xi_1^2 + \frac{p_{\xi_2}^2}{2\mu} + \frac{1}{2}\mu\omega^2\xi_2^2 - \frac{1}{2}\omega_c L_z - g^*\mu_B B S_z \,, \quad (6)$$

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

The Hamiltonian has cylindrical symmetry with respect to the QD axis, i.e., z-axis, which implies that the total orbital angular momentum, L, and its z-component, L_z, are conserved quantities, i.e., good quantum numbers. The total spin of two electrons, i.e., S, and its projection along the z-axis, S_z, are conserved quantities. To obtain the eigen-function and the eigen-energy associate with the D^- centers in QDs under magnetic field, we diagonalize Hamitonian. As we know, the two electrons obey Fermi-Dirac statistics, which means that the electronic part of the total wave function must be antisymmetric, i.e., when $S = 0$ the spatial part of the electronic wave function must be symmetric and when $S = 1$ the spatial part of the electronic wave function must be antisymmetric. Thus, S can be used as a quantum number which indicates the parity of the state.

To obtain the eigen-function and eigen-energies, H is diagonalized in a model space spanned by the translationally invariant harmonic product bases

$$\Phi_{LS} = {}_{[K]}\tilde{A}\big\{ [\phi^{\omega}_{n_1\ell_1}(\vec{\xi}_1)\phi^{\omega}_{n_2\ell_2}(\vec{\xi}_2)]_L \chi_S(s_1, s_2) \big\} \,, \quad (7)$$

where $\phi^{\omega}_{n\ell}(\vec{\xi})$ is a two-dimensional harmonic oscillator state with frequencies ω, 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. In practice calculation, ω serves as an adjustable variational parameter to minimize the eigenvalues. The spin function $\chi_S(s_1, s_2)$ has nothing to do except to determine the parity of the wave functions $\phi^{\omega}_{n_1\ell_1}(\vec{\xi}_1)$ and $\phi^{\omega}_{n_2\ell_2}(\vec{\xi}_2)$. It is clear that the wave function $\phi^{\omega}_{n_2\ell_2}(\vec{\xi}_2)$ is symmetric with respect to exchange of the position of two electrons. Therefore, $\phi^{\omega}_{n_1\ell_1}(\vec{\xi}_1)$ is symmetric (antisymmetric) if $\chi_S(s_1, s_2)$ is antisymmetric (symmetric) to make the total wave function (7) antisymmetric. Thus the triplet and singlet spins of the electrons correspond to symmetric and antisymmetric wave functions over the coordinate $\vec{\xi}_1$.

We define the binding energy of the ν-th quantum state of D^- centres as

$$E_B(D^-) = E(D^0) + E_0 - E(D^-) \,, \quad (8)$$

where $E(D^-)$ is the energy of the ν-th state of the D^- centres in the QDs, E_0 and $E(D^0)$ are, respectively, the lowest energy levels of an electron in QDs, without and with the Coulomb potential. The binding energy defined by (8) possesses the following physical interpretation: this is the minimum energy, which is required to liberate one electron from the bound state of D^- centers. After this dissociation process, the second electron is bound in the ground state of the D^0 center. The condition of stability against dissociation into a neutral donor and a free electron reads $E_B(D^-) \geq 0$.

Using the following parameters, i.e. $m_e^* = 0.067 m_e$ (m_e is the free-electron mass), $\epsilon = 12.4$ and $g^* = -0.44$ for GaAs QDs, we have performed the calculations for the ground state (^1S) and the following bound-excited states: ^3P, ^1D, ^3D, ^1F, and ^3F. Figure 1 shows the binding energies as a function of the magnetic field strength B. The confining energy $\hbar\omega_0$ is set to be $0.506 R_D$ (i.e., 3.0 meV), which corresponds to a QD with characteristic radius $R = (\hbar/m_e^*\omega_0)^{1/2} = 1.988 a_D$. The solid and dashed lines represent the results for the singlet and triplet states, respectively.

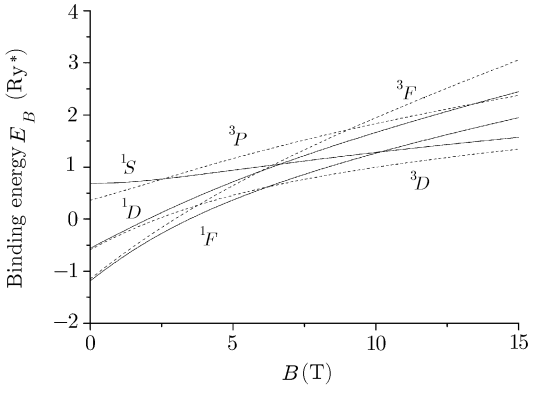

Fig. 1 The binding energies $E_B(D^-)$ (in units of Ry*) of the D^- centre in a QD with $\hbar\omega_0 = 0.506 R_D$ as a function of the magnetic field strength B. The solid and dashed lines represent, respectively, the singlet and triplet states.

Figure 1 shows the following results. (i) The binding energies $E_B(D^-)$ increase as the magnetic field strength B increases. It can be interpreted by the following. On the one hand, the orbit radii of the electrons is proportional to the QD size.[26] When the magnetic field strength B increases, the dot size will decrease and the Coulomb attraction will increase. On the other hand, the Hamilton contains two negative terms $-\omega_c L_z/2$ and $-g^*\mu_B B S_z$,

which are proportional to B and therefore would cause a linear decrease in energy. It is obvious that, for the ground state, these two terms are zero because $L = 0$ and $S = 0$, hence, the binding energy of the ground state slowly increase with increasing B. (ii) When the magnetic field strength less than $B = 2.1$ T, the D^- center confined in a QD possesses two bound states, for $2.1 \leq B < 2.4$ T, there exist three bound states, for $2.4 \leq B < 3.0$ T, there exist four bound states, and for $3.0 \leq B < 3.5$ T, there exist five bound states. When $B > 3.5$ T, as the magnetic field strength B is increased further, the sixth bound state (^{3}D) appears. It is obvious that as the magnetic field strength B is increased further, there are more bound excited states appear. (iii) An important aspect of the D^- centers under the magnetic field is that the ground-state transition can appear as B increases. From Fig. 1, it is readily seen that the first ground-state transition of the D^- center occurs at $B = 2.6$ T (from ^1S state to ^3P state, i.e., singlet $\rightarrow$ triplet state transition) and the second one occurs at $B = 9.1$ T (from ^3P to F^3). It is the competition between the single particle energy and the interacting energy that finally determines the binding energy. We know that the slope of the rising curve depends on L_z. A larger L_z would lead to a larger slope because the negative term $-\omega_c L_z/2$ is stronger. Therefore, when the magnetic field strength B increases, the curve with a larger L_z cross the curve with a smaller L_z because the former is rising faster. Obviously, the crossing would lead to a transition of L of the ground state from one to another. However, the transition is strictly limited to between to magic numbers of L.[27] (iv) When $L \geq 2$, the binding energy differences of the D^- centers is small at $B = 0$ for the same L values. However, as B increases, the binding energy differences increase. We find that the binding energies of the states with $L + S =$even increase more quickly than those of the adjacent states with $L + S =$ odd with increasing B. This feature is a consequence of mechanics symmetry. It has been discussed in previous publications and will not be repeated here.

In conclusion, we have investigated the feature of the binding energies of the ground and the bound-excited states for $L \leq 3$ of the D^- centres confined by a parabolic QD as a function of magnetic field strength. For our D^- center QDs, it was found that there are two bound states in weak magnetic field and there appear to have more bound states with increasing B. The ground-state transition of the D^- centres occurs as a function of B was found. It may be important in the quantitative understanding the optical and magnetic properties of the D^- center QDs.

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