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NEGATIVE DONOR CENTER QUANTUM DOTS IN MAGNETIC FIELDS*

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The method of few-body physics is applied to treat a D^- center quantum dot system in a magnetic field. The magnetic field is applied in the z direction. Using this method, we investigate the energy spectra of low-lying states of D^- center quantum dots as a function of magnetic field. The dependence of the binding energies of the ground-state of the D^- center are calculated as a function of the dot radius with a few values of the magnetic field strength and compared with other results.

Keywords: negative donor center; quantum dot; few-body physics.
PACC: 7320; 7127; 3130

I. INTRODUCTION

A negative hydrogenic donor center (D^-) in semiconductors 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^-).[1] D^- centers 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.[2] Recently there has been much experimental and theoretical interest in the problem of D^- centers in quasi-two-dimensional systems. Since the existence of D^- centers in center-doped GaAs/Al_xGa_{1-x}As multiple quantum wells was first reported by Huant, *et al.*[3] many experimental[4−6] and theoretical[7−13] investigations for D^- centers in quantum wells, quantum dots with and without magnetic fields have been carried out.

A quantum dot (QD) is semiconductor nanostructure with a three-dimensional confinement of electrons.[14] Recently the QD's have been fabricated in different shapes, for example, disk-like (cylindrical) shape[15] and spherical shape.[14,16] In contrast to the various studies on a D^- center in a spherical quantum dot, experimental and theoretical results related to the quantum confinement effect on D^- states in a disk-like QD are still rare. In experimentally realized QD's, the motion in the z direction is always frozen out into the lowest subband. Since the corresponding extent of the wave function is much less than the one in the xy-plane, we can treat the QD's in a disk-like two-dimensional limit. For most QD's, the harmonic oscillator is a very good approximation to describe the lateral confinement of the electrons.[17,18] Therefore, it is interesting to study electronic properties of D^- centers in a disk-like parabolic QD with a finite magnetic field.

In this paper, we propose a procedure to calculate energy spectrum of D^- centers in disk-like QDs with a parabolic lateral confining potential in magnetic fields by using the method of few-body physics. Using this method, we study the energy spectra of low-lying states of D^- centers quantum dots as a function of magnetic field. The dependence of binding energies on the ground-state on the D^- center are calculated as functions of the dot radius for a few values of the magnetic field strength and compared with other results.

II. MODEL AND CALCULATION METHOD

The D^- center in a disk-like QD can be reganded as a system composed of two electrons and a positively charged donor impurity located at the center of the disk potential-well region. A magnetic field threads in the z direction. We assume the validity of the effective-mass approximation and neglect the difference of the electron band masses and dielectric constant between the QD region and the surrounding medium. It is reasonable for the case of the strong confinement and small dielectric-constant difference. However, we should point out that if there is signif-

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icant penetration into the barrier, the effect of the electronic effective mass can be important, and that the effect of the discontinuity of the dielectric constants on the D^- states should be considered for large differences. With the effective-mass approximation, the Hamiltonian of two electrons bound to an ionized donor located at the center of a disk-like parabolic QD can be written as

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

$$V = -\frac{e^2}{\epsilon}\sum_{i=1,2}\frac{1}{r_i} + \frac{e^2}{\epsilon r_{12}}, \quad (2)$$

where $\boldsymbol{r}_i$ ($\boldsymbol{p}_i$) is the position vector (the momentum vector) of the ith electron drawn from the center of the dot; m_e^* is the effective mass of an electron; $r_{12} = |\boldsymbol{r}_1 - \boldsymbol{r}_2|$ is the electron-electron separation; ϵ is the dielectric constant of the medium the electrons are moving in, and ω_0 is the radial confinement frequency. With the symmetric gauge for the magnetic field $\boldsymbol{A} = (B/2)(-y, x, 0)$, the Hamiltonian then reads

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

where $\omega = \sqrt{\omega_0^2 + \omega_c^2/4}$, $\omega_c = eB/(cm_e^*)$ stands for the cyclotron frequency, L_z is the total orbital angular momentum along the z direction. 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.

Introducing the coordinates

$$\boldsymbol{r} = \boldsymbol{r}_{12} = \boldsymbol{r}_1 - \boldsymbol{r}_2, \boldsymbol{R} = (\boldsymbol{r}_1 + \boldsymbol{r}_2)/2, \quad (4)$$

then Eq. (1) can be rewritten as

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

with

$$H_0 = \frac{P^2}{2M} + \frac{1}{2}M\omega^2 R^2 + \frac{p^2}{2\mu} + \frac{1}{2}\mu\omega^2 r^2 \frac{1}{2}W_C L - g^*\mu_B B S_Z, \quad (6)$$

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

The D^- eigenstates 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, 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

$$\Phi_{[K]} = \tilde{A}\{[\phi_{n_1\ell_1}(\boldsymbol{R})\phi_{n_2\ell_2}(\boldsymbol{r})]_L\chi_S\}, \quad (7)$$

where $\chi_S = [\xi(1)\xi(2)]_S$, $\xi(i)$ is the spin state of the ith electron and the spins of two electrons are coupled to S, $\phi_{n\ell}(\boldsymbol{r})$ is a two-dimensional harmonic oscillator state with frequencies ω (ω is considered as an adjustable variational parameter), 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 antisymmetrized. The matrix elements of H are then given by the following expressions:

$$\langle \Phi_{[K]}|H_0|\Phi_{[K']}\rangle = [2(n_1+n_2) + |\ell_1| + |\ell_2| + 2 + \frac{1}{2}W_C L - g^*\mu_B B S_Z,]\hbar\omega\delta_{[K][K']}, \quad (8)$$

$$\langle \Phi_{[K]}|V|\Phi_{[K']}\rangle = U_{n_2n_2'}\delta_{n_1n_1'}\delta_{\ell_1\ell_1'}\delta_{\ell_2\ell_2'} - 2\sum_{[K''],[K''']} B_{[K][K'']} \times B_{[K'][K''']}U_{n_2''n_2'''}\delta_{n_1''n_1'''}\delta_{\ell_1''\ell_1'''}\delta_{\ell_2''\ell_2'''} \quad (9)$$

with

$$U_{nn'} = \int_0^\infty R_{n\ell}(r)\frac{e^2}{\epsilon r}R_{n'\ell}(r)r\mathrm{d}r, \quad (10)$$

$$B_{[K][K']} = \int \Phi_{[K]}(\boldsymbol{R}, \boldsymbol{r})\Phi_{[K']}(\boldsymbol{R}', \boldsymbol{r}')\mathrm{d}\boldsymbol{R}\mathrm{d}\boldsymbol{r}, \quad (11)$$

where $R_{n\ell}(\boldsymbol{r})$ is the radial part of two-dimensional harmonic oscillator function, $B_{[K][K']}$ is the transformation bracket of two-dimensional harmonic product states with two different sets of coordinates. This allows us to reduce the otherwise multi-integral into single-integral. Nonvanishing $B_{[K][K']}$ occurs only when both the states $\Phi_{[K]}(\boldsymbol{R}, \boldsymbol{r})$ and $\Phi_{[K']}(\boldsymbol{R}', \boldsymbol{r}')$ have exactly the same eigen-energy and eigen-angular

momentum. Analytical expression for $B_{[K][K']}$ has already been derived in Ref.[19]. The set of canonical coordinates $(\boldsymbol{R}', \boldsymbol{r}')$ are defined by $\boldsymbol{r}' = \boldsymbol{r}_1$, $\boldsymbol{R}' = \boldsymbol{r}_2$.

The accuracy of the solutions depends on how large the model space is. Since we are interested only in the low-lying states and in the qualitative aspect, the model space adopted is neither very large to facilitate numerical calculation, nor very small to assure the qualitative accuracy. This is achieved by extending the dimension of the model space step by step, and in each step the new results are compared with the previous ones from a smaller space, until satisfactory convergence is achieved. In this paper, the dimension of the model space is constrained by $0 \leq N = 2(n_1 + n_2) + |\ell_1| + |\ell_2| \leq 26$. If N is increased by 2, the ratio of the difference in energy is less than 0.01%.

Ⅲ. NUMERICAL RESULTS

Our numerical computation is carried out for GaAs QD's for which the dielectric constant is taken to be $\epsilon = 12.4$ and the electron effective mass $m_e^* = 0.067m_e$ (m_e is the free-electron mass). The energy and length are measured in units of the effective Rydberg Ry* and Bohr radius a_B^* of a donor in the bulk, respectively. As indicated in Table 1, the convergence for the energy of the ground state of the D^- center QD's with $\hbar\omega_0 = 0.1$ is fast with the number of basic functions. Using the above method, we calculated the energy spectra of the low-lying states of a D^- center as functions of the magnetic field strength (see Fig. 1) for $\hbar\omega_0 = 0.1$. As illustrated in the figures, an important aspect is that the changes of the level ordering and the level differences and then the crossover of two levels can appear as the strength of the magnetic field increases. The physical origin of level crossing is the result of a competition between electron-electron interaction energy, Zeeman splitting, and kinetic energy, leading to a series of incompressible states. This is due to the negative Zeeman term $\frac{1}{2}\omega_c L_z$, which brings levels with higher L below those with lower L values in strong fields. The two cases with $S = 0$ and 1 are depicted separately in Figs. 1(a) and 1(b). Compared with the case in two-electron dots,[20,21] we find that the ground-state transitions of two-electron dot in a magnetic field do not appear, i.e., the ground-state of D^- center in a magnetic field is always the ^1S state. It is obvious that the electronic properties of two-electron systems with and without a positive charge center are different.

Table 1. The convergence of the energy of the ground state of D^- center QD's with the number N_f of the basic functions for a few values of the magnetic field with $\hbar\omega_0 = 0.1$.

N_f/B(Tesla)	0	5	10
195	–1.931918	–2.962311	–2.748878
256	–1.994212	–3.026414	–2.805822
328	–2.031938	–3.063645	–2.835558

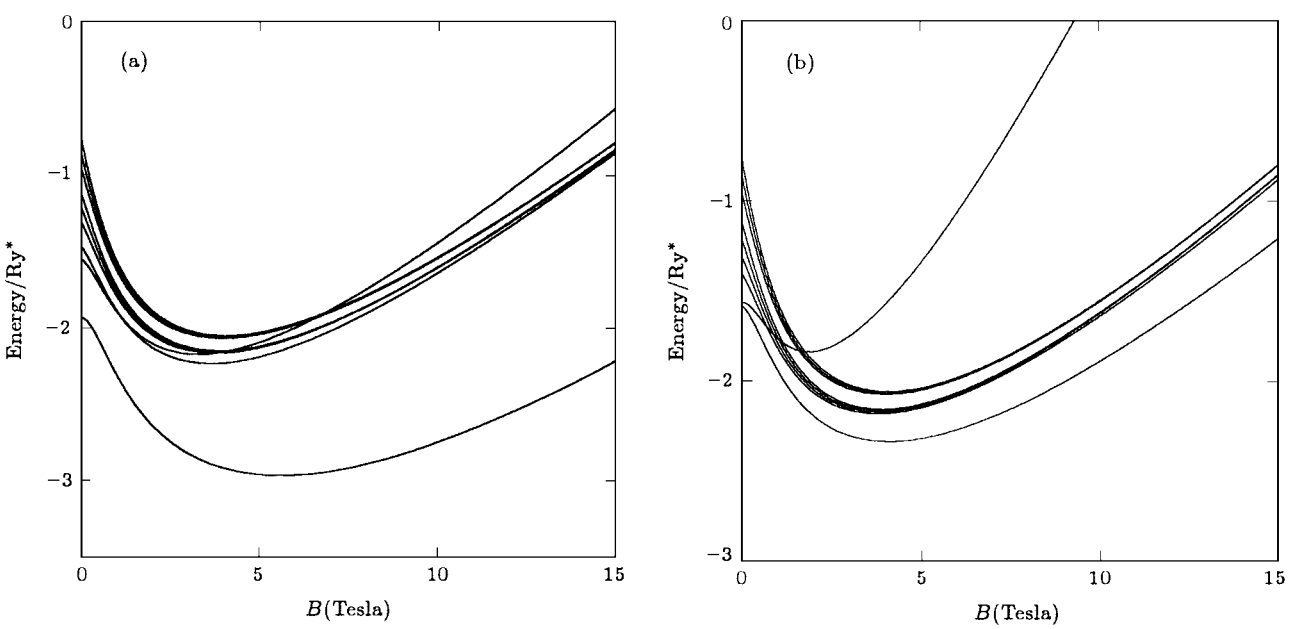


Fig.1. The energy spectra of the low-lying states of the D^- centers in a QD as functions of the magnetic field strength with $\hbar\omega_0 = 0.1$. (a) $S = 0$. The ordering at $B = 0$ is as follows: $L = 0, 1, 2, 3, 4, 5, 6, 7, 8$. (b) $S = 1$. The ordering at $B = 0$ is as follows: $L = 1, 0, 2, 3, 4, 5, 6, 7, 8$.

We define the binding energy of the D^- centers as

$$E_B(D^-) = E(D^0) + E_0 - E(D^-), \qquad (12)$$

where $E(D^-)$ is the D^- ground-state energy in the QD's, 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 for three different magnetic fields corresponding to $B = 0$, $B = 5$T, and $B = 10$T are plotted in Fig. 2. We found that the binding energies of the ground states of D^- centers in QD's increase as the dot radius is reduced. The binding energies are much larger than those (0.0555 and 0.480Ry*) of three-dimensional D^- centers[22] and two-dimensional D^- centers.[23] However, the binding energy of the ground state of D^- centers in QD's in lower magnetic fields reduces with increasing dot radius R more rapidly than in higher magnetic fields. At zero magnetic field, it is interesting to calculate the binding energy of D^- centers and find that it tends to 0.540Ry* at a much larger dot radius R. It is reasonable that the value of the binding energy of two-dimensional D^- centers in QD's is larger than obtained in experiment[3] and from the calculation[24] in quantum-well structures. We have also calculated the binding energies at $R = 4a_B^*$, $8a_B^*$, and $12a_B^*$, which are equal to 0.522Ry*, 0.460Ry*, 0.396Ry* respectively. They are close to the "exact" result (0.480Ry*) obtained by Phelps and Bajaj[23] and that (0.454Ry*) obtained by Zhu *et al.*[25] As shown in Fig. 2, the binding energies of the ground states of D^- centers in QD's increase with increasing magnetic field B. Hence, the binding energies of D^- centers in QD's in a magnetic field are strongly dependent on the confined strength and the strength of the magnetic field.

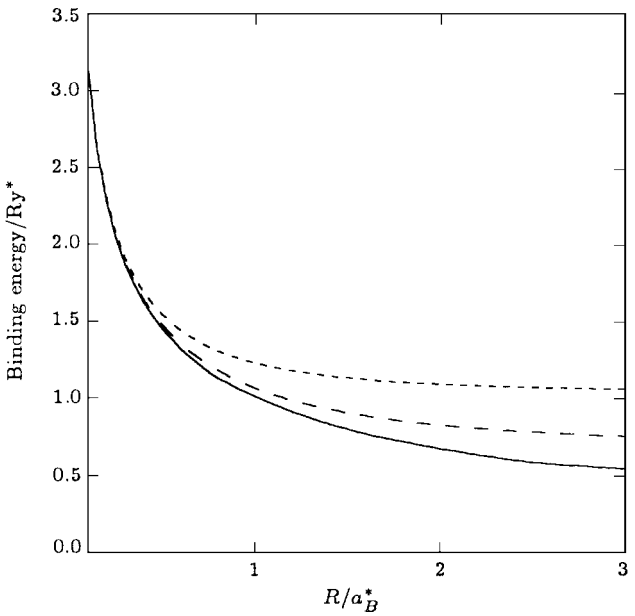


Fig.2. Dependence of the binding energy $E_B(D^-)$ on the QD radius R normalized by the effective Bohr radius a_B^* for a few different values of the magnetic field.

In conclusion, we have used the method of few-body physics and obtained the binding energy spectra of D^- centers in QD's in magnetic fields. The calculated results have shown that the binding energies are strongly dependent on the confinement of QD's and the strength of magnetic field. It may be important in the quantitative understanding of future experimental work involving D^- centers in quantum dots.

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