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Properties of spin polarization state of two-electron system on two-dimensional quantum dots with magnetic field

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Abstract. Influence of the magnetic field on the energy of the spin polarization state of a two-electron system in two-dimensional quantum dots (QDs) is studied by using the method of few-body physics. As example, a numerical calculation is performed for a GaAs semiconductor QD to show the variations of the ground-state energy E_0, the spin-singlet energy $E_1(A)$ and spin-triplet energy $E_1(S)$ of the first excited state and the energy difference (i.e. $\Delta E(A)$ and $\Delta E(S)$) between the first excited and ground states with the effective radius R_0 of the QD and the magnetic field B. The results show that E_0 increases with increasing B, but decreases with increasing R_0; in the magnetic field, the spin-singlet energy $E_1(A)$ of the first excited state splits into two levels as $E_{1+1}(A)$ and $E_{1-1}(A)$, the spin-triplet energy $E_1(S)$ of the first excited state splits into two sets as $E_{1+1}(S)$ and $E_{1-1}(S)$, and each set consists of three "fine structures" which correspond to $M_S=1,0,-1$, respectively; each energy level (set, energy difference) decreases with increasing R_0, but there are great differences among the changes of them with B: $E_{1+1}(A)$, $E_{1+1}^{M_S}(S)$, $\Delta E_{1+1}(A)$, and $\Delta E_{1+1}^{M_S}(S)$ increase significantly with increasing B, but the variations of $E_{1-1}(A)$, $E_{1-1}^{M_S}(S)$, $\Delta E_{1-1}(A)$, and $\Delta E_{1-1}^{M_S}(S)$ with B are relatively slow; the splitting degree of each energy level (set, energy difference) is proportional to the first power of the magnetic field B.

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Key words: quantum dot, method of few-body physics, electron-electron interaction, spin polarization state

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1 Introduction

The progress and rapid development of the growth technology of semiconductor materials greatly promote the widespread study on low-dimensional nanostructures which have been a hotspot in the research field of quantum functional devices[1-8]. The quantum dot (QD) is one kind of artificial microstructure and the electron number in it can increase one by one from 1 by controlling the gate voltage, so the few-electron system can be formed. Kastner *et al.*[9] have regarded the QD as the "artificial atom". The reason is that the appearance of the QD is just like a minimal point structure and the electron in the QD is confined in every direction, so the discrete energy arises, thus the charge and the energy of the QD are quantized. Obviously, like the atomic problem, the study on the energy and its corresponding electronic states of the QD is a basic question. The simplest QD with the electron-electron correlation consists of two electrons, and the two-electron (2e) QD is also called the Helium QD. Xie[10] have studied the states of the barrier D^- centre in a arbitrary strength of magnetic field, which consists of a positive ion located on the z-axis at a distance from the two-dimensional (2D) QD plane and two electrons in the dot plane bound by the ion. Yannouleas *et al.*[11] have investigated the rovibrational spectrum of a 2e 2D parabolic QD. Sun *et al.*[12] and Dong *et al.*[13] have studied the energy spectra and electronic structure of a 2e QD within the effective mass theory. Ruan[14] have derived the transformation bracket relating product states of 2D harmonic oscillator functions with different sets of Jacobian coordinates. Recently, Li *et al.*[15] studies the total energy of the 2e QD and the energy of the electron-electron interaction by using a variational method of Pekar type on the condition of the electron-LO phonon strong coupling in a parabolic QD. In this paper, the influence of the magnetic field on the energy level of the spin polarization state of a 2e system in 2D QDs is studied by using the method of few-body physics. The influence of the magnetic field on the ground-state energy, the spin-singlet energy and spin-triplet energy of the first excited state and the energy difference between the first excited and ground states are discussed concretely.

2 Theoretical model and method

Comparing with the three-dimensional QD, the 2D QD can be controlled (the electron number in the QD) and observed (the spatial distribution of the electron) more easily, and it is more important for theoretical predictions and comparisons to the experimental results. In this paper, two electrons with the effective band mass m_b are confined in a 2D parabolic QD, and the plane of the 2D QD is taken as the $x-y$ plane. The applied magnetic field is in z direction of the QD. Based on the effective mass approximation, the Hamiltonian of the system can be written as

$$H = H_e + H_c + H_S \tag{1a}$$

where

$$\begin{aligned} H_e = & \frac{1}{2m_b}\sum_{j=1}^{2}(\vec{p}_j+e\vec{A}_j)^2+\frac{1}{2}m_b\omega_0^2\sum_{j=1}^{2}\rho_j^2 \\ = & \frac{1}{2m_b}\sum_{j=1}^{2}p_j^2+\frac{1}{2}m_b\omega_e^2\sum_{j=1}^{2}\rho_j^2+\frac{1}{2}\omega_{ce}\sum_{j=1}^{2}L_z^j, \end{aligned} \tag{1b}$$

$$H_c = \frac{e^2}{4\pi\varepsilon\varepsilon_0|\vec{\rho}_1-\vec{\rho}_2|}, \tag{1c}$$

$$H_S = \frac{1}{2}g^*\mu_B B\sum_{j=1}^{2}\sigma_{jz}, \tag{1d}$$

represent the single-article energy of the 2e system, the Coulomb interaction energy between two electrons and the interaction energy between the electronic spin and the external magnetic field, respectively. $A_j = B(y_j,x_j,0)/2$ (where $j=1,2$) is the electronic vector potential. $\vec{p}_j$ and $\vec{\rho}_j$ (where j=1,2) denote the electronic momentum and vector coordinate in $x-y$ plane, respectively. $L_z^j = -i\hbar\partial/\partial\varphi_j$ $(j=1,2)$ is the z-direction component of the angular momentum operator. $\vec{\sigma}=(\sigma_x,\sigma_y,\sigma_2)$ is the Pauli operator. μ_B is the Bohr magneton. ε is the dielectric constant of the medium where the electron moves. $\omega_0=\hbar/(m_b R_0^2)$ represents the confinement frequency of the electron. R_0 is the characteristic length or the effective radius of the QD. g^* is the Lande factor.

For the 2e system with the spin $s=1/2$, the total antisymmetric wave function can be expanded as[14,16]

$$\Psi = A\{\Psi_{n_1m_1}(\vec{\rho}_1)\Psi_{n_2m_2}(\vec{\rho}_2)|S,M_S\rangle\} \tag{2}$$

where $\Psi_{mn}(\vec{\rho})$ is the eigenfunction of the 2D harmonic oscillator with the frequency $\omega_e = \sqrt{\omega_0^2+\omega_{ce}^2/4}$ and the energy $E_{nm}=(2n+|m|+1)\hbar\omega_e\cdot|S,M_S\rangle$. represents the spin wave function of the 2e system (where $\omega_{ce}=eB/m_b, n=0,1,2,\cdots,m=0,\pm1,\pm2,\cdots,S$ is the total spin quantum number and M_S is the total spin magnetic quantum number). A is the antisymmetrization operator. The total antisymmetrization to the wave function adopts the 2D Talmi-Moshinsky coefficient [14]. Then the energy of the 2e system in the state Ψ is

$$E = \langle\Psi|H|\Psi\rangle = E^e+E^c+E^S \tag{3}$$

where E^e, E^c, and E^S represent the single-article energy of the 2e system, the Coulomb interaction energy between two electrons and the interaction energy between the electronic spin and the external magnetic field, respectively. In accordance with Ref. [16], we take the Coulomb interaction term H_c as a perturbation in theoretical derivation.

3 Numerical analysis and discussion

A GaAs semiconductor QD is chosen to perform the numerical calculation and its material parameters are as follows[17]: $m_b = 0.067m_e$, $\varepsilon = 13.1$, $g^* = 0.52$. The concrete results are shown in Figs. 1-5, where the effective Rydberg constant $R_y^* = \hbar^2/(2m_b\alpha_B^*)$ is taken as the unit of energy and the effective Bohr radius $\alpha_B^* = 4\pi\varepsilon\varepsilon_0\hbar^2/(m_b e^2)$ is taken as the unit of length.

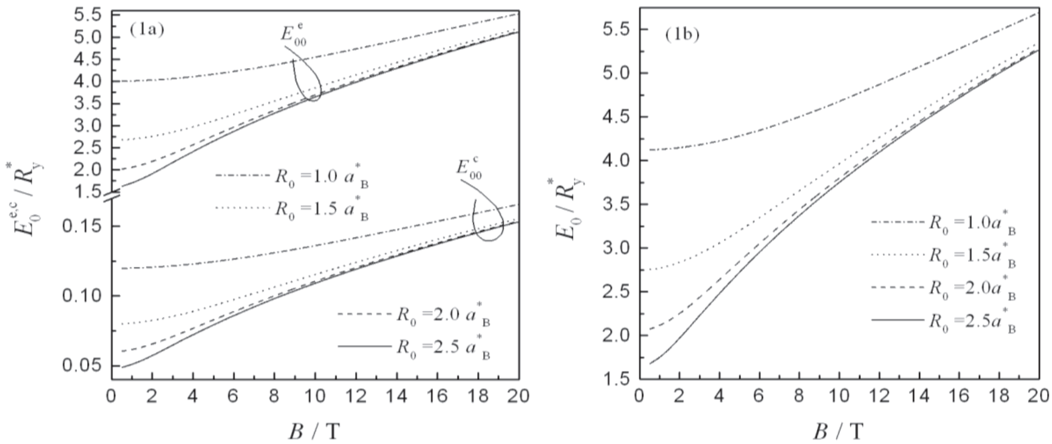

Figure 1: Variation of the ground-state energy E_0 with the effective radius R_0 of the QD and the magnetic field.

Figure 1 shows the variation of the ground-state energy E_0 of 2e system with the magnetic field B at different effective radii R_0 of the QD in the QD. From Fig. (1a), we notice that the single-particle energy E_0^e of 2e system is more larger than the electron-electron interaction energy E_0^c, and the quantitative relation is that E_0^e is 33.4 times larger than E_0^c. This is because two electrons must spin in the opposite direction since the system is in the ground state, and the contribution of the interaction between the spin and magnetic field to the ground-state energy E_0^S is equal to zero. Therefore, E_0^e plays a dominant role in the ground-state energy. It can be also seen form Fig. (1a) that E_0^e and E_0^c both increase with increasing B, but decrease with increasing R_0. In Fig. (1b), the variation of the ground-state energy E_0 is the same as that of E_0^e and E_0^c, and it is obvious that the slopes of $E_0 - B$ curves increase with increasing R_0. The reason is that the effect of the confinement potential on the particle plays a dominant role due to the great confinement strength of the QD on the particle when the QD's radius is smaller, and hence the magnetic field has little influence on the energy of the system, but the QD's radius has great one; when the QD's radius is larger, however, the effect of the confinement potential on the particle plays a secondary role because the confinement strength of the QD on the particle is weakened, thus the magnetic field has relatively great influence on the energy of the system.

Figure 2 shows the variation of the spin-singlet energy $E_1(A)$ of the first excited state with the magnetic field B at different effective radii R_0 of the QD. From Fig. (2a), it can

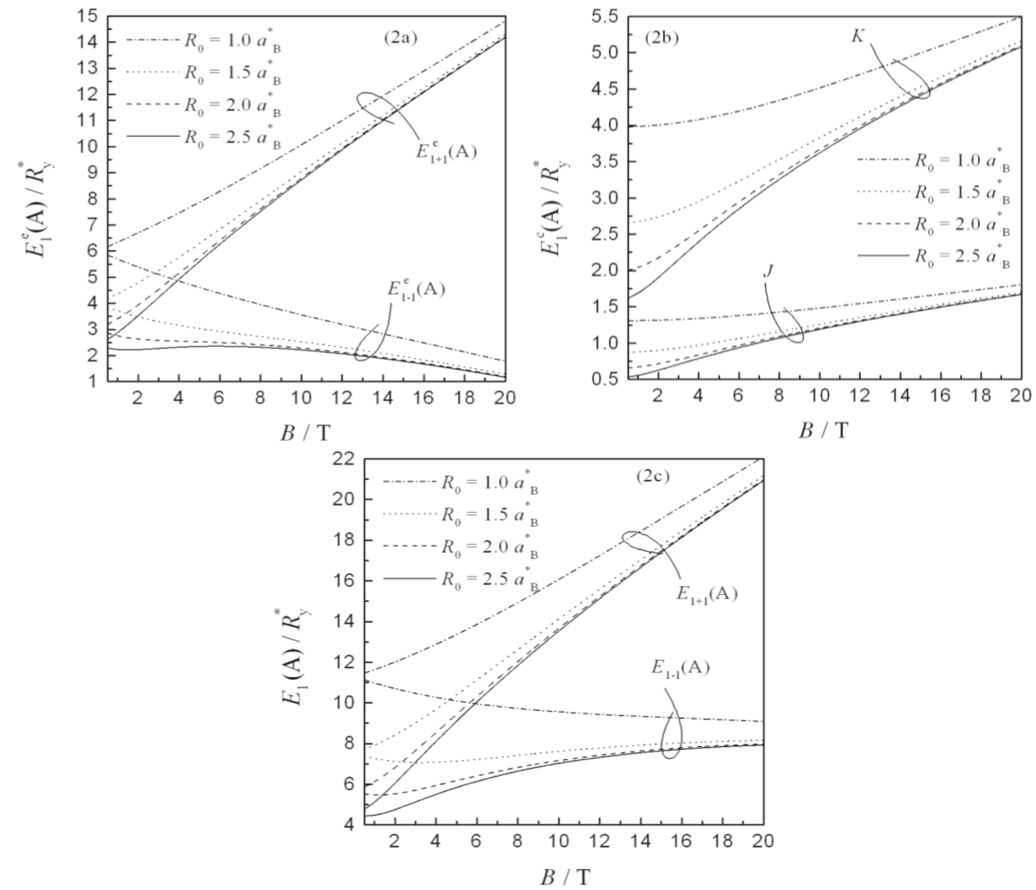

Figure 2: Variation of the spin-singlet energy $E_1(A)$ of the first excited state with the effective radius R_0 of the QD and the magnetic field B.

be seen that the contribution of the single-particle energy of 2e system to the spin-singlet energy of the first excited state $E_1^e(A)$ splits into two lines as $E_{1+1}^e(A)$ and $E_{1-1}^e(A)$ in the magnetic field. With the increase of B, $E_{1+1}^e(A)$ increases, $E_{1-1}^e(A)$ decreases, and the changing amplitude of $E_{1+1}^e(A)$ is greater than that of $E_{1-1}^e(A)$. This splitting is a Zeeman effect caused by additional terms $\pm\hbar\omega_{ee}$, which are produced by the interaction between the magnetic field and symmetric "orbital" motion of the first excited state of single particle. We can see from Fig. (2b) that $E_1^c K+J$ is the contribution of the electron-electron interaction to the spin-singlet energy of the first excited state, where K and J are often called the Coulomb energy and the exchange energy, respectively[16]. K and J are positive and $K > J$. They both increase with increasing B. In addition, the contribution of the interaction between the spin and magnetic field to the ground-state energy E_1^c is still equal to zero because two electrons spin in the opposite direction when the system is in the spin singlet of the first excited state. According to above analysis, it can be easily seen from Fig. (2c) that the spin-singlet energy $E_1(A)$ of the first excited state splits into two lines as $E_{1+1}(A)$ and $E_{1-1}(A)$. The variation of $E_{1+1}(A)$ with B and R_0 is basically similar to that of the ground-state energy E_0, and the only difference is that the influence of the magnetic field is further enhanced by the additional term $+\hbar\omega_{ce}$; however, the variation of $E_{1-1}(A)$ with B and R_0 has some changes, and its concrete It is mainly because the additional term $-\hbar\omega_{ce}$ offsets the influence of the magnetic field to some extent. This conclusion is consistent with the experimental results[18].

Figure 3 shows the variation of the spin-triplet energy $E_1(S)$ of the first excited state with the effective radius R_0 of the QD and the magnetic field B. It can be seen from Fig. 3 that the spin-triplet energy $E_1(S)$ of the first excited state splits into two sets, which consist of six lines. This can be explained as follows: firstly, we can see from Fig.(3a) that the contribution of the single-particle energy to the spin-triplet energy of the first excited state $E_1^e(S)$ splits into two lines as $E_{1+1}(S)$ and $E_{1-1}(S)$ in the magnetic field, and that $E_{1+1}(S)=E_{1+1}(A)$ and $E_{1-1}(S)=E_{1-1}(A)$; Fig. (3b) indicates that the Zeeman effect caused by the interaction between the electronic "spin" motion and the magnetic field makes each above energy level split again into three levels. Hence, the "fine structures" are formed and they correspond to the spin states with $M_S=1,0,-1$, respectively. The energy levels with $M_S=1$ and $M_S=-1$ lie above and below the one with $M_S=0$, respectively. The energy splitting is proportional to the first power of the magnetic field B.

It can be seen from Fig. (3c) that $E_1^c(S)=K-J$ is the contribution of the electron-electron interaction to the spin-triplet energy of the first excited state, and $E_1^c(A)>E_1^c(S)$ due to $K+J>K-J$. This means the spin-singlet energy is higher than the spin-triplet energy of the system, namely, $E_1(A)>E_1(S)$. On the base of above analysis, we can see that $E_1(S)$ consists of two sets of energy levels (six lines) as $E_{1+1}(S)=E_{1+1}^e(S)+K-J+E_1^c(M_S)$ and $E_{1-1}(S)=E_{1-1}^e(S)+K-J+E_1^c(M_S)$. Fig. (3d) shows that $E_{1+1}(S)$ and $E_{1-1}(S)$ both decrease with increasing the effective radius R_0 of the QDand they decrease slowly with increasing R_0 when $R_0>2\alpha_B^*$, then reach a certain value when $R_0\geq 3.5\alpha_B^*$. This indicates that the QD effect almost disappears, and the corresponding radius is called the critical radius; However, $E_{1+1}(S)$ and $E_{1-1}(S)$ increase rapidly with decreasing R_0 when $R_0<2\alpha_B^*$. The qualitative variation of $E_{1+1}(S)$ and $E_{1-1}(S)$ with R_0 is consistent with the results in Ref. [15], and it shows that the phonon effect has no influence on the variation of the energy of 2e system with the radius of the QD. This is because two electrons are confined in a smaller space and the spatial overlap of them increases due to the larger confinement potential of the QD when the radius of the QD is smaller, which make the single-particle energy and the energy of the electron-electron interaction increase. From Fig. (3e), it can be seen that the energy set $E_{1+1}(S)$ increases significantly with increasing B. The reason is that the values of $\hbar\omega_{ce}$, J, and $E_{1+1}^1(S)$ are positive in $E_{1+1}(S)$, and they strengthen the influence of the magnetic field together; In the energy set $E_{1-1}(S)$, with the increase of B, the energy with $M_S=1$ increases a little, the energy with $M_S=-1$ decreases slowly and the change of the energy with $M_S=0$ is not obvious. The main reason is that some negative terms in $E_{1-1}(S)$, such as $-\hbar\omega_{ce}$, $-J$, and the spin-magnetic

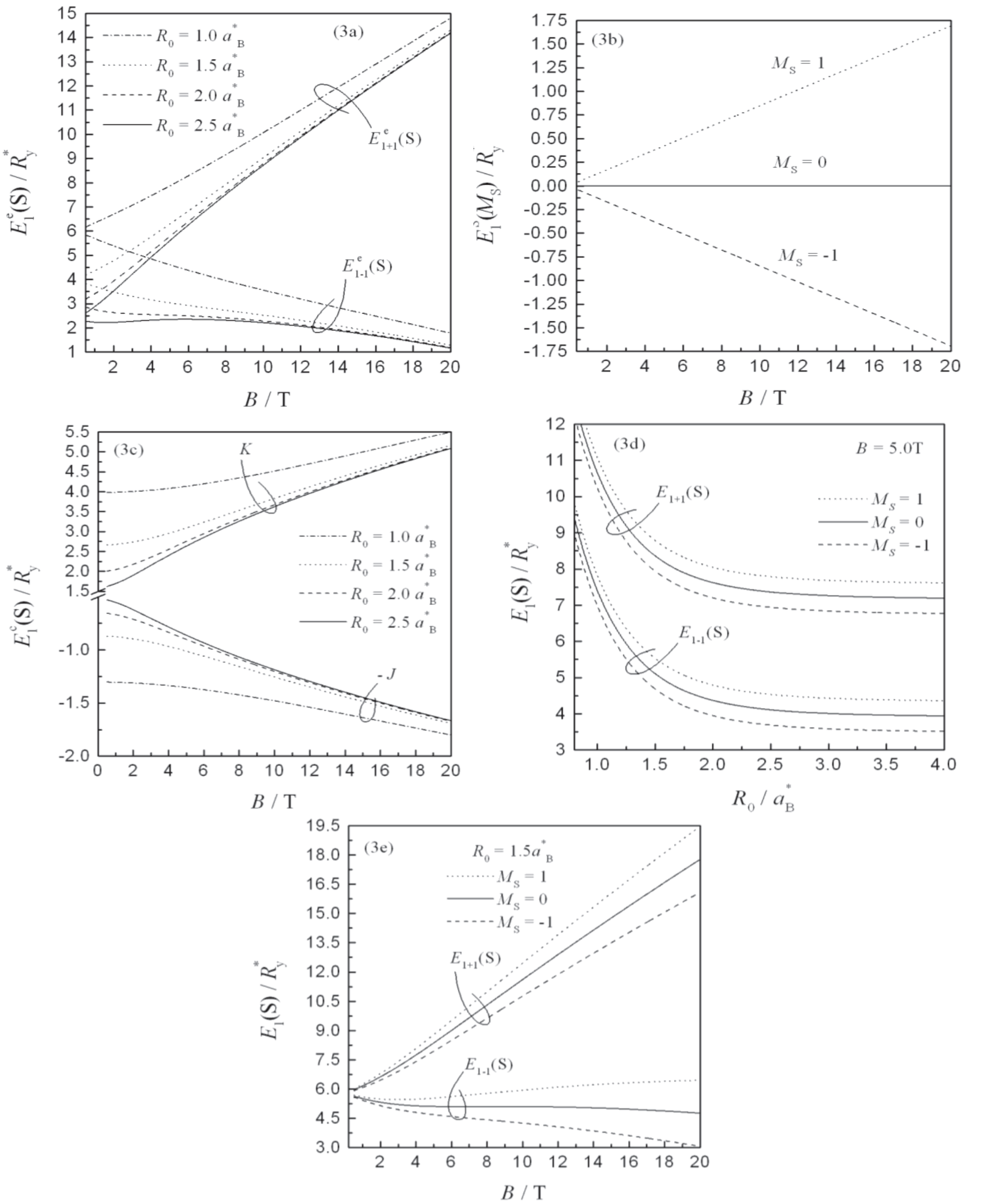

Figure 3: Variation of the spin-triplet energy $E_1(S)$ of the first excited state with the effective radius R_0 of the QD and the magnetic field B.

field interaction energy with $M_S = -1$, offset the influence of the magnetic field.

Figure 4 shows the variation of the energy difference $\Delta E(A)$ between the spin singlet of the first excited state and that of the ground state with the magnetic field B at different effective radii R_0 of the QD. It can be seen from Fig. 4 that the variations of $\Delta E_{1+1}(A) = E_{1+1}(A) - E_0$ and $\Delta E_{1-1}(A) = E_{1-1}(A) - E_0$ with B at different R_0 are similar to that of $E_{1+1}(A)$ and $E_{1-1}(A)$, respectively. The main difference is that the slopes of the curves $\Delta E_{1+1}(A) - B$ and $\Delta E_{1-1}(A) - B$ are smaller than that of $E_{1+1}(A) - B$ and $E_{1-1}(A) - B$, that is, the changing amplitudes of the curves decrease with increasing B. The main reason is that the ground-state energy does not include the Zeeman energy, as a result, the energy difference decreases with increasing B and can not be compensated by the increase of the Zeeman energy.

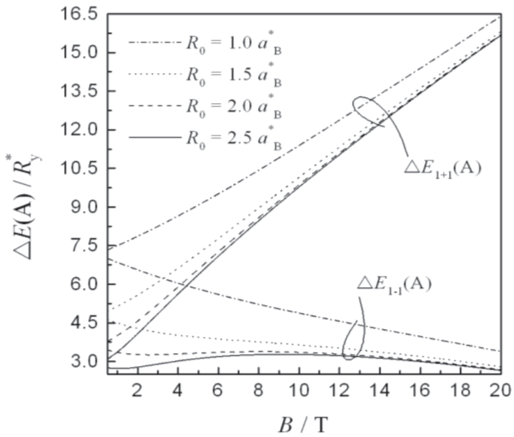

Figure 4: Variation of the energy difference $\Delta E(A)$ between the spin singlet of the first excited state and ground state with the effective radius R_0 of the QD and the magnetic field.

Figure 5 shows the variation of the energy difference $\Delta E(S)$ between the spin triplet of the first excited state and that of the ground state of the system with the magnetic field B and the effective radii R_0 of the QD. It can be seen form Fig. (5a) that $\Delta E_{1+1}(S) = E_{1+1}(S) - E_0$ and $\Delta E_{1+1}(S) = E_{1+1}(S) - E_0$ both decrease with increasing the effective radius R_0 of the QD. The energy difference decreases slowly to a certain value with increasing R_0 when $R_0 > 1.5\alpha^*_B$; but it increases rapidly with decreasing R_0 when $R_0 < 1.5\alpha^*_B$. Obviously, these characteristics come from the variation of $E_{1+1}(S)$ and $E_{1-1}(S)$ with R_0. From Fig. (5b), it can be seen that $\Delta E_{1+1}(S)$ increases with increasing B, $\Delta E_{1+1}(S)$ however decreases with increasing B, and even $\Delta E_{1-1}(S) < 0 (M_S = 0, -1)$ when $B > 9.15$T and $B > 13.4$T, respectively. This indicates that the transition from the spin triplet of the first excited state to the ground state is impossible.

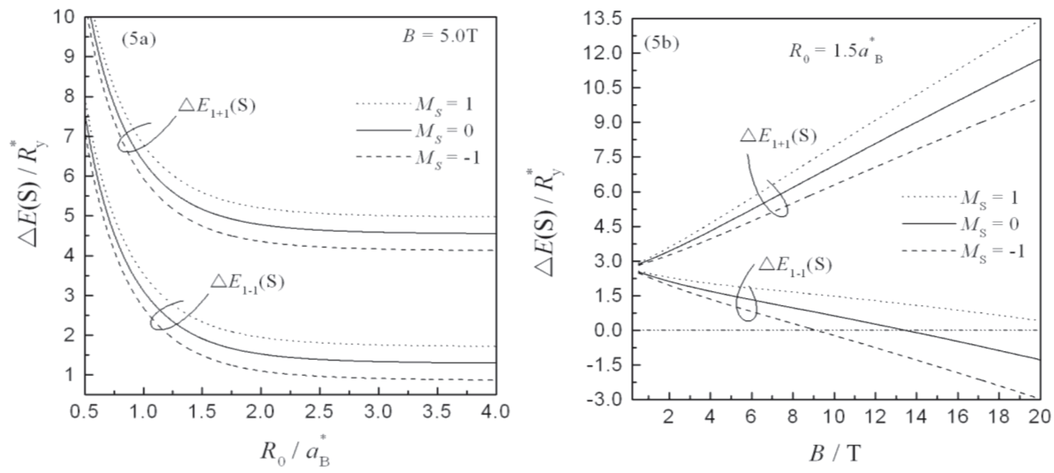

Figure 5: Variation of the energy difference $\Delta E(S)$ between the spin triplet of the first excited state and ground state with the effective radius R_0 of the QD and the magnetic field B.

4 Conclusion

The influence of the magnetic field on the energy of the spin polarization state of a 2e system of two-dimensional QDs is studied by using the method of few-body physics. The conclusions are obtained as follows: (1) The ground-state energy E_0 increases with increasing B, but decreases with increasing R_0. (2) In the magnetic field, the spin-singlet energy $E_1(A)$ of the first excited state splits into two levels as $E_{1+1}(A)$ and $E_{1-1}(A)$, the spin-triplet energy $E_1(S)$ of the first excited state splits into two sets as $E_{1+1}(S)$ and $E_{1-1}(S)$, and each set consists of three "fine structures" which correspond to M_S=1,0,−1, respectively. (3) Each above energy level (set, energy difference) decreases with increasing R_0, but there are great differences among the changes of them with B: $E_{1+1}(A)$, $E_{1+1}^{M_S}(S)$, $\Delta E_{1+1}(A)$ and $\Delta E_{1+1}^{M_S}(S)$ increase significantly with increasing B, but the variations of $E_{1-1}(A)$, $E_{1-1}^{M_S}(S)$, $\Delta E_{1-1}(A)$ and $\Delta E_{1-1}^{M_S}(S)$ with B are relatively slow. (4) The splitting degree of each energy level (set, energy difference) is proportional to the first power of the magnetic field B.

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References

[1] W. Xin, Wuyunqimuge, C. Han, and Eerdunchaolu, Superlattices and Microstructures 61 (2013) 13.
[2] Y. Sun, Z. H. Ding, and J. L. Xiao, J. At. Mol. Sci. 4 (2013) 176.

[3] X. J. Ma and J. L. Xiao, J. At. Mol. Sci. 4 (2013) 138.
[4] H. T. Yang, W. H. Ji, Huhemandula, and W.T. Hu, J. At. Mol. Sci. 4 (2013) 59.
[5] Z. X. Li, and J. L. Xiao, J. At. Mol. Sci. 3 (2012) 360.
[6] W. Xin, Z. M. Gao, Wuyunqimuge, *et al.*, Superlattices and Microstructures. 52 (2012) 872.
[7] Eerdunchaolu and W. Xin, Physica B. 406 (2011) 358.
[8] Eerdunchaolu, Y. Zhang, H. F. Li, and C. Han, Int. J. Mod. Phys. B. 25 (2011) 795.
[9] M. A. Kastner, Rev. Mod. Phys. 64 (1992) 848.
[10] W. F. Xie, J. Phys.: Condens. Matter 12 (2000) 3849.
[11] C. Yannouleas and U. Landman, Phys. Rev. Lett. 85 (2000) 1726.
[12] L. L. Sun, F. C. Ma, and S. S. Li, J. Appl. Phys. 94 (2003) 5884.
[13] Q. R. Dong, S. S. Li, Z.C. Niu, *et al.*, J. Appl. Phys. 96 (2004) 3277.
[14] W. Y. Ruan, J. Math. Phys. 37(1996) 3760.
[15] W. P. Li, J. L, Xiao, J. W. Yin, *et al.*, Chin. Phys. B 19 (2010) 047102.
[16] L. Schiff, Quantum Mechanics. 3-th ed. (McGraw-Hill, Inc., New York, 968). pp.375-376.
[17] S. Adachi, J. Appl. Phys. 58 (1985) R1.
[18] M. Bayer, A. Schmidt, A. Forchel, *et al.*, Phys. Rev. Lett. 74 (1995) 3439.