Singlet-Triplet Transition in Quantum Dots Confined by Triangular and Bowl-Like Potentials: the Effect of Electric Fields *

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We theoretically investigate the energy spectra of two-electron two-dimensional (2e 2D) quantum dots (QDs) confined by triangular potentials and bowl-like potentials in a magnetic field by exact diagonalization in the framework of effective mass theory. An in-plane electric field is found to contribute to the singlet–triplet transition of the ground state of the 2e 2D QDs confined by triangular or bowl-like potentials in a perpendicular magnetic field. The stronger the in-plane electric field, the smaller the magnetic field for the total spin of the ground states in the dot systems to change from $S = 0$ to $S = 1$. However, the influence of an in-plane electric field on the singlet–triplet transition of the ground state of two electrons in a triangular QD modulated by a perpendicular magnetic field is quite small because the triangular potential just deviates from the harmonic potential well slightly. We find that the strength of the perpendicular magnetic field needed for the spin singlet–triplet transition of the ground state of the QD confined by a bowl-like potential is reduced drastically by applying an in-plane electric field.

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Recently much attention has been paid to quantum dots (QDs),[1−3] referred to as the "artificial atoms", and quantum-dot molecules (QDMs) consisting of two or more coupled QDs laterally or vertically. The properties of QDs and QDMs have been studied extensively in both experiments[4−7] and theoretical calculations.[8−12] The most striking feature of two-dimensional semiconductor QDs and QDMs is that the correlation and magnetic field effects are greatly enhanced compared with their normal counterparts, due to their much larger sizes. A very interesting property of two-electron (2e) QDs is the spin singlet–triplet transition of the ground state.[13] Wagner *et al.*[14] predicted theoretically the spin singlet–triplet transition of the ground state of two interacting electrons in a harmonic QD in a perpendicular magnetic field for the first time. The transition between singlet and triplet states in few-electron QDs has been demonstrated in a "vertical" device,[15] and was attributed to the level crossings induced by a magnetic field. In addition to the interesting and fundamental correlation and quantum effects, a tunable transition from a singlet to a triplet ground state, i.e. the control of the exchange splitting relative to the single-particle splitting, is of interest in view of possible quantum computing applications.[16] Therefore, QDs and QDM are very important as candidates for the gate of a solid state quantum computer. A central idea is to use the total spin S of the ground state in QDs and QDM as a qubit.[10,11,17,18]

Recently, Devis *et al.*[19] investigated competitation mechanisms for the singlet–triplet transition in artificial molecules induced by a magnetic field. Kyriakidis *et al.*[20] have shown that such a transition may also be induced by shape deformations of the potential when tuning the gate voltage in laterally defined few-electron QDs. They inferred that the critical magnetic field could be tuned with a gate voltage by introducing nonparabolicity in the confining potential well. Kogan *et al.*[21] demonstrated experimentally that in the Kondo regime, there is a singlet–triplet transition as the shape of the confining potential is varied at zero magnetic field. Chung *et al.*[22] investigated the triplet-singlet transition in a two-dimensional parabolic quantum dot with disorders, which induce the confining potential not to be of a perfect parabolic shape. The shape of the confining potential may affect the electronic structure of quantum dots considerably. In this Letter, we employ this idea and concentrate on 2e 2D QDs confined by triangular[23] or bowl-like[24] potentials in a perpendicular magnetic field with an in-plane electric field. In the framework of effective mass approximation, the energy spectra of the 2e 2D QDs confined by both the potentials are studied with the help of the exact diagonalization method. The spin singlet–triplet transitions of the ground states in these systems are investigated as a function of external magnetic field strength. An in-plane electric field is found to contribute to the singlet–triplet transition of the ground state of the 2e 2D QDs confined by triangular or bowl-like potentials, modulated by a perpendicular magnetic field. The stronger the in-plane electric field, the smaller the magnetic field for the total spin of the ground states in these systems to change from $S = 0$ to $S = 1$. However, the influence of an in-plane electric field on the singlet–triplet transition of the ground state of two electrons in a triangular QD in

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a perpendicular magnetic field is quite small. Nevertheless, we find that the strength of the perpendicular magnetic field needed for the spin singlet–triplet transition of the ground state of the QD confined by a bowl-like potential is reduced drastically by applying an in-plane electric field. Our calculated results might be useful for the applications of quantum dots in future quantum computation and quantum information technologies.

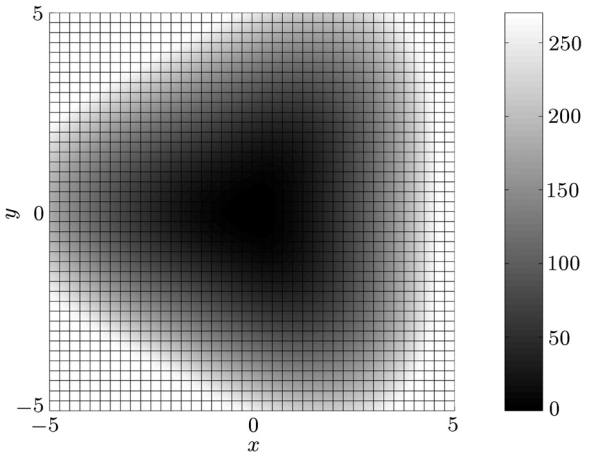

Fig. 1. Schematic diagram of a triangular confinement potential.

Firstly, we consider two electrons, each with an effective mass m^* in the $z = 0$ plane in a 2e 2D QD, in which each electron is confined by a two-dimensional triangular potential[23] (as shown in Fig. 1),

$$V_i(r_i, \theta_i) = \frac{1}{2} m^* \omega_0^2 r_i^2 \Big(1 + \frac{2}{7}\cos(3\theta_i)\Big), \tag{1}$$

where r_i and θ_i are the radius vector and the polar angle of each electron in polar coordinates, respectively. Additionally a perpendicular magnetic field B is applied along the z-axis while an in-plane electric field F along the x-axis. Therefore, the total Hamiltonian of the system can be given by

$$H = \sum_{i=1}^{2} \frac{\Big(\boldsymbol{P}_i - \frac{e}{c}\boldsymbol{A}\Big)^2}{2m^*} + \sum_{i=1}^{2} V_i(r_i, \theta_i) - \sum_{i=1}^{2} eFx_i + \frac{e^2}{\kappa|\boldsymbol{r}_1 - \boldsymbol{r}_2|}, \tag{2}$$

where $\kappa = 4\pi\epsilon_0\epsilon_r$ and $\boldsymbol{A}$ is the vector potential of the magnetic field (along the z-axis) taken in the symmetric gauge $\Big(\boldsymbol{A} = \frac{1}{2}\boldsymbol{B} \times \boldsymbol{r} = \frac{1}{2}B[-y, x, 0]\Big)$. The total Hamiltonian can be separated into three parts,

$$H = H_0 + H' + \frac{e^2}{\kappa|\boldsymbol{r}_1 - \boldsymbol{r}_2|},$$
$$H' = \sum_{i=1}^{2} \frac{1}{2} m^* \omega_0^2 r_i^2 \frac{2}{7}\cos(3\theta_i), \tag{4}$$

where H' is the perturbation Hamiltonian and H_0 is exactly the Hamiltonian of a 2e 2D QD confined by a circular harmonic well in a perpendicular magnetic field together with an in-plane electric field, without the Coulomb interaction between the two electrons,

$$H_0 = \sum_{i=1}^{2} H_i - eF\sum_{i=1}^{2} x_i, \tag{5}$$
$$H_i = \frac{p_i^2}{2m^*} + \frac{1}{2}m^*\Big(\omega_0^2 + \frac{1}{4}\omega_c^2\Big)r_i^2 - \frac{1}{2}\omega_c l_{zi}. \tag{6}$$

The eigenstates of H_i are the well-developed Fock–Darwin states. Similar to Eq. (3) in Ref. [11], the full many-body wave function with total spin S of the triangular QD can be expanded as[11]

$$\Psi_S(r_1, r_2) = \sum_{i\le j} \alpha_{ij}\{\phi_i(r_1)\phi_j(r_2) + (-1)^S\phi_i(r_2)\phi_j(r_1)\}, \tag{7}$$

where α_{ij} is the coefficient vector. One can find that it is symmetric for $S = 0$ and antisymmetric for $S = 1$ according to the Pauli exclusion principle. The energy spectra of the ground state of the 2e2D QD confined by a triangular potential well in a magnetic field can be calculated by exact diagonalization. We have checked the convergence by varying the number of basis functions and found that it is sufficient to obtain the energy eigenvalues of the total Hamiltonian (3) by taking the wave functions of the lowest six single-particle states as the basis functions in exact diagonalization. We use the material parameters of usual GaAs, i.e., electron effective mass $m^* = 0.067m_0$ and effective dielectric constant $\epsilon_r = 12.7$ in our calculation.

As illustrated in Fig. 2, a circular bowl-like confinement potential[24] is given by

$$V_i(\boldsymbol{r}_i) = \begin{cases} \frac{1}{2}m^*\omega_0^2 r_i^2, & r_i \leqslant r_0, \\ V_0, & r_i > r_0. \end{cases} \tag{8}$$

The Hamiltonian of the 2e 2D QD confined by this potential in a perpendicular magnetic field and an in-plane electric field reads

$$H = \sum_{i=1}^{2} \frac{\Big(\boldsymbol{p}_i - \frac{e}{c}\boldsymbol{A}\Big)^2}{2m^*} + \sum_{i=1}^{2} V_i(\boldsymbol{r}_i) - \sum_{i=1}^{2} eF(x_i + y_i) + \frac{e^2}{\kappa|\boldsymbol{r}_1 - \boldsymbol{r}_2|}, \tag{9}$$

which can also be divided into three parts,

$$H = H_0 + H' + \frac{e^2}{\kappa|\boldsymbol{r}_1 - \boldsymbol{r}_2|}, \tag{10}$$
$$H_0 = \sum_{i=1}^{2} H_i - eF\sum_{i=1}^{2}(x_i + y_i), \tag{11}$$

$$H' = \begin{cases} 0, & r_1 \leqslant r_0, r_2 \leqslant r_0, \\ V_0 - \dfrac{1}{2}m^*\omega_0^2 \boldsymbol{r}_2^2, & r_1 \leqslant r_0, r_2 > r_0, \\ V_0 - \dfrac{1}{2}m^*\omega_0^2 \boldsymbol{r}_1^2, & r_1 > r_0, r_2 \leqslant r_0, \\ 2V_0 - \dfrac{1}{2}m^*\omega_0^2(\boldsymbol{r}_1^2 + \boldsymbol{r}_2^2), & r_1 > r_0, r_1 > r_0, \end{cases} \tag{12}$$

where H' is the perturbation Hamiltonian and H_0 is exactly the Hamiltonian of the 2e 2D QD confined by a circular harmonic well in a magnetic field and an in-plane electric field. The eigenstates and eigenenergies of H_0 can be calculated analytically. Then the full many-body wave function of two electrons in the bowl-like QD can be expanded with those eigen functions of H_0. By diagonalizing the Hamiltonian[10] the energy spectrum of the 2e 2D QD confined by the bowl-like potential is obtained numerically.

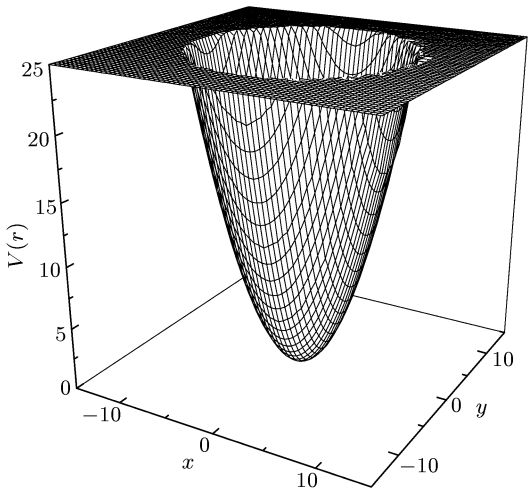

Fig. 2. Schematic diagram of a bowl-like confinement potential.

For the 2e 2D QD confined by a triangular potential shown in Fig. 1, the energy split between the triplet ($S = 1$) and singlet ($S = 0$) ground states ΔE as a function of the magnetic field without an in-plane electric field ($F = 0 \times 10^5$(V/m)) is illustrated in Fig. 3. Comparing with the energy difference between triplet and singlet ΔE of the circular 2e 2D QD confined by a parabolic potential,[11] we find the similar behaviour at the weak magnetic field, but different behaviour at the strong magnetic field, i.e. the ground state of the 2e 2D triangular QD remains the triplet state at high magnetic field. For weak magnetic field, the ground state of the system is the spin singlet $S = 0$. The ground state spin is flipped to $S = 1$ at the crossing point of $B = 8.85T$ as the strength of the magnetic field increases. The spin singlet–triplet transition of the ground state in this 2e 2D triangular quantum dot is also involved with the several lowest energy levels of the noninteracting single particle. Due to the smaller deformation of the triangular potential, compared with the circular parabolic potential at the frequency of harmonic potential $\omega_0 = 6$ meV, the single particle states of the triangular QD are similar to the Fock–Darwin states. The several lowest single particle energy levels group together to form the lowest Landau level as the magnetic field increases. The difference between the two lowest single particle states becomes smaller than the exchange energy, and the system spin-polarizes.[11] For the strong magnetic field, the energy split ΔE becomes smaller and the spin of the ground state remains $S = 1$. The influence of an in-plane electric field on the spin singlet–triplet transition of the ground state of the triangular QD in a magnetic field is also shown in Fig. 3. The crossing points of ΔE with the x axis in Fig. 3 for different electric fields are very close to each other because the triangular confinement potential deviates just slightly from the harmonic potential well. This means that we can use the ground states with total spin $S = 0$ and $S = 1$ of the triangular QD to construct a magnetic-field-modulated qubit. However, a fairly strong magnetic field is needed to control the singlet–triplet transition no matter what the strength of the in-plane electric field is.

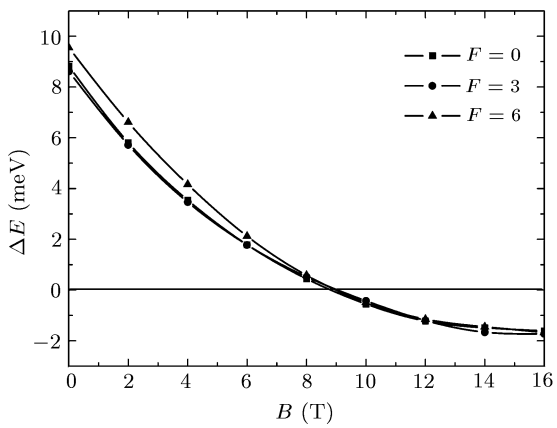

Fig. 3. Energy difference between triplet ($S = 1$) and singlet($S = 0$) ground states ΔE of a two-electron two-dimensional QD confined by a triangular potential as a function of the magnetic field B in the presence of the in-plane electric field $F = 0, 3, 6 \times 10^5$(V/m).

For a bowl-like confinement potential shown in Fig. 2, the energy spectra of the 2e 2D QDs confined by this circular bowl-like potential in a perpendicular magnetic field are investigated by the exact diagonalization. In this study the circular-parabolic confinement potential of the QDs is cut off at $r_0 = 5a^*$, jointed by a constant potential $V_0 = 1/2m^*\omega_0^2 r_0^2$. For different in-plane electric fields, the energy differences ΔE between triplet ($S = 1$) and singlet ($S = 0$) ground states as a function of the magnetic field B are plotted in Fig. 4. Without the in-plane electric field, the ground state spin switches from $S = 0$ to $S = 1$ at the crossing point of $B = 8.9$ T as the strength of magnetic field increases. When applying an electric field parallel to the $x-y$ plane on the bowl-like QD, we find that the crossing point of the singlet–triplet transition

of the ground state of the system is reduced drastically. This is mainly due to the squeeze of the wave functions of two electrons in QD. When the electric field is increased, two electrons are pushed to be closer to each other, which increases the Coulomb interaction between two electrons. The equilibrium between the Coulomb interaction and the in-plane electric field will reach, as the electric field becomes strong enough. The wave functions of two electrons may overflow the bowl-like confinement potential of the QD. However, the wave functions of two electrons in QD confined by the triangular potential can hardly overflow the confinement potential because the triangular confinement potential deviates just slightly from the parabolic potential well and the in-plane electric field just pushes two electrons together and makes them a displacement. The stronger the in-plane electric field, the smaller the magnetic field for the total spin of the ground state in the QD confined by the bowl-like confinement potential to change from $S = 0$ to $S = 1$. For the electric field $F = 3 \times 10^5$(V/m) and $F = 6 \times 10^5$(V/m), the crossing points are at 8.5 and 4.8 T, respectively. This means that we can control the spin singlet–triplet transition of the ground state of the QD confined by a bowl-like potential in a perpendicular magnetic field by applying an in-plane electric field. In addition, this implies that the 2e 2D QD confined by a bowl-like potential is more promising as a candidate for the gate of a quantum computer. Our theoretical results may be useful for those experimental works on the singlet–triplet transition of the ground state of asymmetric QDs and QDM.

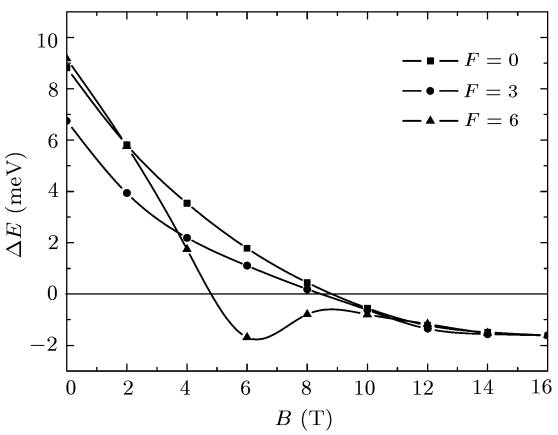

Fig. 4. Energy difference ΔE between the triplet ($S = 1$) and singlet ($S = 0$) ground states of the two-electron two-dimensional QD confined by a bowl-like potential as a function of the magnetic field B in the presence of the in-plane electric field $F = 0, 3, 6 \times 10^5$(V/m).

In summary, we have investigated theoretically the electronic structure of the 2e 2D QDs confined by a triangular potential or a bowl-like potential in a magnetic field. The energy spectra of the 2e 2D QDs in these potentials are studied by exact diagonalization within the framework of effective mass theory. The total spin $S = 0$ and $S = 1$ of the ground state in these systems is also found as a function of external magnetic field strength. An in-plane electric field is found to contribute to the spin singlet–triplet transition of the ground state of 2e 2D QDs confined by triangular or bowl-like potentials in a perpendicular magnetic field. The stronger the in-plane electric field, the smaller the magnetic field needed for the total spin of the ground states in the dot systems to change from $S = 0$ to $S = 1$. However, the influence of an in-plane electric field on the singlet–triplet transition of the ground state of two electrons in a triangular QD is quite small because the triangular potential just slightly deviates from the harmonic potential well. However, we find that the crossing point of the singlet–triplet transition of the ground state of the QD confined by the bowl-like potential is reduced drastically by applying in-plane electric fields. This implies that these magnetic-field-modulated 2e 2D QDs, confined by triangular or bowl-like potentials can be exploited as a prototypical solid state system, are important as candidates for the gate of a quantum computer.

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