Symmetry and size effects on energy and entanglement of an exciton in coupled quantum dots*

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(Received 6 August 2012; revised manuscript received 16 October 2012)

We study theoretically the essential properties of an exciton in vertically coupled Gaussian quantum dots in the presence of an external magnetic field. The ground state energy of a heavy-hole exciton is split into four energy levels due to the Zeeman effect. For the symmetrical system, the entanglement entropy of the exciton state can reach a value of 1. However, for a system with broken symmetry, it is close to zero. Our results are in good agreement with previous studies.

Keywords: exciton, coupled Gaussian quantum dot, symmetry, entanglement entropy

PACS: 71.35.Ji, 73.21.La, 73.22.Gk **DOI:** 10.1088/1674-1056/22/4/047101

1. Introduction

A system consisting of coupled quantum dots (CQDs) is called an artificial molecule.[1–3] CQDs are interesting because they lead to the appearance of additional spectral lines. Moreover, they are very useful because of their potential applications not only in quantum device design, but also in the currently active field of quantum information processing.[4–7] It has been proposed that quantum bits (qubits) can be represented by either electron spin states[8–10] or exciton states.[11,12] Since the entanglement of qubits plays an important role in quantum communication and quantum computation, it is essential to study entanglement in these systems.[9,13] For exciton states, Bayer *et al.*[12,14] have theoretically predicted that there is a large entanglement in symmetric CQDs. However, in a system with broken symmetry, which may be induced by strain or alloy fluctuation,[15,16] the entanglement of exciton states has been found to be very small for both small and large inter-dot distances. Several experiments on optical signatures[12,17–19] and several theoretical studies[15,16,20] have been devoted to determining the effects of system asymmetry and external field on exciton entangled states.

In this paper, we report on exciton states with emphasis on the energy of the radiative interband transition, the binding energies, and the behavior of entanglement in CQDs in the presence of an external magnetic field. By optimizing the structural and band parameters of the CQDs, the behavior of the entanglement can be modulated, which is important for producing a stable and controllable quantum information process. This will lead to a better understanding on the properties and the applications of the exciton in low-dimensional semiconductor systems and quantum computation.

2. Theoretical model

In our model, an exciton is located in the CQDs. The lateral confinement potential in the xy plane is assumed to be a harmonic oscillator configuration. Such a parabolic lateral confinement is known to mimic most of the important features of various self-assembled quantum dots (QDs) and gives results that are in good agreement with those of experiments.[9,19] Along the longitudinal direction, i.e., the z direction, the external magnetic field is applied, and the carriers are confined by the Gaussian potential that is based on the Gaussian distribution of indium concentration

$$X(z_i) = X_0 \exp\left(-(z_i - a/2)^2/{Z_1}^2\right) + X_0 \exp\left(-(z_i + a/2)^2/{Z_2}^2\right), \quad (1)$$

where $i =$ e, h, and X_0 is the indium concentration at the center of the dot, a is the distance between the centers of the two QD's, and Z_1 (Z_2) is the half thickness of the right (left) QD. In Fig. 1, the geometry of the CQDs along the z direction and the shape of the Gaussian potential are shown schematically. When Z_1 is equal to Z_2, the system is symmetrical. Otherwise, the symmetry is destroyed. The wetting-layer thickness is expressed as T_{WL}, the barrier thickness is defined as $t = a - Z_1 - Z_2$, and the spacer thickness is given

*Project supported by the National Natural Science Foundation of China (Grant Nos. 61176089 and 10905016) and the Natural Science Foundation of Hebei Province, China (Grant Nos. A2011205092 and A2011208010).

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by $d = t + 2Z_2 - T_{\rm WL}$. The conduction-valence-band offset ratio for the InAs/GaAs interface has been estimated to be 70/30.[21] Therefore, we can take the longitudinal confinement potential to be parameterized as follows:

$$V_{\rm e}(z_{\rm e}) = -0.7\triangle E_{\rm g} X(z_{\rm e}) \tag{2}$$

for the electron and

$$V_{\rm h}(z_{\rm h}) = -0.3\triangle E_{\rm g} X(z_{\rm h}) \tag{3}$$

for the hole, where $\triangle E_{\rm g} = E_{\rm g}^{\rm GaAs} - E_{\rm g}^{\rm InAs}$, with $E_{\rm g}^{\rm GaAs}$ and $E_{\rm g}^{\rm InAs}$ being the GaAs and InAs energy gaps, respectively. For the sake of simplicity, we neglect the dielectric constant discontinuity and the effective-mass mismatch in the dot and the barrier materials. The Hamiltonian is given by

$$\begin{aligned} H_{\rm X} =& \frac{1}{2m_{\rm e}^*}\left(\boldsymbol{P}_{\rm e} + \frac{e}{c}\boldsymbol{A}\right)^2 + \frac{1}{2m_{\rm h}^*}\left(\boldsymbol{P}_{\rm h} - \frac{e}{c}\boldsymbol{A}\right)^2 \\ &+ \frac{1}{2}m_{\rm e}^*\omega_{\rm e}^2(x_{\rm e}^2 + y_{\rm e}^2) + \frac{1}{2}m_{\rm h}^*\omega_{\rm h}^2(x_{\rm h}^2 + y_{\rm h}^2) \\ &+ V_{\rm e}(z_{\rm e}) + V_{\rm h}(z_{\rm h}) - \frac{e^2}{\varepsilon r_{\rm eh}} \\ &+ \mu_{\rm B} g_{\rm e}^* \boldsymbol{B}\cdot\boldsymbol{S}_{\rm e} - \mu_{\rm B} g_{\rm h}^* \boldsymbol{B}\cdot\boldsymbol{S}_{\rm h}, \end{aligned} \tag{4}$$

where $m_{\rm e}^*$ ($m_{\rm h}^*$) is the effective mass of the electron (hole) in the conduction (valence) band; $\boldsymbol{A}$ is the vector potential of the magnetic field, which can be written as $\boldsymbol{A} = \boldsymbol{B}\times\boldsymbol{r}/2$ in the Coulomb gauge; $\omega_{\rm e}$ ($\omega_{\rm h}$) is the harmonic oscillator frequency for the electron (hole); ε is the dielectric constant; $r_{\rm eh} = \sqrt{(x_{\rm e}-x_{\rm h})^2 + (y_{\rm e}-y_{\rm h})^2 + (z_{\rm e}-z_{\rm h})^2}$ is the separation between the electron and hole. The last two terms are the Zeeman energies, which describe the interaction between the spins of the carriers and the magnetic field. Here $\mu_{\rm B}$ is the Bohr magneton, $g_{\rm e}^*$ ($g_{\rm h}^*$) is the electron (hole) effective gyromagnetic ratio, and $\boldsymbol{S}_{\rm e}$ ($\boldsymbol{S}_{\rm h}$) is the spin vector operator of the electron (hole).

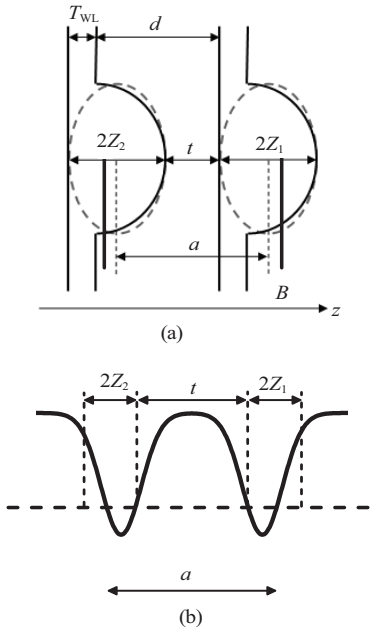


Fig. 1. Schematic illustration of the CQDs. Plot (a) shows the geometry of the CQDs, and the dashed line shows the contour of the indium-concentration Gaussian distribution function. Plot (b) gives the profile of the confinement potential in the growth direction.

With the one-dimensional effective potential model,[22,23] we can obtain the one-dimensional effective Hamiltonian for the lowest energy states

$$\begin{aligned} H_{\rm X}^{\rm eff} =& E_{\rm e} + E_{\rm h} - \frac{\hbar^2}{2m_{\rm e}^*}\frac{\partial^2}{\partial z_{\rm e}^2} - \frac{\hbar^2}{2m_{\rm h}^*}\frac{\partial^2}{\partial z_{\rm h}^2} \\ &+ V_{\rm e}(z_{\rm e}) + V_{\rm h}(z_{\rm h}) - V_{\rm eff}(z_{\rm e} - z_{\rm h}) \\ &+ \mu_{\rm B} g_{\rm e}^* B S_{\rm ez} - \mu_{\rm B} g_{\rm h}^* B S_{\rm hz}, \end{aligned} \tag{5}$$

where

$$E_{\rm e} = \hbar\sqrt{e_{\rm s}^2 B^2/4m_{\rm e}^{*2}c^2 + \omega_{\rm e}^2}$$

and

$$E_{\rm h} = \hbar\sqrt{e_{\rm s}^2 B^2/4m_{\rm h}^{*2}c^2 + \omega_{\rm h}^2}$$

are the ground state energies of the single electron and the single hole in xy plane, respectively;

$$\begin{aligned} V_{\rm eff}(z_{\rm e} - z_{\rm h}) =& \frac{e_{\rm s}^2\sqrt{\pi}}{\varepsilon\sqrt{\dfrac{\hbar}{m_{\rm e}^*\sqrt{e_{\rm s}^2B^2/4m_{\rm e}^{*2}c^2 + \omega_{\rm e}^2}} + \dfrac{\hbar}{m_{\rm h}^*\sqrt{e_{\rm s}^2B^2/4m_{\rm h}^{*2}c^2 + \omega_{\rm h}^2}}}} \\ &\times {\rm erfcx}\left(\frac{|z_{\rm e} - z_{\rm h}|}{\sqrt{\dfrac{\hbar}{m_{\rm e}^*\sqrt{e_{\rm s}^2B^2/4m_{\rm e}^{*2}c^2 + \omega_{\rm e}^2}} + \dfrac{\hbar}{m_{\rm h}^*\sqrt{e_{\rm s}^2B^2/4m_{\rm h}^{*2}c^2 + \omega_{\rm h}^2}}}}\right) \end{aligned} \tag{6}$$

is the one-dimensional effective Coulomb interaction potential, here

$${\rm erfcx}(x) = \exp(x^2){\rm erfc}(x) = \frac{2}{\sqrt{\pi}}\exp(x^2)\int_x^\infty \exp(-t^2)\,{\rm d}t$$

is the exponentially scaled complementary error function.

The exciton energy eigenvalue $E_{\rm X}$ is used to determine the energy of the radiative interband transition $E_t = \triangle E_{\rm g} + E_{\rm X}$, and the ground state binding energy $E_{\rm X}^B = E({\rm e}) + E({\rm h}) - E_{\rm X}$ ($E({\rm e})$ and $E({\rm h})$ are the energies of an electron and a hole in the CQDs, respectively).

For two distinguishable particles, their entanglement is quantified by the von Neumann entropy,

$$S(\rho_{\rm e}) = -{\rm tr}(\rho_{\rm e} \log_2 \rho_{\rm e}), \tag{7}$$

where $\rho_{\rm e} = {\rm tr}_{\rm h}|\Psi(\boldsymbol{r}_{\rm e}, \boldsymbol{r}_{\rm h})\rangle\langle\Psi(\boldsymbol{r}_{\rm e}, \boldsymbol{r}_{\rm h})|$ is the reduced density matrix of the electron ($|\Psi(\boldsymbol{r}_{\rm e}, \boldsymbol{r}_{\rm h})\rangle$ is the wave function of the exciton). The non-zero von Neumann entropy indicates the existence of entanglement between the positions of the electron and the hole.

3. Results and discussion

In our calculation, we have chosen parameters appropriate for InAs QDs in a GaAs matrix: $m_{\rm e}^* = 0.0404 m_0$, $m_{\rm h}^* = 0.350 m_0$, where m_0 is the free electron mass. $g_{\rm e}^* = -0.81$, $g_{\rm h}^* = -0.74$, $X_0 = 0.67$, $T_{\rm WL} = 0.54$ nm, $E_{\rm g}^{\rm GaAs} = 1.5196$ eV, $E_{\rm g}^{\rm InAs} = 0.4105$ eV, $\hbar\omega_{\rm e} = \hbar\omega_{\rm h} = 212.5$ meV, and $\varepsilon = 15.0$.[19,24] The z component of the spin angular momentum of the electron is $\pm 1/2$. Accordingly, the spin of the heavy hole takes on values of $\pm 3/2$. We have used a mesh of 500×500 grid points to guarantee the precision.

Figure 2 shows the changes in the exciton energies in the symmetric system as functions of various system parameters. In Fig. 2(a), the dependence of the exciton ground state energies on the magnetic field is given for the case $d = 6$ nm and $Z_1 = Z_2 = 0.92$ nm. We can see that there is a fourfold degeneracy in the energy at $B = 0$ that is lifted when the magnetic field is nonzero. This is because of the Zeeman interaction between the exciton spin and the magnetic field. When the spin orientations are $S_{\rm ez} = 1/2$ and $S_{\rm hz} = -3/2$, the Zeeman splitting yields the lowest exciton energy level. Figure 2(b) shows the dependence of the radiative transition energies on the spacer thicknesses and compares the results with experimental data extracted from Ref. [18]. It may be seen that the calculated transition energies agree very well with the measured positions of the photoluminescence lines. With decreasing interdot distance the exciton recombination lines exhibit a clear red shift. This is because the exciton energy decreases with decreasing spacer thicknesses. This is due mainly to the reduction in the quantum confinement of the electron and the hole. Figure 2(c) shows the ground state binding energies of the exciton as a function of the interdot barrier thickness t. The binding energies first decrease and then increase. This is because for small barrier thicknesses the tunneling of the carriers is very strong, and the coupled Gaussian potential is thus similar to a single quantum well. As a result, the larger t is, the smaller the binding energy, until a minimum occurs. For the case in which t is fixed, the smaller $Z_1(Z_2)$ is, the stronger the spacial confinement is and the larger the binding energy is.

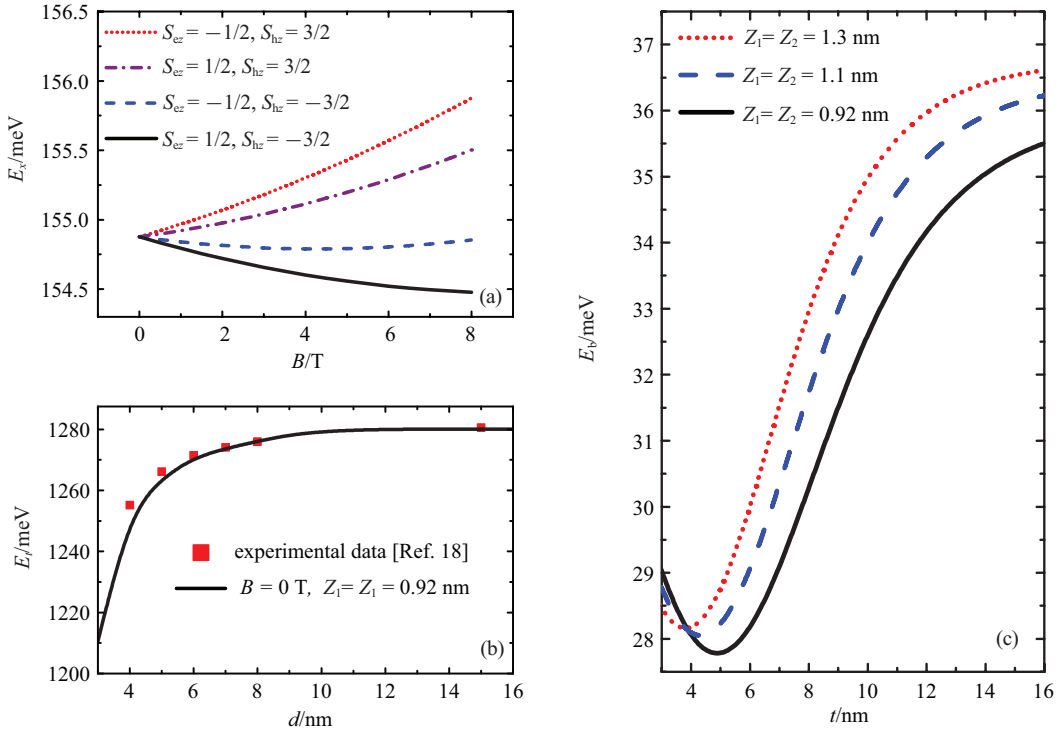


Fig. 2. (color online) In the symmetric system, (a) ground state energies of the exciton as a function of the magnetic field for $d = 6$ nm and $Z_1 = Z_2 = 0.92$ nm; (b) radiative transition energies as a function of the spacer thicknesses for $B = 0$ T and $Z_1 = Z_2 = 0.92$ nm, compared with experimental data extracted from Ref. [18]; (c) binding energies as a function of the interdot barrier thickness for $B = 8$ T.

Continuing to increase the barrier thickness, the tunneling of the carriers decreases and the electron and the hole more easily locate in the same QD, which leads to enhancement of the binding energy. For fixed t, a smaller value of $Z_1(Z_2)$ results in stronger tunneling of the carriers, i.e., the probability of the electron and the hole being located in different QDs increases, which increases the average distance between the electron and the hole and decreases the binding energy.

In Fig. 3(a) the entanglement entropies of the exciton as a function of the barrier thickness in symmetric CQDs are plotted. It can be seen that the entanglement entropies increase monotonically with increasing barrier thickness and for the same barrier thickness, the larger the QD's thickness, the stronger the entanglement. To facilitate understanding of the physical reasons for these relationships, in Fig. 3(b) we plot the wave function distributions of the exciton for four representative barrier thicknesses. For $t = 2.7$ nm, the exciton state is composed of the intradot states $|00\rangle$ and $|11\rangle$ and the interdot states of $|01\rangle$ and $|10\rangle$ in almost equal proportions. Note that in this representation, the first (second) index of $|ij\rangle$ gives the position of the electron (hole), and "0" represents the left QD and "1" represents the right one.

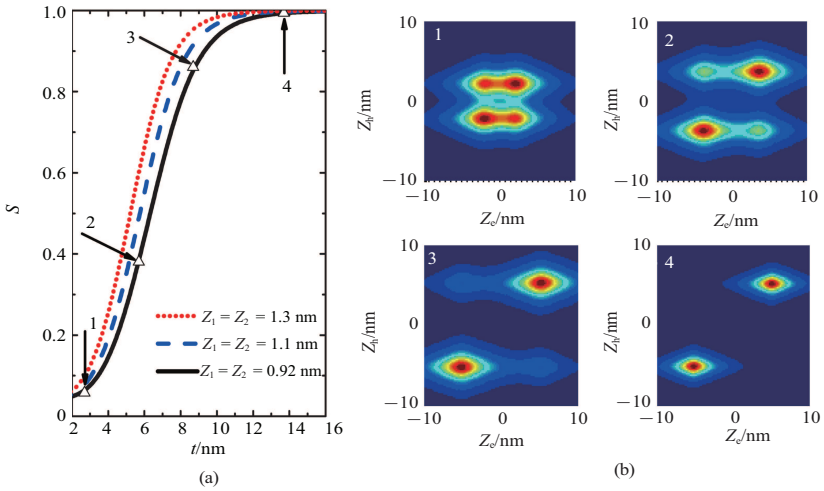


Fig. 3. (color online) (a) Entanglement entropy of the exciton as a function of the interdot barrier thickness in symmetric CQDs with $B = 8$ T. Part (b) shows the wave function of the exciton as a function of the electron and hole coordinates for the four locations marked in part (a).

In this case, the exciton state is close to the unentangled state $(|00\rangle + |10\rangle + |01\rangle + |11\rangle)/2$, so its von Neumann entropy is very small. With increasing barrier thickness, the tunneling of the carriers gradually weakens. The Coulomb attractive interaction makes the electron and the hole more and more likely to occupy the intradot states $|00\rangle$ and $|11\rangle$. That is to say, the exciton states gradually approach the "Bell states" $(|00\rangle \pm |11\rangle)/\sqrt{2}$. When $t > 15$ nm, the probability of the exciton being located in the interdot states $|01\rangle$ and $|10\rangle$ is almost 0; the entanglement entropy is 1 and "Bell states" emerge. These results are in agreement with the theoretical prediction that there is large entanglement within a symmetrical model for the exciton[12,14] and offers the theoretical proof for the design and application for quantum computation.

However, for the asymmetrical CQDs the entanglement of the exciton state is very small, as can be seen from Fig. 4.

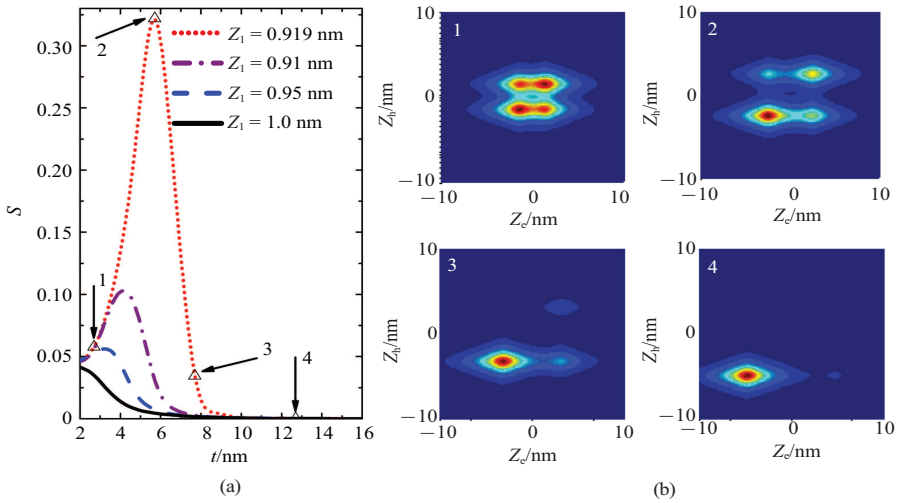


Fig. 4. (color online) (a) Entanglement entropy of the exciton as a function of the interdot barrier thickness in asymmetrical CQDs with $Z_2 = 0.92$ nm and $B = 8$ T. The symbols and part (b) have the same meaning as those in Fig. 3.

Even though the difference of two QDs' thicknesses is only 0.001 nm, the entanglement entropy changes to a great extent. Comparing with symmetrical CQDs, we see from Fig. 4(b) that with the increasing barrier thickness the electron and the hole both tend to occupy the wider QD, i.e., the exciton state principally contains the $|11\rangle$ state. The $|11\rangle$ state is completely unentangled, so its entanglement is zero for the large barrier thickness. These results are consistent with Ref. [15].

4. Conclusion

In conclusion, we have investigated a number of essential properties of exciton states in CQDs under the influence of an applied magnetic field, including the ground state energies, the radiative transition energies, the entanglement, and the wave function distributions. The numerical results indicate that symmetry and size have significant influence on the energy and entanglement of an exciton in CQDs. Our results are in good agreement with previous studies. We hope our results are helpful in designing and fabricating practical quantum computer devices.

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