Signature of symmetry of laterally coupled quantum dots in far-infrared spectrum*

Gu Li-Ying(谷利英)[a], Li Yan-Fang(李艳芳)[a)b)†],
Chu Wei-Dong(楚卫东)[b], and Wei Ying-Hui(卫英慧)[a]

[a] *College of Materials Science and Engineering, Taiyuan University of Technology, Taiyuan* 030024, *China*
[b] *Institute of Applied Physics and Computational Mathematics, Beijing* 100088, *China*

(Received 31 March 2011; revised manuscript received 21 June 2011)

We study the effect of structure asymmetry on the energy spectrum and the far-infrared spectrum (FIR) of a lateral coupled quantum dot. The calculated spectrum shows that the parity break of coupled quantum dot results in more coherent superpositions in the low-lying states and exhibits unique anti-crossing in the two-electron FIR spectrum modulated by a magnetic field. We also find that the Coulomb correlation effect can make the FIR spectrum of coupled quantum dot without strict parity deviate greatly from Kohn theorem, which is just contrary to the symmetric case. Our results therefore suggest that FIR spectrum may be used to determine the symmetry of coupled quantum dot and to evaluate the degree of Coulomb interaction.

Keywords: structure symmetry, far-infrared spectrum, coupled quantum dot, Coulomb interaction

PACS: 73.21.La, 75.75.–c, 78.40.Fy **DOI:** 10.1088/1674-1056/21/2/027301

1. Introduction

In recent years, the coupled quantum dot (CQD), generally called QD molecule (QDM), has been one of the most interesting systems in nano-meter science.[1−5] In such a system, optical and transport properties related to the control of quantum coherent state have been studied experimentally and theoretically. In the optics and the electronics of CQDs, energy level mixing and superposition of states are key quantum properties. By varying external parameters, for example, by varying magnetic or electrical field, one can control several energy levels into proximity. Then, depending on the characteristics of the resonance point, quantum coherent superposition possibly occurs and shows level anti-crossing.[4−8]

The geometric symmetry of a CQD is one of the key factors which influences the coherent property of electron state at a resonance point. For high symmetric CQD whose wave function has a strict parity, the property of the resonance point is determined by the parity of quantum state. If the approaching levels have the same (opposite) parities, they will show anti-crossing crossing. However, most real CQDs hardly consist of identical QDs and then do not possess strict parities. The broken parity will greatly change the electron behaviour at a resonance point, which has been observed experimentally.[5] In the present paper, using the variation-diagonalization method,[9] we present the electronic structure and FIR spectrum of a CQD consisting of two laterally coupled QDs. By setting the two dots with different sizes, we investigate the effect of the broken parity of CQD on the magnetic-field-modulated coherent superposition of electron states. We find that the signature of lowered symmetry of CQD can be clearly shown as anti-crossing in the FIR spectrum. Furthermore, the feature of anti-crossing is closely related to the Coulomb interaction between electrons. Our results are useful to study the quantum control based on CQDs.

2. Hamitonian and formula

The Hamiltonian of two electrons in a two-dimensional laterally CQD with a magnetic field perpendicular to the plane of the dot can be written as

$$H = H_{\rm e1} + H_{\rm e2} + \frac{e^2}{4\pi\varepsilon_0\varepsilon_r\,|\boldsymbol{r}_{\rm e1} - \boldsymbol{r}_{\rm e2}|}, \qquad (1)$$

*Project supported by the National Natural Science Foundation of China (Grant No. 11074025), the National Basic Research Program of China (Grant No. 2011CB922200), and a grant from the China Academy of Engineering Physics.
†Corresponding author. E-mail: liyf1230@sohu.com
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where H_{e1} and H_{e2} are the single-electron Hamiltonian

$$H_e = \frac{\left(\boldsymbol{p} + \frac{1}{2}e\boldsymbol{B} \times \boldsymbol{r}_e\right)^2}{2m_e^*} + V_c\left(\boldsymbol{r}_e\right). \tag{2}$$

We employ the parabolic potential $V_c(\boldsymbol{r}_e)$ to describe the confinement of the coupled dots as

$$V_c = \min\left(\frac{1}{2}m_e^*\omega_1^2\left(\left(x - \frac{d}{2}\right)^2 + y^2\right)\right.$$
$$\left.\frac{1}{2}m_e^*\omega_2^2\left(\left(x + \frac{d}{2}\right)^2 + y^2\right)\right), \tag{3}$$

where ω_1, ω_2, and d are respectively the confinement strengths of the two dots and the distance between them. The radius of a QD can be defined by $R_i = \sqrt{\hbar/(m^*\omega_i)}$.

In order to obtain the eigenstate Φ_i of the single-electron Hamiltonian Eq. (1), we use the eigenstate of the trial Hamiltonian

$$H_{e0} = \frac{\left(\boldsymbol{p} + \frac{1}{2}e\boldsymbol{B} \times \boldsymbol{r}_e\right)^2}{2m_e^*} + V_0(\boldsymbol{r}_e),$$

where $V_0 = \frac{1}{2}m_e^*\alpha^2(x^2 + y^2)$ as a set of variational basis to diagonalize Eq. (2), with α being the variational parameter of the trial Hamiltonian. This is the so-called variational-diagonalization method[9] which is a powerful tool to obtain the eigenstates of coupled nanostructures.

Using the single-electron eigenstates of Eq. (2), we can construct the two-electron basis of spin singlets and triplets and then diagonalize the two-electron Hamiltonian Eq. (1) to obtain the two-electron eigenstate $|\,\Psi_i\rangle$ of CQD. In the electric-dipole approximation, optical absorption coefficient is proportional to transition intensity which can be calculated using the following formula:[10]

$$A \propto c\omega \sum_{ji} |\,\langle\Psi_f\,|\,\boldsymbol{e}\cdot\boldsymbol{d}\,|\,\Psi_i\rangle\,|^2\,\delta(\omega - \omega_{if})(F_i^0 - F_f^0), \tag{4}$$

where $\boldsymbol{e}$ is the complex polarization vector of external field, $\boldsymbol{d} = \boldsymbol{r}_1 + \boldsymbol{r}_2$ is the dipole operator of two electrons, F^0 is the Fermi distribution function of equilibrium state and $\omega_{if} = (E_f - E_i)/\hbar$. In the following discussion, we consider unpolarized light with two circular polarizations: left handed ω_- and right handed ω_+ with $\boldsymbol{e} = \sqrt{1/2}(\boldsymbol{e}_x \pm \mathrm{i}\,\boldsymbol{e}_y)$. In addition, for simplicity, we take absolute zero of temperature, i.e. $F_{i=G}^0 = 1$ and $F_f^0 = 0$.

3. Results and discussion

3.1. Parity and energy level structure

In our study, we consider a GaAs CQD and use material parameters $m_e^* = 0.067m_e$ and $\varepsilon_r = 12.4$. The dot size parameters are taken as $\omega_1 = \omega_2 = 3$ meV ($\omega_1 = 3$ meV and $\omega_2 = 3.5$ meV) for symmetric (asymmetric) CQD, which correspond to effective dot radius $R_1 = R_2 = 20$ nm ($R_1 = 20$ nm and $R_2 = 18.5$ nm).

For a lateral CQD, the absence of the rotational symmetry makes the angular momentum unconserved. However, each eigenstate has a definite parity if the CQD is formed by two identical dots.

We first discuss the relation between the symmetry of CQD and the single-electron energy spectrum. In Fig. 1 we plot the single-electron energy spectra with magnetic filed modulation and the some wave functions of symmetric and asymmetric CQDs. For the symmetric case, the parity of each single-electron state can be labeled by ±1, where $+1$ (-1) represents symmetric (anti-symmetric) state under spatial inversion. Because of the rotational symmetry of a uniform magnetic field, the modulation magnetic field does not change the parity of state, see the wave functions of Φ_3 with $B = 0$ and 2 T in the inset of Fig. 1(a). In Fig. 1(a), it is clearly seen that the parity of state determines the coherent property at the resonance point. Anti-crossing (such as $A_{2,6}$) appears as states with same parity encounter under the modulation of the field, which marks coherent superposition of states. In contrast, there are only possible crossings between the states (such as $C_{2,3}$) with different parities, which means that the coherent superposition cannot occur. For CQD consisting of non-identical dots, the electron wave function is lacking in space inversion symmetry, which can be seen in Fig. 1(b) as an example. Though the inversion symmetry is broken slightly, the symmetry-broken, which means that the lack of parity of the system can strongly change the coherent property at the resonance point as shown in Fig. 1(b). It is very obvious that all crossings will become anti-crossings due to the symmetry break. For example, $C_{2,3}$ in Fig. 1(a) becomes $A_{2,3}$ in Fig. 1(b) with considerable splitting. It can be seen that the influence of parity break on quantum coherent superposition in the CQD system is essential. Such an effect also exists in CQD with two electrons.

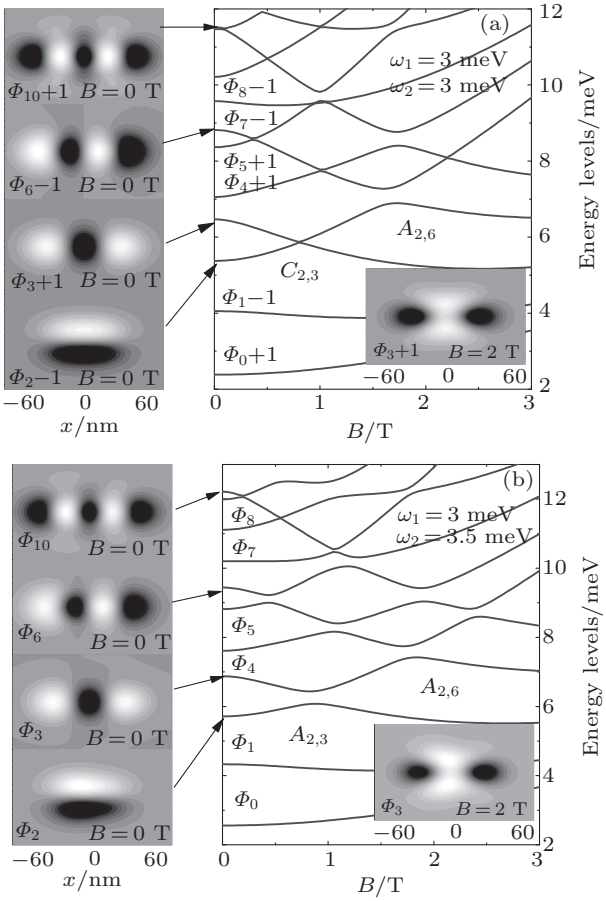


Fig. 1. Single-electron energy levels and several wave functions of symmetric (a) and asymmetric (b) coupled quantum dots in magnetic field. $\omega_{1,2}$ are the confinement strengths of the two dots. The signs + and − in (a) represent even and odd parities respectively.

For a symmetric CQD with two electrons, the system also has a definite parity because the inversion asymmetric Coulomb potential does not change the parity. A two-electron basis has an even (odd) parity if it is formed by the single-electron states with same (different) parities. Then the eigenstates of two electrons in a symmetric CQD will have an even (odd) parity if it is constructed by the basis with even (odd) parity. In Fig. 2, we show the energy spectra of singlets and triplets of symmetric and asymmetric CQDs in magnetic field and label both the parity and the main single-electron components (only the single-electron components) of each two-electron state for the symmetric (asymmetric) case. Similar to the single-electron case, the parity of two-electron states in a symmetric CQD determines the coherent behaviour at each resonance point and all crossings become anti-crossings in the asymmetric case. From the transition intensity plotted in the energy spectrum, we can see clearly the coherent superposition at anti-crossings which is shown as a mixture between light and dark states. Among the anti-crossings of asymmetric CQDs, we pay special attention to $A_{1,3}$ in the singlet case and $A_{2,3}$ in triplet case, which respectively correspond to crossings $C_{1,3}$ and $C_{2,3}$ in Figs. 2(a) and 2(b). Obviously, they will be the signatures of symmetry and spin states of two electrons in FIR spectrum.

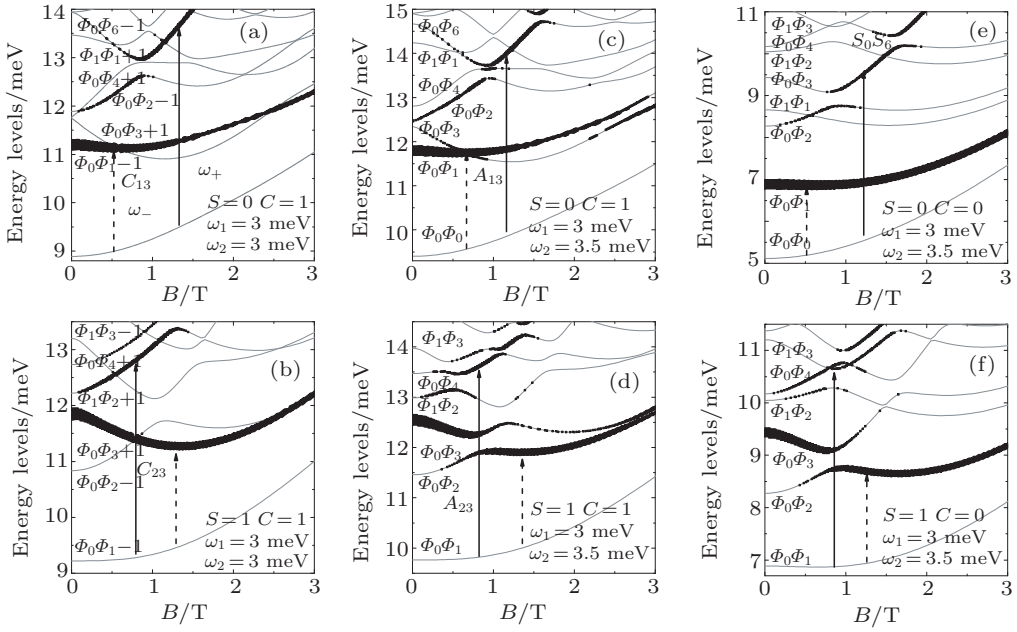


Fig. 2. Two-electron energy levels of symmetric and asymmetric coupled quantum dots in magnetic field. $S = 0$ and 1 correspond to the singlet and triplet. $C = 1$ and 0 correspond to the cases with and without the Coulomb interaction respectively. $\Phi_i\Phi_j$ represents the main single-electron component of the two-electron states. The signs + and − in (a) and (b) represent the parities of the two-electron states in symmetric coupled dots. The thickness of each energy level represents its FIR transition intensity and the dash and solid arrows label the left and the right rotation light FIR transitions.

3.2. Parity and FIR spectrum

The magnetic-field-modulated quantum coherent behaviour can be observed in the FIR spectrum of CQD. In Fig. 3 we show the FIR spectra of symmetric and asymmetric CQDs. For a quantum dot with symmetric parabolic confinement, Kohn theorem says that the FIR spectrum is determined only by the confinement strength and independent of the interaction between electrons.[11] However, the FIR spectrum of CQD will deviate from the Kohn theorem due to the decrease of the symmetry. For a symmetric coupled dot, the FIR spectrum of left rotation circularly polarized light obeys the Kohn theorem, but there are anti-crossings and additional secondary transitions in FIR of right rotation circularly polarized light, which is also found in Ref. [12]. For the asymmetric coupled dot, the deviation from Kohn theorem is more obvious. There are more anti-crossings emerging in the right rotation light spectrum. And it is interesting that there are strong anti-crossings in the left rotation light spectrum.

We can understand the FIR spectrum of CQD by analyzing the FIR transition rules. In Fig. 2, the thickness of the energy levels represents the intensity of the FIR transitions from ground state. The FIR transition is mainly a first-order single-electron transition process. For example, in a low energy region, the left (right) rotation mode of singlet in symmetric CQD corresponds to the single-electron transition from Φ_0 to Φ_1 (Φ_2). And for triplet in symmetric CQD, the left rotation mode corresponds to the transition $\Phi_1 \rightarrow \Phi_3$, while the two right rotation modes respectively correspond to $\Phi_0 \rightarrow \Phi_2$ and $\Phi_1 \rightarrow \Phi_4$, which leads to a compleicated structure of FIR spectrum.

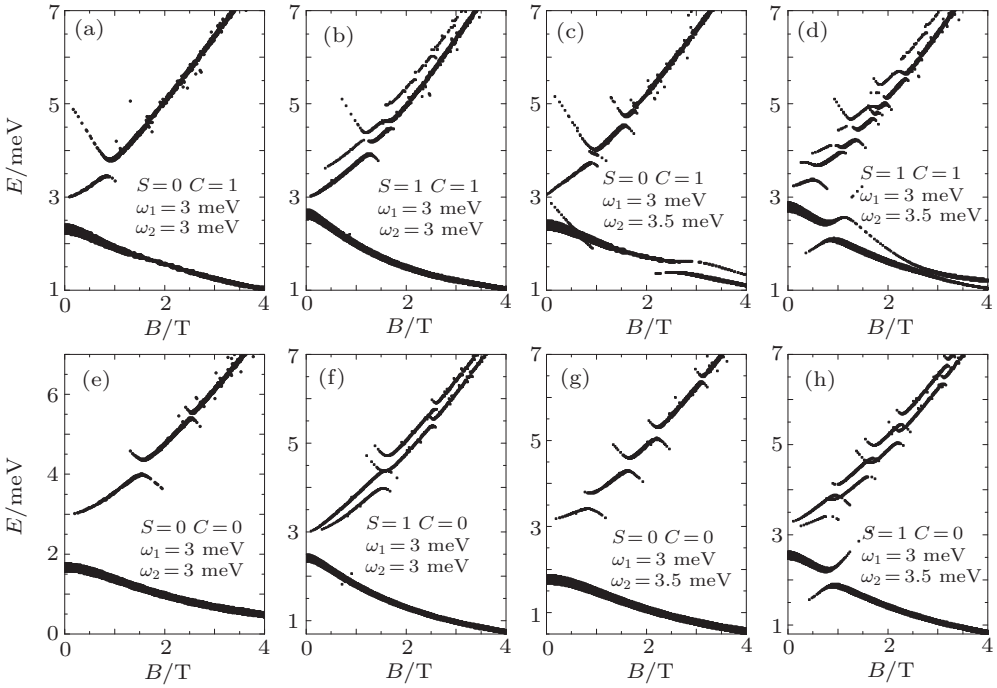


Fig. 3. FIR spectra of symmetric and asymmetric couple quantum dots in magnetic field. The thickness of each line is proportional to the FIR intensity. The meanings of S, C and $\omega_{1,2}$ are the same as those in Fig. 2.

For the asymmetric CQD, the decrease of the symmetry results in more anti-crossings in both right and left rotation light excited spectra and then the property of FIR deviates from the Kohn theorem strongly. Especially, the anti-crossings appearing in the left rotation mode of the FIR are purely the result of the parity break of CQD. This can be further confirmed by changing the interdot distance of CQD (see Fig. 4). By comparing Figs. 4(a) and 4(b) with Fig. 3(a), one can find that the structure of the FIR spectrum of symmetric coupled dot is almost unchanged with the variation of the inter-dot distance. For asymmetric CQD, the different interdot distances bring about the changes of the number and the position of anti-crossing (comparing Fig. 3(c) with Figs. 4(a) and 4(b)). However, the anti-crossing

on left rotation mode in FIR spectrum always exists. Therefore, the anti-crossing on the left rotation mode of FIR spectrum can be used as a signature of parity break of CQDs.

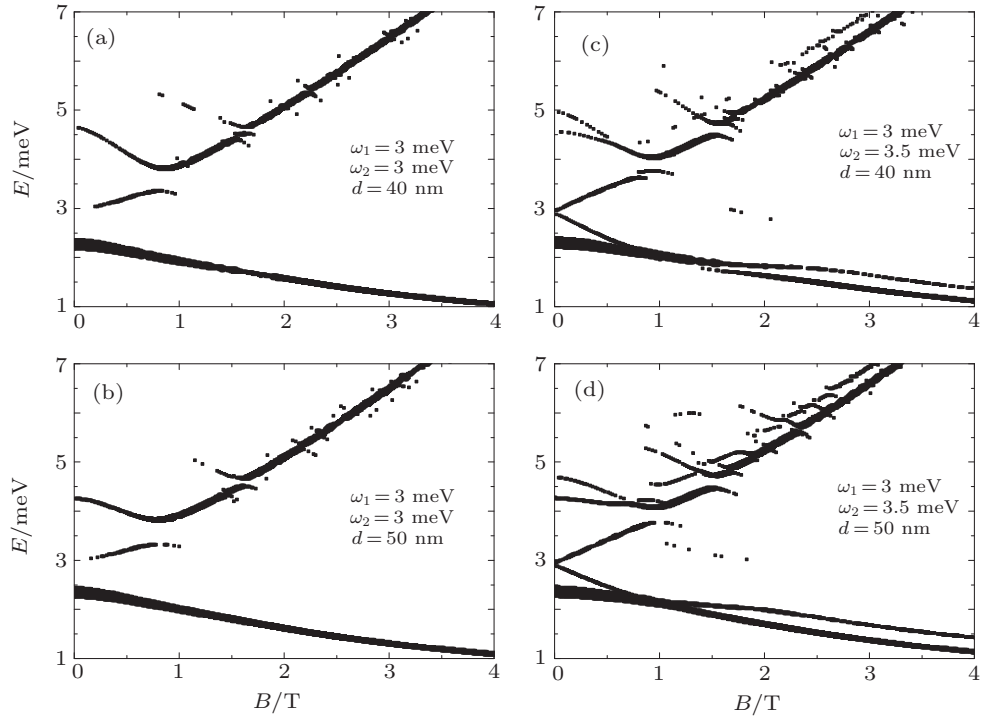


Fig. 4. FIR spectra of singlets of symmetric and asymmetric coupled quantum dots with different values of inter-dot distance d.

3.3. Coulomb interaction and the structure of FIR spectrum

For the symmetric CQDs, the study by Marlo *et al.*[12] suggested that the Coulomb interaction makes the effective potential more analogous to parabolic ones, then the FIR spectrum will be more similar to the one obeying the Kohn theorem. Our study also confirms such a conclusion. Comparing Fig. 3(a) with Fig. 3(e) and Fig. 3(b) with Fig. 3(f), we can see that the Coulomb interaction reduces the number of anti-crossings and weakens the secondary transitions in the right rotation light FIR spectra, which just means the reduction of the deviation from the Kohn theorem. However, this is not true for the asymmetric CQD. Figures 3(g) and 3(h) show the FIR spectra of singlets and triplets for asymmetric CQDs without the Coulomb interaction. By comparing them with the cases with the Coulomb interaction in Figs. 3(c) and 3(d), one can find that the interaction increases the number of anti-crossings and changes their positions. A more important feature is that there are two anti-crossings in the left rotation mode in both spectra of singlets and triplets if there is the Coulomb interaction but only one survives in the spectrum of triplets if there is no Coulomb interaction. Thus, the Coulomb interaction makes the FIR transition deviate from the Kohn theorem more severely. In order to understand it further, we plot the energy levels and the intensities of the FIR transitions of asymmetric coupled dots without the Coulomb interaction each as a function of magnetic field in Figs. 2(e) and 2(f). Comparing them with Figs. 2(c) and 2(d) we find that the Coulomb interaction greatly changes the level space and order because different states may have greatly different Coulomb energies. This leads to the change of splitting and position of anti-crossings. In fact, the FIR spectra of two electrons without Coulomb interaction are just those of one electron. In other words, there is significant difference between single- and double-electron FIR spectra in asymmetric CQDs.

4. Summary

We investigated the effects of the symmetry of lateral CQD on the structure of electronic energy level and FIR spectrum. For the CQD with spatial in-

version symmetry, each state has a definite parity. The coherent superposition modulated by a magnetic field occurs between states with the same parity and manifests itself as anti-crossing in the FIR spectrum. The existence of the parity in the symmetric CQD leads to the fact that the anti-crossings only emerge in the right rotation mode of the FIR spectrum. For asymmetric CQD, the absence of parity makes the anti-crossings also emerge in the left rotation light FIR spectrum, which can be taken as an obvious signature of parity break of CQD. We also find that the Coulomb interaction can make the FIR spectrum of asymmetric CQD deviate from the Kohn theorem more severely, which is just contrary to the symmetric case. These results provide a method for extracting information about CQD structure, coherent superposition and many-body correlation effects using FIR spectrum.

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