Vol 17 No 4, April 2008
1674-1056/2008/17(04)/1400-05

Chinese Physics B

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Evaluation of electron–electron interactions in coupled quantum dots by using far-infrared spectra*

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(Received 17 September 2007; revised manuscript received 19 November 2007)

We have studied the far-infrared spectra of two-electron vertically coupled quantum dots in an axial magnetic field by exact diagonalization. The calculated results show an obvious difference in role between the interactions for spin $S = 1$ and for spin $S = 0$. The results support the possibility to evaluate the interactions by far-infrared spectroscopy in vertically coupled quantum dots.

Keywords: coupled quantum dots, electron–electron interactions, far-infrared spectra
PACC: 7320D, 7360J

1. Introduction

A semiconductor quantum dot is physically similar to a set of atomic electrons bound to a nucleus, and for this reason its structure is sometimes termed 'artificial atom'. To extend the atomic analogy further, quantum dots are considered as 'artificial molecules',[1] if they are coupled together. Two coupled quantum dots containing two electrons allow for fundamental quantum experiments not accessible in real molecules with the further prospect of quantum control of the electronic properties. Electron tunnelling from one quantum dot to another typically occurs on the nanosecond time scale, which opens a door for the precise manipulation and measurement of electronic states.[2] Such devices may thus serve as building blocks for future quantum processors.[3,4] Recently coupled quantum dots have received increasing attention triggered by the experimental verification of controlled qubit operations induced by electromagnetic switches.[5,6]

Since the first calculations which uncovered the role of the electron–electron interaction were performed for a single dot in 1990[7] and 1991,[8] correlation effects of electrons confined in quantum dots have been studied from many different theoretical perspectives by using a great variety of approaches.[9] Based on exact diagonalization techniques, it has been shown that the two-electron ground state exhibits a phase transition from a singlet to a triplet state at finite magnetic-field strengths due to interactions.[10−12] Marlo *et al* [13] studied the effects of electron–electron correlations and confinement potential on the far-infrared (FIR) spectra of two-electron coupled quantum dots and found the interactions to shift the spectra towards those of high-symmetry parabolic quantum dots. The stability diagrams of a one- and two-electron coupled quantum dots were calculated for much larger interdot separations 30 and 60 nm in an associated exponential double-well potential.[14] Recently, the electronic structures of a laterally coupled two-electron quantum dot molecule have been computed for different confinement strengths and for varying interdot separations and external electromagnetic fields.[15] Guo[16] studied a density matrix of two interacting particles with a kinetic coupling derived in bipartite entangled state representation.

In view of the fact that the interaction plays a vital role in the two electron system, we evaluate the strength of interaction by certain means. In this paper, we draw inspiration from the effects of electron–electron correlations on FIR spectrum[13] and observe how FIR spectra are modified when the interactions are taken into account in two-electron InAs vertically coupled quantum dots in an axial magnetic field. Moreover, we analyse the reason why the modification

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occurs and the results support the possibility to evaluate interaction effect by FIR spectroscopy in vertically coupled quantum dots.

2. Theoretical model

Figure 1 shows vertically coupled quantum dots, which consist of two InAs/GaAs double self-assembled quantum discs. Each disc grows on a wetting layer (WL) with a thickness of W containing the GaAs barrier material. Both the quantum discs have the same height H (typically 1–2 nm) and the same radius R (typically 7–12 nm). The separation between the two wetting layers, D, forms a quantum tunnelling barrier with a thickness of $D-H$, and the conduction band offset between the quantum discs and the surrounding material forms a confining potential (V_0) for the quantum discs. The material parameters of the quantum discs and WLs have their effects through the effective Rydberg Ry=$m_{\rm e}e^4/2\epsilon^2\hbar^2$ and the effective Bohr radius $a_{\rm B}=\epsilon\hbar^2/m_{\rm e}e^2$, where $m_{\rm e}$ and ϵ are the effective mass of an electron and the dielectric constant, respectively. Throughout this paper, we use R and $a_{\rm B}$ as the units of energy and length, respectively.

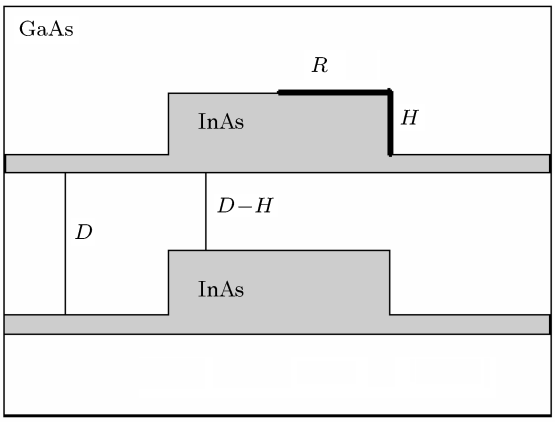


Fig.1. Schematic of InAs vertically coupled quantum dots consisting of two InAs/GaAs double self-assembled quantum discs each with radius R and height H, and a wetting layer separation D in between.

In the effective mass approximation, the Schrödinger equation for one electron in cylindrical coordinates is expressed as

$$\hat{H}\psi(r,\theta,z)=E\psi(r,\theta,z), \tag{1}$$

where

$$\hat{H}=-\frac{1}{r^2}\left(r\frac{\partial}{\partial r}r\frac{\partial}{\partial r}+\frac{\partial^2}{\partial\theta^2}\right)+\frac{eB}{c}l_z+\frac{e^2B^2}{4c^2}r^2 -\frac{\partial^2}{\partial z^2}+V(r,z), \tag{2}$$

with the potential $V(r,z)=-V_0$ between the WL and quantum discs, and $V(r,z)=0$ in the barrier. Since the heights of both quantum discs are much smaller than their radii, the electron motion in the growth direction is strongly confined. In the adiabatic approximation, the wavefunction is written as $(1/\sqrt{2})\mathrm{e}^{\mathrm{i}m\theta}g_{\rm r}^{\rm v}(z)f_{\rm m}^{\rm v}(r)$. The details of the computational procedure can be found elsewhere.[17]

To investigate the variation of the two-electron levels of vertically-assembled quantum discs versus the axial magnetic field, the spin-free Hamiltonian of the system can be expressed as

$$\hat{H}=\hat{H}_1+\hat{H}_2+\frac{e^2}{\epsilon r_{12}}, \tag{3}$$

where $\hat{H}_1$ and $\hat{H}_2$ are single-electron Hamiltonians of the system and remain in the formalism of Eq.(1). The Zeeman coupling $E_{\rm Z}=g^*\mu_{\rm B}BS_{\rm Z}$ of the magnetic field to $S_{\rm Z}$ can be neglected. We have obtained numerically the eigenstates of the single-electron part of Eq.(3), $\psi(r,\theta,z)=(1/\sqrt{2})\mathrm{e}^{\mathrm{i}m\theta}g_{\rm r}^{\rm v}(z)f_{\rm m}^{\rm v}(r)$, thus the two-electron wavefunction with total spin S can be expanded as

$$\Psi_{\rm S}(r_1,r_2)=\sum_{i\leqslant j}\alpha_{i,j}\{\psi_i(r_1,\theta_1,z_1)\psi_j(r_2,\theta_2,z_2) +(-1)^S\psi_i(r_2,\theta_2,z_2)\psi_j(r_1,\theta_1,z_1)\}, \tag{4}$$

which is symmetric for $S=0$ and antisymmetric for $S=1$. Coefficient vector α_1 and corresponding energy E_l for the lth eigenstate are found from a generalized eigenvalue problem in which the Hamiltonian matrix elements can be calculated numerically. Six lowest levels for one set of structure parameters are plotted in Fig.2.

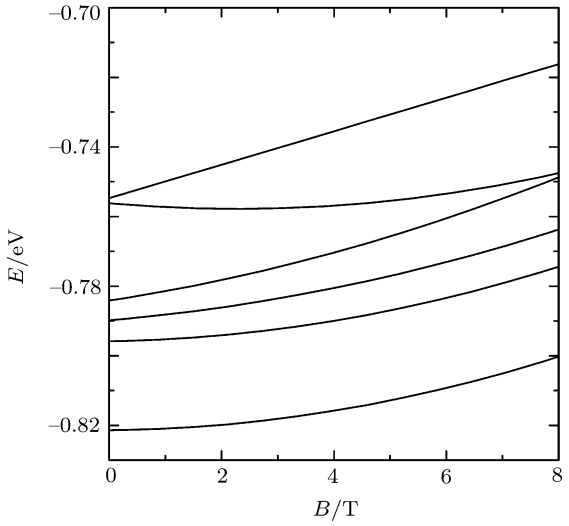


Fig.2. The six lowest two-electron states versus axial magnetic field B, with H=2 nm, D=7.5 nm and R=12 nm.

Using the golden rule within the electric-dipole approximation for the perturbing electromagnetic field, the transition probability from the ground state to the lth excited state can be calculated as[13]

$$A_{l,\pm} \propto |\langle \Psi_l | \mathrm{e}^{\mathrm{i}\phi} \sum_{i=1}^{2} r_i | \Psi_0 \rangle|^2 \delta(E_l - E_0 - \hbar\omega), \quad (5)$$

where we have used the right- or the left-handed circular polarization of the field, denoted respectively by '+' or '−'.

3. Results and discussion

Figures 3 and 4 show the dependences of the calculated FIR spectrum on axial magnetic field B with a confining potential V_0=1 eV, corresponding to the band offset between InAs and GaAs, and the effective mass m_e=0.023 m_0 for unstrained InAs. The calculated FIR spectrum is presented with the structure parameters: H=2 nm, D=7.5 nm and R=12 nm. When the transition probability is less than 95% of the maximum value, it will be suddenly weaken to 0, thus we do not plot the transition probability. One should note that the transition probabilities between different spins are zero, and thus S is conserved in the allowed transitions. We present the results for unpolarized light, averaging over the two circular polarizations.

As a general feature of the calculated spectra, one can see that each spectrum has a major component with two branches for unpolarized light, where the higher one (ω_+) has a positive dispersion and the lower one (ω_-) a negative dispersion. In Fig.3, the calculated FIR spectrum is shown for the total spin $S = 1$ and that for total spin $S = 0$ in Fig.4. By comparing the interaction spectrum with the non-interaction one, we can analyse the effect of the interactions on the effective potential from two aspects. On the one hand, the interactions lead to the splitting of zero-field resonances and the splitting can be explained by the two-electron levels. In Fig.2, the two-electron levels possess the zero-field splitting in contrast to the non-interaction two-electron levels due to the interactions. According to Eq.(5), the zero-field splitting between the two-electron levels can lead directly to the splitting of zero-field resonances. On the other hand, the resonance energy as a function of the magnetic field becomes less linear due to the interactions, as can be explained by the nonlinearity of the two-electron levels. These results show the interactions lower the symmetry of the effective potential. Comparing the results of vertically coupled quantum dots with the results of laterally coupled quantum dots,[13] we can find that anticrossings for vertically coupled quantum dots are not very obvious. No obvious anticrossing shows that the interactions lower the symmetry of the effective potential but not seriously. The reason is that the effective potential of a vertical molecule is provided with a higher symmetry. So we can come to a conclusion: when effective potential possesses a high-level symmetry, the interactions lower the level of its symmetry; when effective potential possesses a low-level symmetry, the interactions raise the level of its symmetry.

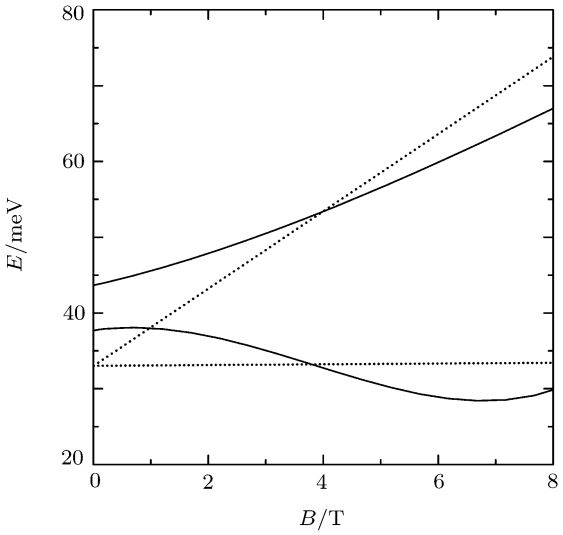


Fig.3. FIR spectrum (for $S = 1$) of vertically coupled quantum dots with H=2 nm, D=7.5 nm and R=12 nm. Spectrum shows the energy of absorbed light as a function of axial magnetic field B. The higher branch corresponds to ω_+ and the lower one corresponds to ω_-. The dotted lines are for the situation without the interactions.

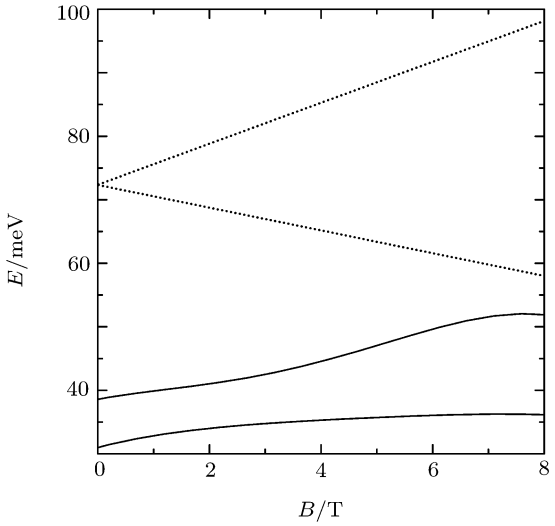


Fig.4. FIR spectrum (for $S = 0$) of vertically coupled quantum dots with H=2 nm, D=7.5 nm and R=12 nm. Spectrum shows the energy of absorbed light as a function of axial magnetic field B. The higher branch corresponds to ω_+ and the lower one corresponds to ω_-. The dotted lines are for the situation without the interactions.

In the following, we investigate the effect of the interactions on the resonance energies (see Fig.5). There exists an obvious difference in role between the interactions for spin $S = 1$ and for spin $S = 0$. The interactions reduce the resonance energy for spin $S = 0$ obviously, whereas for spin $S = 1$ the effect of the interactions on the resonance energies is much less weak. The difference can be explained by the single-electron states and the double-electron states. For spin $S = 0$, the double-electron ground state is mainly composed of two lowest single-electron states. However, the two electrons of the $S = 1$ ground state cannot occupy the lowest single-electron state simultaneously according to the Pauli exclusion principle. Thus the interaction energy of the $S = 0$ ground state is greater than that of the $S = 1$ ground state, which leads the ground energy of the $S = 0$ state to increase obviously, and then for spin $S = 0$ the resonance energy decreases obviously. Just because the role of the interactions in the $S = 0$ state, the curves for spin $S = 0$ and those for spin $S = 1$ are pressed together (see Fig.5). These analyses suggest that for spin $S = 0$ the resonance energy decreases as the interactions become stronger. This result is significant, because it allows probing the interactions by FIR spectroscopy in vertically coupled quantum dots.

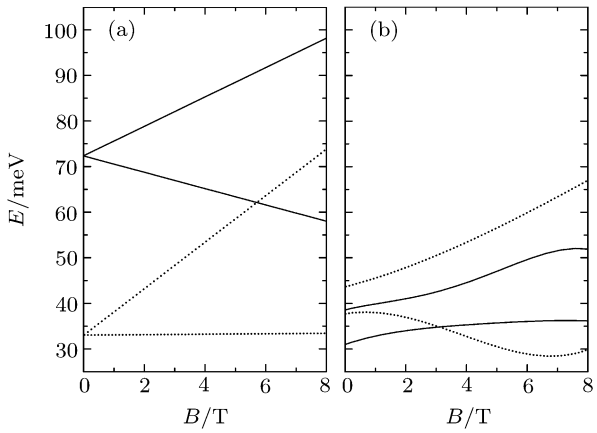


Fig.5. FIR spectra of vertically coupled quantum dots with H=2 nm, D=7.5 nm and R=12 nm: (a) the non-interacting spectrum and (b) the interacting spectrum. Spectra show the energy of absorbed light as a function of axial magnetic field B, where the solid lines represent the $S = 0$ state and the dotted lines are for the $S = 1$ state.

4. Conclusion

We have carried out the numerical calculation of the FIR spectra of two-electron InAs vertically coupled quantum dots by exact diagonalization and evaluate the interactions by using the FIR spectra. The effective potential of vertically coupled quantum dots is provided with a higher symmetry than that of lateral coupled quantum dots. When the effective potential of vertically coupled quantum dots possesses a high-level symmetry, the interactions lower the level of its symmetry; when the effective potential of vertically coupled quantum dots possesses a low-level symmetry, the interactions raise the level of its symmetry. There exists an obvious difference in role between the interactions for spin $S = 1$ and for spin $S = 0$ and the result supports the possibility to evaluate the interactions by using FIR spectroscopy in vertically coupled quantum dots.

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