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Singlet–triplet oscillations and far-infrared spectrum of four-minima quantum-dot molecule

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Abstract

We study ground states and far-infrared spectra (FIR) of two electrons in four-minima quantum-dot molecule in magnetic field by exact diagonalization. Ground states consist of altering singlet and triplet states, whose frequency, as a function of magnetic field, increases with increasing dot–dot separation. When the Zeeman energy is included, only the two first singlet states remain as ground states. In the FIR spectra, we observe discontinuities due to crossing ground states. Non-circular symmetry induces anticrossings, and also an additional mode above ω_+ in the spin-triplet spectrum. In particular, we conclude that electron–electron interactions cause only minor changes to the FIR spectra and deviations from the Kohn modes result from the low-symmetry confinement potential.

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1. Introduction

Many experimental and theoretical studies have revealed interesting properties of few-electron quantum dots (QDs) [1]. Rich spectrum of crossing energy levels as a function of magnetic field and strong interaction effects are nowadays rather well understood in a symmetric confinement potential. Recently, the focus has turned into understanding the properties of quantum dots in less symmetric confinement potentials. In a circular-symmetric confinement potential the center of mass and relative variables decouple, which makes especially the excitation spectra trivial [2]. In a less symmetric confinement this condition is lifted. However, it is not clear how the symmetry of the confinement and interaction effects show up in the far-infrared excitation spectra (FIR) of a low-symmetry QD.

In this work, we examine ground states and far-infrared excitation spectra of two electrons in four-minima confinement potential. Ground state of four-minima quantum-dot molecule (QDM)

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consist of altering spin-singlet ($S=0$) and spin-triplet ($S=1$) states as a function of magnetic field. On contrary to two-minima QDM [3], the second singlet region in four-minima QDM can be observed at the greatest inter-dot distances studied even if the Zeeman energy is included. In FIR spectra, we observe anticrossings in Kohn modes and an additional mode above ω_+ in spin-triplet spectrum. Crossing ground state levels induce discontinuities in the two-body FIR spectra. In particular, as in two-minima QDM [4], we conclude that electron–electron interactions cause only minor changes to the FIR spectra and deviations from the Kohn modes result in from the low-symmetry confinement potential.

2. Model and method

We model the two-electron QDM by a 2D Hamiltonian

$$H = \sum_{i=1}^{2}\left(\frac{(-i\hbar\nabla_i - \frac{e}{c}\mathbf{A})^2}{2m^*} + V_c(\mathbf{r}_i)\right) + \frac{e^2}{\varepsilon r_{12}}, \qquad (1)$$

where V_c is the external confinement potential:

$$V_c = \frac{1}{2}m^*\omega_0^2 \min[(\mathbf{r}+\mathbf{L}_i)^2]. \qquad (2)$$

The potential consists of four parabolas with minima at positions $\mathbf{L}_i = (\pm L, \pm L)$. We use the GaAs material parameters $m^*/m_e = 0.067$ and $\varepsilon = 12.4$, and the confinement strength $\hbar\omega_0 = 3.0\,\mathrm{meV}$. $\mathbf{A}$ is the vector potential of the magnetic field (along the z axis) taken in the symmetric gauge. The Hamiltonian is spin free and the Zeeman energy can be included in the total energy afterwards, $E_Z = g^*\mu_B B S_Z$ ($g^* = -0.44$ for GaAs).

We construct two-body wave functions, with total spin S:

$$\Psi_S(\mathbf{r}_1,\mathbf{r}_2) = \sum_{i\leqslant j}\alpha_{i,j}\{\phi_i(\mathbf{r}_1)\phi_j(\mathbf{r}_2) + (-1)^S\phi_j(\mathbf{r}_1)\phi_i(\mathbf{r}_2)\}, \qquad (3)$$

using 2D gaussians ($\phi_i(\mathbf{r}) = x^{n_{x_i}}y^{n_{y_i}}\mathrm{e}^{-r^2/2}$) as a single particle basis. (See Ref. [3] for more details). The Hamiltonian matrix is diagonalized numerically.

In the calculation of far-infrared spectra we use Fermi golden rule within electric-dipole approximation to calculate the transition probability from the ground state (E_0) to excited states (E_l):

$$\mathscr{A}_{l,\pm} \propto \left|\left\langle \Psi_l \left| \mathrm{e}^{\pm i\phi}\sum_{i=1}^{2}\mathbf{r}_i \right| \Psi_0 \right\rangle\right|^2 \delta(E_l - E_0 - \hbar\omega), \qquad (4)$$

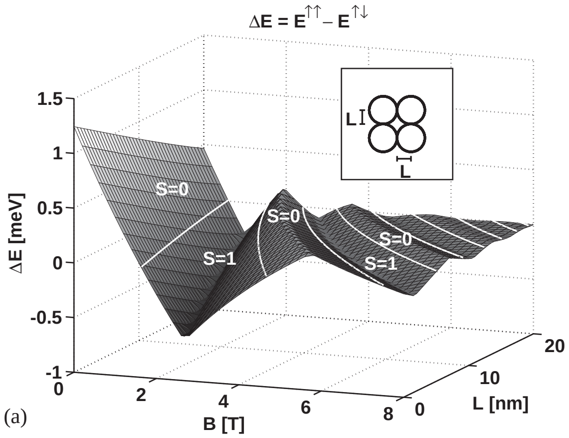
where $\pm$ refers to two circular polarizations.

3. Singlet–triplet oscillations

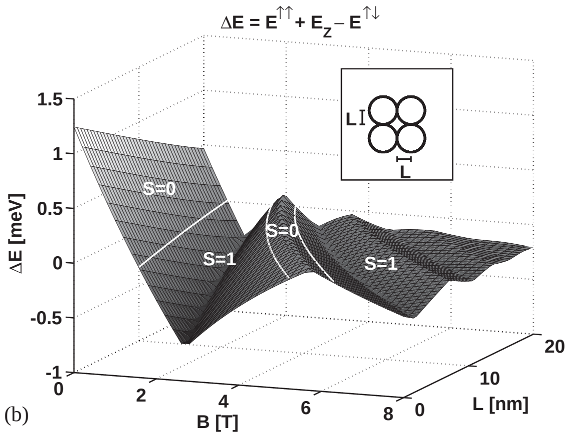
The energy differences of the lowest triplet and singlet states are plotted in Fig. 1 as a function of magnetic field (B) at different inter-dot spacings ($L = [0, 20]\,\mathrm{nm}$). Ground state of the four-minima QDM consist of altering singlet ($S=0$) and triplet ($S=1$) states. At small magnetic field the ground state of the two-electron QDM is spin-singlet ($S=0$), which changes to spin-triplet ($S=1$) as the magnetic field is increased. The first singlet–triplet transition can be understood with simple occupation of the lowest single-particle states: In the singlet state the two electrons occupy the lowest energy eigenstate with opposite spins ($S=0$). As the magnetic field increases, the energy difference of the lowest and the second lowest single-particle levels decreases. At some point the exchange energy in the spin-triplet state becomes larger than the energy difference between the adjacent energy levels. Thus, the singlet–triplet transition occurs and the adjacent eigenlevels are occupied with electrons of parallel spins ($S=1$).

However, the true solution of two-electron QDM is much more complicated than the occupation of single-particle levels and the inclusion of the exchange energy. Interaction between the electrons changes the situation drastically. As a signature of complex many-body features a second singlet state at higher magnetic field is observed in double-minima QDM [3].

In four-minima QDM we do not only find a second singlet region at higher magnetic field, but also a third, fourth, and even a fifth singlet state at the inter-dot spacings studied ($L \leqslant 20\,\mathrm{nm}$). Actually, it is interesting to note that especially at



(a)



(b)

Fig. 1. Triplet singlet energy difference ($\Delta E = E^{\uparrow\uparrow} - E^{\uparrow\downarrow}$) in two-electron four-minima quantum dot molecule as a function of magnetic field and dot–dot separation L. In (a) the energy difference is plotted without Zeeman energy and in (b) with Zeeman energy. Insets show geometry of four-minima QDM.

large inter-dot spacings rapid singlet–triplet oscillations are seen as a function of magnetic field. However, when the Zeeman term (which lowers the spin-triplet energy) is included in the energy, the subsequent singlet states after the second $S = 0$ are no longer ground states as can be seen in Fig. 1(b).

It is surprising to see how stable the second singlet is in four-minima QDM. Even if the Zeeman energy is included, there remains a 0.7–1 T magnetic field window of the second $S = 0$ state at the greatest distance studied. The energy difference of $L = 10$ nm QDM can be examined in Fig. 2(d). The third singlet region at $B \approx [6, 7.5]$ T is no longer ground state if the Zeeman term is included as the lower curve indicates. However, the second singlet persist as a ground state to the largest L studied as Fig. 1(b) indicates. This is contrary to two-minima QDM where the second singlet state is observed only at very small inter-dot distances ($L \leqslant 2.5$ nm) if the Zeeman term is included [3].

Ten lowest energy levels of $L = 10$ nm QDM as a function of magnetic field are shown in Fig. 2 (a–c) for single-particle, spin-singlet and spin-triplet states, respectively.

4. Far-infrared spectra

The calculated FIR spectra of $L = 10$ nm QDM are shown in Fig. 3 for spin-singlet in (a) and spin-triplet in (c). For the comparison we also plot non-interacting two-electron spectra for the symmetric wave function (non-interacting $S = 0$) and for the antisymmetric wave function (non-interacting $S = 1$) in Fig. 3(b) and (d), respectively. Fig. 3(b) also represents the single-particle FIR spectra of the QDM.

The linewidth at the corresponding energy (in meV) in FIR spectra indicates the transition probability from the ground state to an excited state and it is also plotted below each spectrum (in arbitrary units). E.g. in $S = 0$ spectrum (a) the upper ω_+ mode has rather constant transition probability till the first anticrossing, where the transition probability of the lower part of the anticrossing rapidly decreases as a function of B, whereas the upper part increases at the same time. The vertical lines in (a) and (c) mark the magnetic field values where the singlet–triplet or triplet–-singlet transition is observed. They also mark regions of observable spectra, which is $S = 0$ at magnetic field values $B \approx [0, 1]$ T and $B \approx [3, 4]$ T, and $S = 1$ outside these regions. In the non-interacting spectra no ground state transitions occur. The open circles represent Kohn modes of parabolic QD with $\hbar\omega_0 = 3$ meV confinement.

Anticrossings in the upper ω_+ branch are seen in the singlet, triplet and non-interacting spectra. These result from the non-circular confinement potential. Discontinuities in the interacting spectra

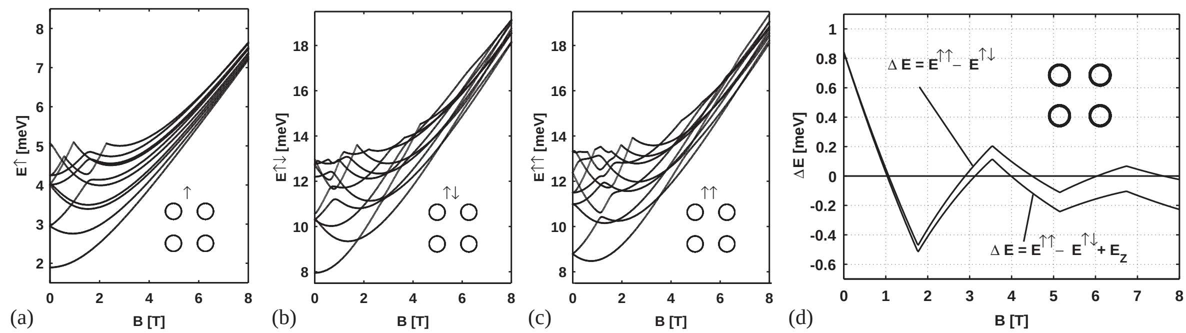


Fig. 2. Ten lowest energy levels of $L = 10\,\mathrm{nm}$ QDM for (a) single-particle, (b) spin-singlet ($S = 0$), and (c) spin-triplet ($S = 1$) states. Triplet–singlet energy difference of $L = 10\,\mathrm{nm}$ QDM is plotted in (d).

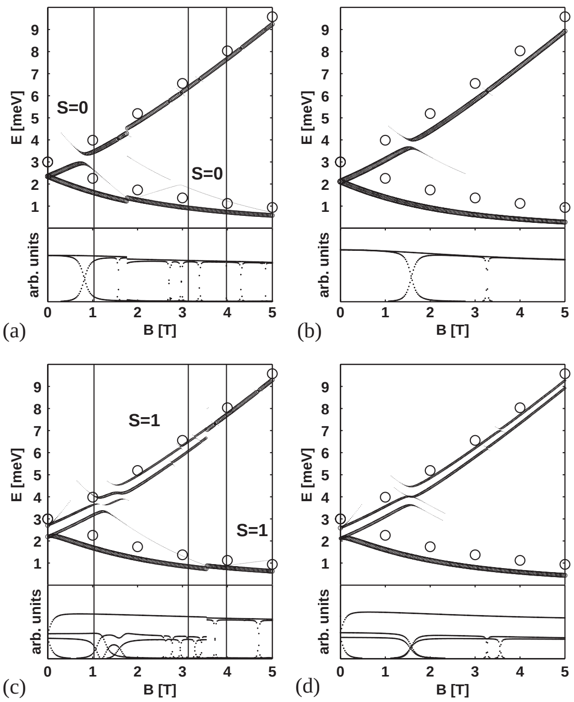


Fig. 3. Far-infrared spectra of $S = 0$ in (a), $S = 1$ in (c) and corresponding non-interacting spectra in (b) and (d) for $S = 0$ and $S = 1$, respectively.

at $B \approx 1.2\,\mathrm{T}$ in $S = 0$ and at $B \approx 3.5\,\mathrm{T}$ in $S = 1$, can be identified to crossing ground states (see also Fig. 2(b) and (c)). However, these crossings are observed in the magnetic field values where the ground state is of the other spin type. At higher magnetic field ($B > 8\,\mathrm{T}$) one could see discontinuities in the spin-polarized system ($S = 1$) resulting from the crossing ground state levels in the spin-triplet spectra. Otherwise only discontinuities in the observable spectra result from altering singlet and triplet FIR spectra.

As x and y excitations are degenerate, there occurs no zero-field splittings of the Kohn modes which were observed in the two-minima QDM [4]. In the spin-triplet spectra the upper branch is split to two modes separated by a clear energy gap. Similar type of splittings of the upper branch are also seen in other types of non-circular potentials [4,5]. The comparison of the interacting and non-interacting QDMs shows remarkably similar spectra. In the non-interacting spectra anticrossings are at slightly higher B and modes are slightly lower in energy than the interacting modes. As the Coulomb repulsion is present in the interacting case, electrons feel effectively steeper confinement resulting slightly higher excitation energies. Only notable difference is in the triplet spectra, where the double structure of the ω_+ changes to single peak after $B \approx 3.5\,\mathrm{T}$ in the interacting case. Otherwise, interacting and non-interacting spectra are so similar that we can conclude that the FIR spectra reflects mainly the single-particle excitations of electrons in the low-symmetry confinement and only minor changes are induced by the electron–electron interactions.

5. Summary

To summarize, we have calculated the ground state of two electrons in four-minima quantum-dot molecule as a function of magnetic field. Our exact diagonalization calculations reveal a complicated two-body ground state structures of altering singlet and triplet states as a function of magnetic field. In the far-infrared spectra we observe anticrossings and an additional mode in the spin-triplet state both arising from the non-circular confinement potential. We conclude that electron–electron interactions have only a minor effect on the FIR spectra of four-minima QDM.

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