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Three interacting electrons in vertically coupled quantum dots

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Abstract

We study a three-electron system in a double-layer quantum dot under a magnetic field by means of the exact diagonalization of the Hamiltonian matrix. Discontinuous ground-state energy transitions induced by an external magnetic field are reported. Series of magic numbers of the angular momentum which minimize the ground-state electron–electron interaction energy have been obtained.

1. Introduction

A quantum dot (QD) consists of an artificial structure in which electrons are confined in all three spatial dimensions and thus have a fully quantized energy spectrum. A set of electrons held in such a structure is conceptually similar to a set of atomic electrons bound to a nucleus, and for this reason QDs are sometimes termed 'artificial atoms' [1, 2]. Usually, one considers two-dimensional (2D) or disc-like QDs with the lateral size much larger than the extent in the growth direction. These dots have typically a disc-like shape with a lateral confinement potential that to a good approximation is parabolic. Most theoretical and experimental studies have so far been focused on the electronic structure of a single disc-like QD [3–5]. The most striking feature of 2D QDs is that the correlation and magnetic field effects are greatly enhanced compared with their normal counterparts. This feature makes quantum confined semiconductors very promising for possible device applications in microelectronics, non-linear optics, and many other fields.

The electron–electron interaction in QDs has a profound influence on the ground state, which occurs in a magnetic field only at certain magic values of the total angular momentum L and total spin S [3]. In 1993 Yang *et al* [6] investigated the phase diagrams, and the most important finding was the discovery of the transition of the quantum numbers L and S of the ground state in accord with the variation of the strength B of the magnetic field. This definitely implies a phase transition, i.e., a transition of structures. Thereby, when the magnetic field continuously increases, jumps in a number of physical properties such as the optical properties [7], electronic heat capacity [3], and magnetization [8] from one plateau to another plateau will occur.

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In an effort to understand the fractional quantum Hall effect, Laughlin [9] first studied the states of a three-electron system in two dimensions in a strong magnetic field and confined by a parabolic potential. Laughlin explicitly constructed the spin-polarized correlated states in the lowest Landau level and showed that they approximated the exact eigenstates well. The ground states turned out to be incompressible since only 'magic numbers' of the angular momentum $L = 3k$ ($k = 1, 2, 3, \ldots$) of the ground state minimize the Coulomb repulsion. In 1995 Ruan *et al* [4] studied the effect of quantum mechanical symmetry in determining the features of 2D three-electron QDs and showed the origin of the magic numbers.

Recently, attention has been focused on double-layer few-electron systems [10–12] (artificial molecules), where the additional degree of freedom enriches the physics. It is then intriguing to consider what happens if we laterally confine a double-layer few-electron system to form vertically coupled QDs. Because fascinating correlation effects are known to occur in double 2D (bilayers) systems and double 1D systems (double quantum wires [13]), we can expect to find interesting phenomena in double 0D systems (double dots), which are the subject of the present work. Such a double QD, with one state per dot, has recently been proposed as a possible candidate for the two-qubit entanglement required for quantum computation.

In 1993 Bryant [14] studied the energy spectra, charge densities, and correlation functions for interacting two-electron systems in coupled dots as functions of the applied bias. In 1996 Oh *et al* [15] studied the electronic structure in coupled QDs with one or two electrons in magnetic fields. They were interested in the spin transitions of the ground state and the optical transitions between the energy levels. In 1998 Kaputkina and Lozovik [16] studied the energy spectra for interacting two-electron systems in horizontally and vertically coupled QDs as functions of QD separation, lateral confinement, and magnetic field. They considered each dot as a strictly 2D system. Tokura *et al* [17] next investigated the electron states in two vertically coupled QDs using an exact diagonalization method. In this paper we will concentrate on a three-electron QD system consisting of double-layer QDs, investigated by means of exact numerical diagonalization. Such a system is the simplest that includes both intra-dot and inter-dot interactions. In addition to the interesting and fundamental correlation and quantum effects, this system is very important as a candidate for use as the gate of a quantum computer.

2. The model and the method

The system that we study is a double dot containing three electrons. We assume that the upper dot contains electrons 1 and 2 and the lower dot contains electron 3. In both dots the electron motion is perfectly 2D, and the lateral confining potential within each layer is assumed to be parabolic, $\frac{1}{2}m^*\omega_0^2 r^2$. The dots are separated in the vertical direction with their centres aligned on a common axis. The external magnetic field is assumed to be lying along the z-direction. The electron–electron interaction is taken to be the unscreened Coulomb potential. We assume that the electrons can exchange between the two dots when the distance d is small. The Hamiltonian for the three electrons with the same effective mass m_e^* in a double-layer QD is given by

$$H = \sum_{i=1}^{3}\left[\frac{1}{2m_e^*}\left(\vec{p}_i + \frac{e}{c}\vec{A}_i\right)^2 + \frac{1}{2}m^*\omega_0^2 r_i^2\right] + V_{intra} + V_{inter} - g^*\mu_B B S_z, \quad (1)$$

with

$$V_{intra} = \frac{e^2}{4\pi\epsilon}\frac{1}{r_{12}}, \quad (2)$$

$$V_{inter} = \frac{e^2}{4\pi\epsilon}\left(\frac{1}{\sqrt{r_{13}^2 + d^2}} + \frac{1}{\sqrt{r_{23}^2 + d^2}}\right), \quad (3)$$

where the momentum, position vector, and vector potential associated with the ith electron are given by $\vec{p}_i$, $\vec{r}_i$, and $\vec{A}_i$ respectively, ω_0 is the confining strength of the QD, V_{intra} and V_{inter} are respectively the intra-dot and inter-dot electron–electron interactions, g^* is the effective Landé factor, μ_B is the Bohr magneton, S_z is the z-component of the total spin, d is the distance between the vertically coupled dots. With the symmetric gauge for the vector potential $\vec{A} = \frac{1}{2}B(-y, x, 0)$, the Hamiltonian can then read [6, 14]

$$H = \sum_{i=1}^{3}\left(\frac{p_i^2}{2m_e^*} + \frac{1}{2}m_e^*\omega^2 r_i^2\right) + V_{intra} + V_{inter} + \frac{1}{2}\omega_c L_z - g^*\mu_B B S_z, \tag{4}$$

where $\omega = \sqrt{\omega_0^2 + \omega_c^2/4}$, $\omega_c = eB/m_e^*$ is the cyclotron frequency, L_z is the total orbital angular momentum along the z-direction.

A set of the centre-of-mass (cm) and canonical relative coordinates are introduced to describe the motion of the particles: $R_{cm} = \sum_{i=1}^{3}\vec{r}_i/3$, $\vec{\xi}_1 = \vec{r}_2 - \vec{r}_1$, $\vec{\xi}_2 = \vec{r}_3 - (\vec{r}_1 + \vec{r}_2)/2$. Equation (4) can then divided into two independent parts:

$$H = H_{cm} + H_r, \tag{5}$$

where

$$H_{cm} = \frac{P_{cm}^2}{2M} + \frac{1}{2}M\omega^2 R_{cm}^2, \tag{6}$$

is for the cm motion and $M = 3m_e^*$ is the total mass. It is trivial (simply a harmonic oscillation). H_r is for the relative motion:

$$H_r = H_0 + V_{intra} + V_{inter}, \tag{7}$$

with

$$H_0 = \sum_{\nu=1}^{2}\left(\frac{p_\nu^2}{2\mu_\nu} + \frac{1}{2}\mu_\nu\omega^2\xi_\nu^2\right) + \frac{1}{2}\omega_c L_z - g^*\mu_B B S_z, \tag{8}$$

where $\mu_1 = m_e^*/2$ and $\mu_2 = 2m_e^*/3$.

For a disc-like QD, the eigenstates of H_r are classified according to the total angular momentum L and the total spin S. To obtain the eigenfunctions and eigenenergies associated with relative motion, H_r is diagonalized in a model space spanned by the translationally invariant 2D harmonic product bases $\{\Phi_{[K]} \equiv \tilde{A}[\phi_{n_1\ell_1}(\vec{\xi}_1)\phi_{n_2\ell_2}(\vec{\xi}_2)\chi^S_{S_{12}}]_L\}$, where $[K]$ denotes the set of quantum numbers $(n_1, \ell_1, n_2, \ell_2)$, $\chi^S_{S_{12}} = [(\eta(1)\eta(2))_{S_{12}}\eta(3)]_S$, $\phi_{n\ell}(\vec{\xi})$ is a 2D harmonic oscillator state with frequencies ω and energy $(2n + |\ell| + 1)\hbar\omega$. $\eta(i)$ is a spin state of a single electron and S_{12} is the spin of the electrons 1 and 2. In practical calculations, ω serves as a variational parameter for minimizing the energies. $\tilde{A}$ is an anti-symmetrizer. The anti-symmetrization and the calculation of the related matrix elements are realized by using the 2D Talmi–Moshinsky coefficients [18]. It is notable that the basis functions do not form an orthogonal set due to the anti-symmetrization; hence, in practical calculations, an additional procedure of orthogonalization is needed to extract linearly independent basis functions. The matrix elements of H_r are then given by the following expressions:

$$\langle\Phi_{[K]}|H_0|\Phi_{[K']}\rangle = \{[2(n_1 + n_2) + |\ell_1| + |\ell_2| + 2]\hbar\omega + \tfrac{1}{2}\omega_c L_z - g^*\mu_B B S_z\}\delta_{[K],[K']} \tag{9}$$

$$\langle\Phi_{[K]}|V_{intra}|\Phi_{[K']}\rangle = U^I_{n_1,n_1'}\delta_{\ell_1,\ell_1'}\delta_{n_2,n_2'}\delta_{\ell_2,\ell_2'} \tag{10}$$

with

$$U^{I}_{n,n'} = \int_0^\infty R_{n\ell}(\xi)\frac{e^2}{4\pi\epsilon\xi}R_{n'\ell}(\xi)\xi\,\mathrm{d}\xi \tag{11}$$

where $R_{n\ell}$ is the radial part of a 2D harmonic oscillator function. We let $\vec{\xi}_1' = \vec{r}_2 - \vec{r}_3$, $\vec{\xi}_2' = \vec{r}_1 - (\vec{r}_2 + \vec{r}_3)/2$. Let us define

$$B_{[K],[K']} = \int \Phi_{[K]}(\vec{\xi}_1, \vec{\xi}_2)\Phi_{[K']}(\vec{\xi}_1', \vec{\xi}_2')\,\mathrm{d}\vec{\xi}_1\,\mathrm{d}\vec{\xi}_2, \tag{12}$$

which is the transformation bracket of two 2D harmonic product states with two different sets of relative coordinates. Then

$$\langle\Phi_{[K]}|V_{inter}|\Phi_{[K']}\rangle = 2\sum_{[K''][K''']} B_{[K],[K'']}B_{[K'],[K''']}U^{II}_{n_1'',n_1'''}\delta_{\ell_1'',\ell_1'''}\delta_{n_2'',n_2'''}\delta_{\ell_2'',\ell_2'''} \tag{13}$$

where

$$U^{II}_{n,n'} = \int_0^\infty R_{n\ell}(\xi)\frac{e^2}{4\pi\epsilon\sqrt{\xi^2+d^2}}R_{n'\ell}(\xi)\xi\,\mathrm{d}\xi. \tag{14}$$

Evidently, the introduction of $B_{[K],[K']}$ can help to reduce the other multiple integral into a single integral. Non-vanishing $B_{[K],[K']}$ occurs only when the two states $\Phi_{[K]}(\vec{\xi}_1, \vec{\xi}_2)$ and $\Phi_{[K']}(\vec{\xi}_1', \vec{\xi}_2')$ have exactly the same eigenenergy and eigenangular momentum. An analytical expression for $B_{[K],[k']}$ has already be derived in [18]. The accuracy of the solutions depends on how large the model space is. Since we interested only in the low-lying states and in the qualitative aspects, the model space adopted is neither very large—to facilitate numerical calculation—nor very small—to ensure qualitative accuracy. This is achieved by extending the dimension of the model space step by step; in each step the new results are compared with previous results from a smaller space, until satisfactory convergence is achieved. In this paper, the dimension of the model space is constrained by $0 \leqslant N = 2(n_1 + n_2) + |\ell_1| + |\ell_2| \leqslant 24$. If N is increased by 2, the ratio of the difference in energy is less than 0.01%.

3. Numerical results

In what follows the energy unit is meV and the length unit is nm. We used the following parameters: $m_e^* = 0.067\,m_e$ (m_e is the mass of the free electron), $\epsilon = 12.4$, and $g^* = -0.44$, which are typical for a GaAs system, and a confinement strength $\hbar\omega_0 = 1.0$ meV is adopted. First we calculated the correlation energy spectra of the low-lying states for the single-dot case, i.e., $d = 0$, as a function of the external magnetic field (see figure 1) for two different values of the total spin: (a) $S = 3/2$ and (b) $S = 1/2$. It is the competition between the single-particle energy and the interaction energy that finally determines the total energy. The existence of the Zeeman term $\omega_c L_z/2$ (negative) enables states with larger L to be possibly even lower in energy than those with smaller L. As a result, the lowest state of a spin configuration moves to states with larger L as magnetic field increases. However, the transition is strictly limited to being between two magic values of L. It is readily seen that the magic series for the three-electron single QD is $L = 3k$ if $S = 3/2$, where k is an integer, or $L \neq 3k$ if $S = 1/2$. The arising of magic angular momenta in three-electron QDs can be easily explained from an analysis of symmetry [4, 19].

To see intuitively the effect of inter-dot correlation, we set $d = 10.0$ nm and $\hbar\omega_0 = 1.0$ meV (i.e., a double-layer QD) and plotted in figure 2 the correlation energy spectrum of the low-lying states for the fully polarized system ($S = 3/2$). We find that the ground-state transition is qualitatively the same as those of a three-electron single dot; and as the distance d increases, the ground-state transitions shift to higher magnetic field. This can be interpreted

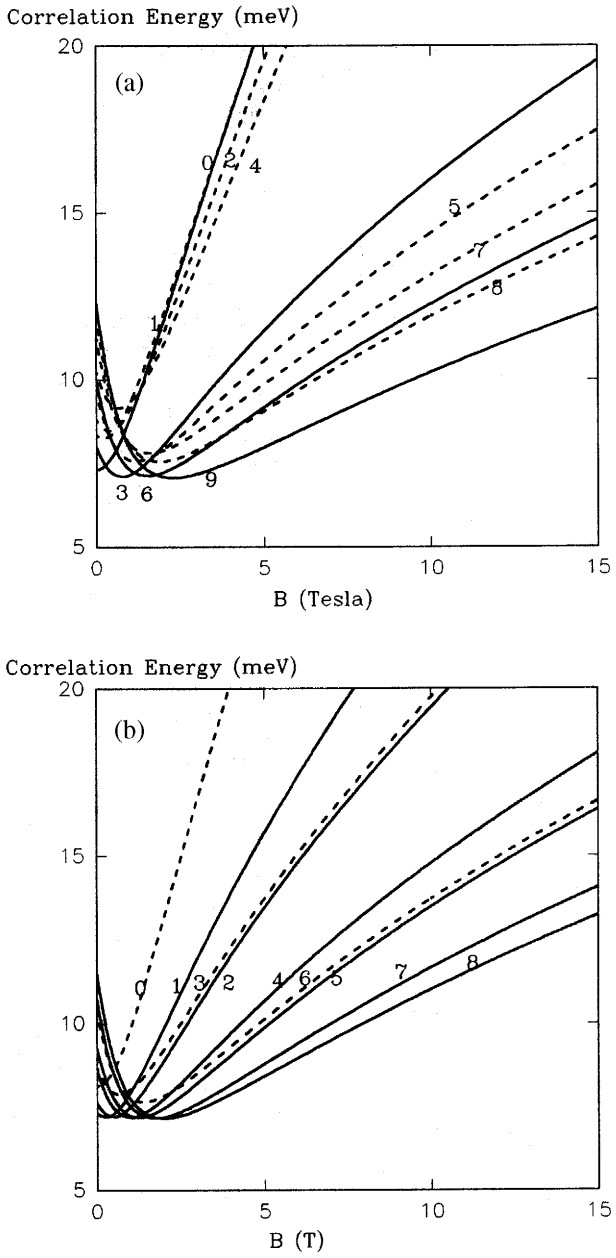

Figure 1. Correlation energy spectra of the state with lowest L as functions of magnetic field; (a) $S = 3/2$; (b) $S = 1/2$. The solid curves are associated with magic numbers L; the dashed curves are associated with non-magic values of L. The numbers in the figures label the angular momenta of the state. The parameters are taken as appropriate for GaAs; $\hbar\omega_0 = 1.0$ meV and $d = 0$.

as follows. The orbital radii of the electrons are proportional to the QD size and the quantum number of the angular momentum [20]. When the magnetic field increases, the dot size will decrease and the electrons will in turn jump to higher orbits with higher angular momentum

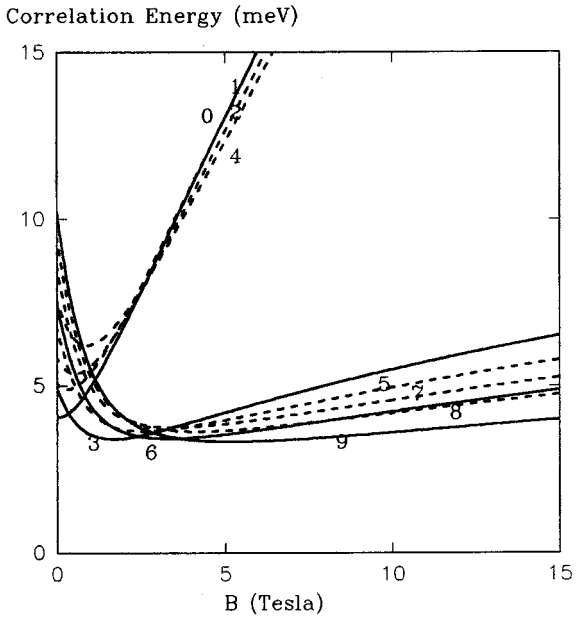

Figure 2. As figure 1(a), but for $d = 10.0$ nm.

to avoid repulsive interaction energy. When the distance d increases, the repulsive interaction energy decreases and the electrons jump to higher orbits at higher magnetic field.

It is interesting to compare the above results with those obtained when the distance d between the vertically coupled dots is larger, such that the two dots become independent. Obviously, for a larger separation, the electron tunnellings between the two dots can be negligible. In this case, the spin S_{12} of the electrons 1 and 2 is a good quantum number. In figure 3 we plotted the correlation energy spectra of the low-lying states for the fully polarized system (i.e., $S_{12} = 1$) as functions of the external magnetic field B with $d = 100.0$ nm and $\hbar\omega_0 = 1.0$ meV. They is qualitatively the same as those for a two-electron single QD. The two-electron single-dot system has been studied in great detail by Merkt *et al* [21]. As is required by the Pauli principle, $L = 2k + 1$ if $S_{12} = 1$ and $L = 2k$ if $S_{12} = 0$. Obviously, in figure 3, it is readily seen that the ground transitions occur in the sequence of values $L = 2k + 1$ as the magnetic field is increased. For a fully polarized three-electron system, it is the sequence of $L = 2k + 1$, and $L \neq 3k$—which can become the lowest state for uncoupled dots—fails to become the lowest state for coupled dots. The physical origin is that the equilibrium configuration of the three-electron system in coupled dots is an equilateral triangle with the particles at the vertices when their positions are vertically projected onto the same x–y plane, but that of two-electron systems in QDs is a linear chain with the particles on the two ends. If the wavefunction is smoothly (without nodal lines) distributed around the above equilibrium configurations, the binding will be averagely strong and the internal motion will appear only as a gentle oscillation around the equilibrium configuration. The total energy can then be minimized. Due to quantum mechanical symmetry confinement, there are only certain states with the magic angular momenta that can form the above equilibrium configurations. Obviously a cyclic permutation is equivalent to a rotation by 120° in an equilateral triangle configuration and a permutation is equivalent to a rotation by 180° in a linear chain configuration; hence, the magic number sequences of three-electron coupled QDs and uncoupled QDs are different.

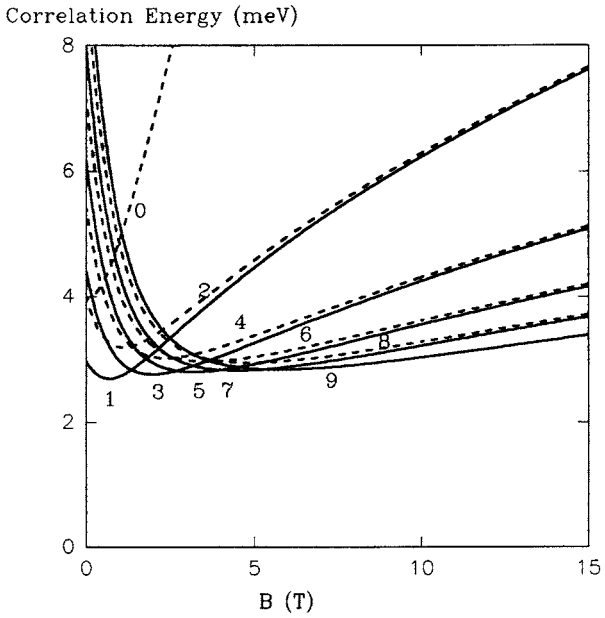

Figure 3. As figure 1(a), but for $d = 100.0$ nm.

In conclusion, we have numerically diagonalized the Hamiltonian of three interacting electrons in a double-layer QD with parabolic potentials under a magnetic field. We have found magic numbers intrinsic to vertically coupled QDs. As for the single-dot systems, the ground-state transitions of vertically coupled QDs have been found to occur only at certain magic values of L, showing a selection rule for the total angular momentum L. As the distance d between the two-layer dots increases, the ground-state transitions shift to higher magnetic field. The inter-dot correlation leads to some sequences of possible disappearances of ground states which are present for uncoupled dots.

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