Transition of the ground state in a coupled N-layer quantum dot

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ABSTRACT

An exact method is proposed to diagonalize the Hamiltonian of an N-layer quantum dot containing N electrons in arbitrary magnetic fields. For $N = 4$, energy spectra of the dot are calculated as a function of the applied magnetic field. We find discontinuous ground-state energy transitions induced by an external magnetic field in the case of strong coupling. However, in the case of weak coupling, the transition does not occur and the angular momentum remains zero.

Keywords: : quantum dot, ground-state transition

There has been growing interest in the physics of quantum dots (QDs) in recent years[1,2] because of the rapid development of fabrication technology. Quantum dots confine electrons in all three spatial dimensions and the many-body effects of electron-electron interactions show a broad range of electronic structures similar to those of real atoms. The discrete energy spectrum of the artificial atom depends on the number of electrons N and the size of confinement D. Both can be controlled by experiments, and the competition between quantum confinements and Coulomb interactions determines the physical properties of a QD. Since they offer the possibility of applications in future optoelectronic devices and optical memories, it is most interesting to study the electronic structure in QDs.

Discrete energy levels of few-electron systems confined in a QD are studied from the transport measurements.[3,4] Distinct periodic structure of the Coulomb-regulated conductance peaks is seen as a function of the magnetic field, and the magnetic field dependence of single-particle levels can be deduced from these peaks. These single-electron spectroscopic techniques allow direct measurements of the QD levels as a function of magnetic fields. The ground state of an N-electron system in magnetic fields has been measured up to $N = 35$.[5] The results are found to be consistent with the confinement of a cylindrically symmetric parabolic potential $m_e\omega_0^2 r^2/2$. Excited states are investigated more recently by the analysis of photoluminescence excitation spectra.[6,7]

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 been so far focused on the electronic structure of a single disc-like QD[8,9]. In such cases, the QD energy levels are mainly determined by the lateral electronic motion. The effects of thickness has been discussed only in the case of polaronic states.[10]

The electron-electron interaction in QDs has 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.[11] As the field strength increases the magic number jumps, causing discontinuities in the magnetization.[12] Further studies of the many-electron ground state in a parabolic QD shows the capacitance oscillation as a function of the electron number due to the shell structure.[13] A numerical calculation of the QD energy spectra for $N = 5$ and 6 in the strong field limit reveals a number of fine structures associated with ground-state level crossings, implying the existence of structural phase transitions.[14] As a matter of fact, when the magnetic field continuously increases, discontinuities are found in the magnetization[15,16] and electronic heat capacity,[17] as well as in the oscillator strength and other optical properties.[18]

Recently, a coupled QD that could be considered as an artificial molecule has attracted much attention[19–21], the added degree of freedom is expected to enrich the physics. Rich electronic structures and optical properties, and a variety of structural phase transitions are predicted in such systems. The main feature in this system is the effects of dot-dot and electron-electron interactions on the electronic structure. 1993 Bryant[22] studied the energy spectra, charge densities, and correlation functions for interacting two-electron systems in coupled dots as functions of the applied bias. In 1999 Oh et al[23] 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[24] studied the energy spectra for interacting two-electron system in horizontal and vertical coupled QDs as functions of QD separation, lateral confinement, and magnetic field. They considered each dot as a strictly 2D system. Tokura et al[25] next investigated the electron states in two vertically coupled

QDs using an exact diagonalization method. From a theoretical point of view, it would be very interesting further to clarify the effect of interdot separation and external magnetic field on multilayer vertically coupled QDs. However, most of previous work has focused on double-layer QD systems, and only few works related to the multiple QD systems, e.g., Benjamin and Johnson[3] has given an analytical investigation of the multiple QD system through some assumptions and approximations of the interlayer interactions. Zhang et al[4] have numerically calculated the energy spectrum of the low-lying states of a vertically coupled three-layer QD system, which each layer contains one electron. Thus, it is then intriguing to ask when the layer number further increases what happens in QDs. We propose in this paper a procedure of exact diagonalization to study N-layer QDs. The low-lying energy levels as well as the ground state electronic structure are calculated systematically as a function of magnetic fields of arbitrary strength.

Consider a coupled collinear N-layer QD containing a total of N electrons, where the interlayer separation d and the internal magnetic field B are varied. We assume that each QD contains only one electron. The lateral potential $\frac{1}{2}m_e\omega_0^2 r^2$ that confines the electrons in the xy-plane is assumed to be identical in each layer, where m_e is the electron effective mass and ω_0 measures the strength of the parabolic confinement. The external magnetic field is assumed to be along the z-direction. With the symmetric gauge, the Hamiltonian takes the form

$$H = \sum_{i=1}^{N}\left(\frac{p_i^2}{2m_e} + \frac{1}{2}m_e\omega_0^2 r_i^2\right) + V_{inter} + \frac{1}{2}\omega_c L_z - g^*\mu_B B S_z, \quad (1)$$

with

$$V_{inter} = \frac{e^2}{\epsilon}\sum_{i<j}^{N}\frac{1}{\rho_{ij}}, \quad (2)$$

where $\rho_{ij} = \sqrt{|\vec{r}_i - \vec{r}_j|^2 + [(i-j)d]^2}$. The z-component of the total orbital (spin) angular momentum is denoted by L_z (S_z). g^* stands for the Lande factor and μ_B the Bohr magneton. The electron frequency is by $\omega = \sqrt{\omega_0^2 + \omega_c^2/4}$ where $\omega_c = eB/m_e$ is the cyclotron frequency.

To treat the N-particle system, we introduce a set of the center of mass (c.m.) coordinates and a set of Jacobi coordinates, which is a set of $(N-1)$ independent vectors $\vec{\xi}_i$. Each $\vec{\xi}_i$ represents the displacement of the c.m. of one subset of the N-electron system from the c.m. of another subset in such a way that no two Jacobi vectors are connected to the same c.m.. Associated with each Jacobi vector, a reduced mass μ_i is defined for the pair of clusters whose centers of mass are joined by $\vec{\xi}_i$. The center of mass motion is completely separated from the relative motion in this approach, and the multiple integration can be reduced to single integrals by means of the Jacobi coordinates and Talmi-Moshinsky transformation coefficients. The advantage of this method is particularly remarkable in dealing with few-body problems such as the QDs. When the number of electrons is larger, it is more convenient to use the usual second-quantization method, which includes excitations of the c.m. as well. Eq. (1) can then divided into two independent parts

$$H = H_{cm} + H_r, \quad (3)$$

where

$$H_{cm} = \frac{P_{cm}^2}{2M} + \frac{1}{2}M\omega^2 R_{cm}^2, \quad (4)$$

is for the c.m. motion and $M = Nm_e$ is the total mass. It is trivial (simply a harmonic oscillation). H_r is for the relative motion:

$$H_r = H_0 + V_{inter}, \quad (5)$$

with

$$H_0 = \sum_{\nu=1}^{N-1}\left(\frac{p_\nu^2}{2\mu_\nu} + \frac{1}{2}\mu_\nu\omega^2\xi_\nu^2\right) + \frac{1}{2}\omega_c L_z - g^*\mu_B B S_z. \quad (6)$$

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 eigen-functions and eigen-energies associated with relative motion, H_r is diagonalized in a model space spanned by the translationally invariant two-dimensional harmonic product bases with a variational parameter ω.

To see intuitively the effect of inter-dot correlation, we set $N = 4$ and $d = 10.0nm$ (for the case of strong coupling) and $\hbar\omega_0 = 3.6meV$ (i.e., a vertically coupled four-layer QD) and plotted in Fig. 1 the energy spectrum of the low-lying states for the fully polarized system ($S = 2$). We find that ground-state transition is qualitative the same as those of a four-electron single dot[5], and as the distance d increases, the ground-state transitions shift to the higher magnetic field, e.g., the first ground-state transition for a four-electron single QD occurs at $B = 1.0T$ and that for a vertically four-layer QD with $d = 10nm$ occurs at $B = 2.5T$. On the other hand, we find that the second ground-state transition does not occur in the domain of $B \leq 15T$. It can be interpreted by the following. The orbit radii of the electrons is proportional to the QD size and the quantum number of the angular momentum. When the magnetic field increases, the dot size will decrease and the electrons will in turn jump to higher orbits with higher angular momentum to avoid repulsive interaction energy. When the distance d increases, the repulsive interacting energy decreases and the electrons jump to higher orbits at higher magnetic field.

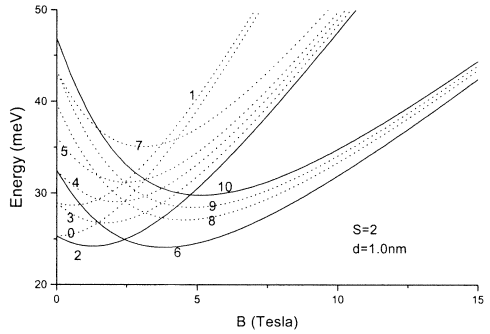

Figure 1: Energy spectra of the low-lying state as function of magnetic field for the fully polarized system ($S = 2$). The solid lines are associated with magic numbers L, the dashed lines are associated with non-magic numbers L. The numbers in the figures label the angular momentum of the state. Parameters are taken appropriate for GaAs, $\hbar\omega_{\square} = 3.6meV$ and $d = 10.0nm$.

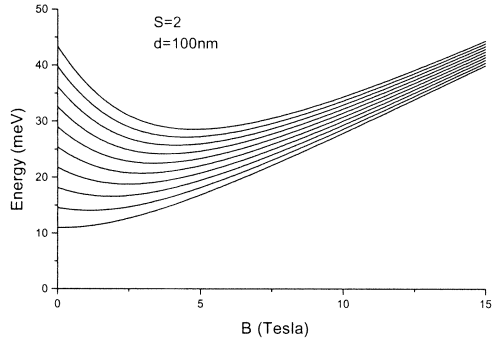

Figure 2: The same as Fig. 1 except for $d = 100.0nm$.

It is interesting to compare the above results with those when the distance d between the vertically coupled dots is larger so that the four dots become independent, such that the Coulomb repulsion interaction become weaker. In Figure 3 we plotted the energy spectrum of the low-lying states for the fully polarized system as a function of the external magnetic field B with $d = 100.0nm$ (for the case of weak coupling) and $\hbar\omega_{\square} = 3.6meV$. Figure 2 shows that no transition in the domain of $B \leq 15T$ is found if d is large, i.e., in the case of weak coupling, the angular momentum L of the ground state does not change in accordance with the change of the magnetic field B and remains zero as a single-electron QD. Obviously, for a larger separation, the electron tunnelling between the two dots can be negligible. The origin of the magic numbers is the quantum constraint arising from the Pauli principle.[Œ] However, there is not the similar origin in our system considered.

Acknowledgment: This work is financially supported by the National Natural Science Foundation under Grant No. 10275014.

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