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Ground-State Properties of Quantum Dots with a Magnetic Field

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The transitions in the spin and orbital angular momentum of the ground state of two interacting electrons, parabolically confined in the quantum dot, in a magnetic field of arbitrary strength are studied.

1. Introduction

With recent progress in nanofabrication technology, it has been possible to confine electrons in all three spatial dimensions in semiconductor structures called quantum dots (QDs). In such small structures the electrons are fully quantized into a discrete spectrum of energy levels. The confinement in z-direction, which is the growth direction, is assumed to be stronger than that in the xy-plane, so that the dots can be viewed as two-dimensional disks. The growing interest in this field is motivated by the physical effects and the potential device applications, both as electronic memories as well as optoelectronic devices to which many experimental [1 to 5] and theoretical [7 to 20] works have been devoted. The effects of a magnetic field, which plays a useful role in identifying the absorption features, on the states of interacting electrons, impurities [13], and excitons [15 to 20] confined in the QD have been intensively studied. Maksym and Chakraborty [6] have studied the eigenstates of interacting electrons, parabolically confined in the QD, in a magnetic field perpendicular to the plane of the QD and found that the Coulomb interaction has an important effect on the magnetic field dependence of the energy spectrum. When the potential is quadratic the far-infrared (FIR) spectroscopy is unable to detect the Coulomb interaction by virtue of the generalized Kohn theorem. Wagner et al. [7] have also considered two interacting electrons, parabolically confined, in a perpendicular magnetic field in addition to the spin and predict oscillations between the spin-singlet and spin-triplet ground states, Pfannkuche et al. [8] have discussed the properties of the helium quantum dot in a magnetic field by using Hartree, Hartree-Fock, and exact treatments, Ferconi and Vignale [9] have presented a study of ground-state energies and density profiles of quantum dots, with large number of electrons in a magnetic field using the current-density-functional theory (CDFT). Merkt [10] has studied the FIR spectroscopy of quantum dots. Maksym and Chakraborty [6] and De Groote et al. [11] have investigated the thermodynamic properties of quantum dots such as heat capacity and magnetization as sensitive probe to the ground-state transitions.

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In this work we will calculate the enery spectra of two interacting electrons in the quantum dot in a magnetic field taking into account the effect of spin and parabolic confinement. We will also investigate the important role of the electron–electron interaction energy in the angular momentum transitions of the ground state of the quantum dot system.

2. The Hamiltonian

The effective-mass Hamiltonian for an interacting pair of electrons confined in a quantum dot by a parabolic potential of the form $m^*\omega_0 r^2/2$ in a magnetic field applied parallel to the z-axis (and perpendicular to the plane of the quantum dot where the electrons are confined) in the symmetric gauge, is written as $H = H_{\text{space}} + H_{\text{spin}}$; H_{space} and H_{spin} depend only on spatial and spin coordinates, respectively. Explicitly,

$$H_{\text{space}} = \sum_{i=1}^{2} \left[-\frac{\hbar^2 \nabla_i^2}{2m^*} + \frac{1}{2} m^* \omega^2 r_i^2 + \frac{\hbar\omega_c}{2} L_i^z \right] + \frac{e^2}{\varepsilon |\boldsymbol{r}_1 - \boldsymbol{r}_2|} \tag{1}$$

and

$$H_{\text{spin}} = g^* \mu_B B \sum_i S_{i,z} , \tag{2}$$

where the two-dimensional vectors $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ describe the positions of the first and the second electron in the xy-plane, respectively, L_i^2 and $S_{i,z}$ stand for the z-components of the orbital and angular momentum and spin for each electron, respectively, $\mu_B = e\hbar/2m_e$, g^*, $\omega_c = eB/m^*c$, m^*, and ε are the Bohr magneton, Landé factor, the cyclotron frequency, effective mass, and dielectric constant of the medium, respectively. The frequency ω depends on both the magnetic field B and the confinement frequency ω_0, and is given by

$$\omega = \left(\omega_0^2 + \frac{\omega_c^2}{4} \right)^{1/2} . \tag{3}$$

Upon introducing the center-of-mass $\boldsymbol{R} = (\boldsymbol{r}_1 + \boldsymbol{r}_2)/\sqrt{2}$ and the relative coordinates $\boldsymbol{r} = (\boldsymbol{r}_1 - \boldsymbol{r}_2)/\sqrt{2}$, the Hamiltonian in (1) decoupled to center-of-mass motion Hamiltonian

$$H_R = -\frac{\hbar^2}{2m^*} \nabla_R^2 + \frac{m^*}{2} \omega^2 R^2 + \frac{\hbar\omega_c}{2} L_z^R \tag{4}$$

and the relative motion Hamiltonian

$$H_r = -\frac{\hbar^2}{2m^*} \nabla_r + \frac{m^*}{2} \omega^2 r^2 + \frac{\hbar\omega_c}{2} L_z^r + \frac{e^2}{\sqrt{2}r} . \tag{5}$$

Equation (4) describes the Hamiltonian of the harmonic oscillator with the well-known eigenenergies,

$$E_{n_{cm}, m_{cm}} = (2n_{cm} + |m_{cm}| + 1)\, \hbar\omega + \frac{\hbar\omega_c}{2} m_{cm} \tag{6}$$

labeled by the radial ($n_{cm} = 0, 1, 2, \ldots$) and the azimuthal ($m_{cm} = 0, \pm 1, \pm 2, \pm 3, \ldots$) quantum numbers. Antisymmetry of the two-electron wavefunction requires that for even m they are singlets and for odd m triplets with the Zeeman energy term $E = g^* \mu_B B S_z$, and the total spin $S_z = [1 - (-1)^m]/2$ represents a good quantum number for the system. The total energy states of the Hamiltonian, $E = E_R(n_{cm}, m_{cm}) + E_r(m_r, m) + E_{\text{spin}}(S_z)$, are labeled by

the cm and relative quantum numbers, $|n_{cm}, m_{cm}; n_r, m\rangle$. The problem is reduced to obtaining eigenenergies $E_{n_r,m}$ of the relative motion Hamiltonian.

The eigenenergies are obtained with the help of the $1/N$ expansion method. The shifted $1/N$ expansion method, N describing the spatial dimensions, is a pseudoperturbative technique in the sense that it proposes a perturbation parameter that is not directly related to the coupling constant [15, 21 to 23]. We give here the essential steps which lead to the energy expression.

The method starts by writing the radial Schrödinger equation for an arbitrary cylindrically symmetric potential, in an N-dimensional space, as

$$\left[-\frac{d^2}{dr^2}+\frac{(k-1)\,(k-3)}{4r^2}+V(r)\right]\psi(r)=E_r\psi(r)\,, \tag{7}$$

where $k=N+2m$.

In order to get useful results from the $1/\bar{k}$ expansion, where $\bar{k}=k-a$ and a is a suitable shift parameter, the large-$\bar{k}$ limit of the potential must be suitably defined [21]. Since the angular momentum barrier term behaves like $\bar{k}^2$ at large $\bar{k}$, so the potential should behave similarly. This will give rise to an effective potential which does not vary with $\bar{k}$ at large values of $\bar{k}$ resulting in a sensible zeroth-order classical result. Hence (7) in terms of the shift parameter becomes

$$\left[-\frac{d^2}{dr^2}+\frac{\bar{k}^2[1-(1-a)/\bar{k}]\,[1-(3-a)/\bar{k}]}{4r^2}+\frac{V(r)}{Q}\right]\psi(r)=E_r\psi(r)\,, \tag{8}$$

where

$$V(r)=\frac{\sqrt{2}}{r}+\frac{1}{4}\,\omega^2r^2+m\,\frac{\omega_c}{2} \tag{9}$$

and Q is a scaling constant to be specified from (11). The shifted $1/N$ expansion method consists in solving (8) systematically in terms of the expansion parameter $1/\bar{k}$. The leading contribution to the energy comes from

$$\bar{k}^2V_{\text{eff}}(r_0)=\frac{\bar{k}^2}{r_0^2}\left(\frac{1}{4}+\frac{r_0^2V(r_0)}{Q}\right), \tag{10}$$

where r_0 is the minimum of the effective potential, given by

$$2r_0^3V'(r_0)=Q\,. \tag{11}$$

It is convenient to shift the origin to r_0 by the definition

$$x=\bar{k}^{1/2}(r-r_0)/r_0 \tag{12}$$

and expanding (8) about $x=0$ in powers of x. Comparing the coefficients of powers of x in the series with the corresponding ones of the same order in the Schrödinger equation for the one-dimensional anharmonic oscillator, we determine the anharmonic oscillator frequency, the energy eigenvalue, and the scaling constant in terms of $\bar{k}$, Q, r_0, and the potential derivatives. The anharmonic frequency parameter is

$$\bar{\omega}=\left[3+\frac{V''(r_0)}{V'(r_0)}\right]^{1/2} \tag{13}$$

and the energy eigenvalues in powers of $1/\bar{k}$ (up to third order) read as

$$E_{n_r,m} = \frac{\sqrt{2}}{r_0} + \frac{1}{4}\,\omega r_0^2 + m\,\frac{\omega_c}{2} + \frac{\bar{k}^2}{4r_0} + \frac{1}{r_0^3}\left[\frac{(1-a)\,(3-a)}{4} + \gamma_1\right] + \frac{\gamma_2}{\bar{k}r_0^2}\,. \tag{14}$$

The explicit forms of γ_1 and γ_2 are given in the Appendix. The shift parameter a, which introduces an additional degree of freedom, is chosen so as to make the first term in the energy series of order $\bar{k}$ vanish, namely,

$$\frac{\bar{k}}{r_0^2}\left[\left(n_r + \frac{1}{2}\right)\bar{\omega} - \frac{(2-a)}{2}\right] = 0\,. \tag{15}$$

By requiring agreement between $1/\bar{k}$ expansion and the exact analytic results for the harmonic and Coulomb potentials, from (15) we obtain

$$a = 2 - (2n_r + 1)\,\bar{\omega}\,, \tag{16}$$

where n_r is the radial quantum number related to the principal n and magnetic m quantum numbers by the relation $n_r = n - |m| - 1$. Energies and lengths in (7) to (16) are expressed in units of R^* and a^*, respectively.

For the two-dimensional case, $N = 2$, (11) takes the following form:

$$\sqrt{2r_0 V'(r_0)} = 2 + 2m - a = Q^{1/2}\,. \tag{17}$$

Once r_0 (for a particular quantum state and confining frequency) is determined, the task of computing the energy is relatively simple.

3. Results and Conclusions

Our results for QDs made of GaAs/AlGaAs are presented in Fig. 1 and 2 and Table 1. We have displayed in Fig. 1, the energies of the states $|00;\,0m\rangle$, $m = 0, -1, -2, \ldots, -10$, for two interacting electrons parabolically confined in the quantum dot of size $l_0 = 3a^*$ as a

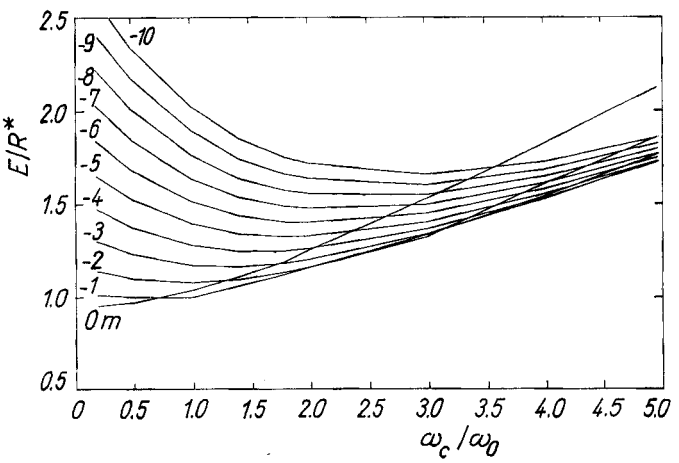

Fig. 1. The total eigenenergies of the states $|00;\,0m\rangle$, $m = 0, -1, -2, \ldots, -10$, for two interacting electrons, parabolically confined in the quantum dot of size $l_0 = 3a^*$ and $g^* = 0$ (for GaAs $a^* = 98.7$ Å and $R^* = 5.83$ meV)

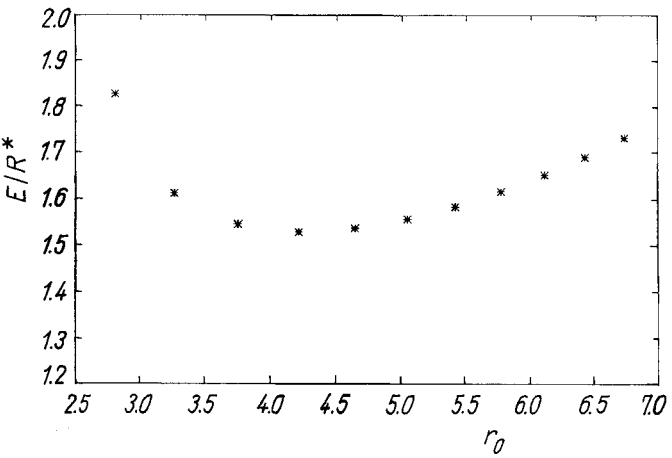

Fig. 2. The total eigenenergies of the states $|00; 0m\rangle$, $m = 0, -1, -2, \ldots, -10$, against the roots r_0 for a quantum dot of size $l_0 = 3a^*$ and $\omega_c/\omega_0 = 4$

function of the ratio ω_c/ω_0 and for $g^* = 0$. As the magnetic field increases the energy of the state $m = 0$ enhances while the energy of the states with non-vanishing azimuthal quantum number m decreases, thus leading to a sequence of different ground states.

These results are in agreement with the findings of Wagner et al. [7]. The level-crossings, which appear in the spectra, can be understood from the dependence of the Coulomb and kinetic energies, for a particular value of the ratio ω_c/ω_0, on the azimuthal quantum number $|m|$. The dominant contribution to the relative energy $E_{n_r,m}$ of the system is coming from the first term, namely,

$$V(r_0) = \frac{\sqrt{2}}{r_0} + \frac{1}{4}\left(\omega_0^2 + \frac{\omega_c^2}{4}\right) r_0^2 .$$

The roots r_0, which are evaluated for quantum states $|00; 0m\rangle$, $m = 0, -1, -2, \ldots, -10$ and $\omega_c/\omega_0 = 4$, are listed in Table 1. As is clearly seen from the table, the root r_0 increases as $|m|$ increases and as a result the electron–electron interaction term decreases. On the other hand, the magneto-confining energy increases. The decrease in the Coulomb interaction energy does not compensate completely the increase in the kinetic energy of the system and the net result is that the total energy of the system as a function of r_0 has a minimum as shown in Fig. 2. As a result of this competition, the spin and orbital angular momenta of the ground state of the interacting system change with increasing magnetic field.

In conclusion, we have obtained the energy spectra of two interacting electrons, parabolically confined in the quantum dot in a magnetic field. We have discussed the effects of the Coulomb interaction and the spin on the energy level-crossings in the quantum dots. The

Table 1

The values of the roots r_0 calculated for quantum states with non-vanishing azimuthal quantum numbers (m), $\hbar\omega_0 = 1.3$ meV and $\omega_c/\omega_0 = 4$

m	0	−1	−2	−3	−4	−5	−6	−7	−8	−9	−10
r_0	2.799	3.263	3.752	4.215	4.644	5.044	5.418	5.770	6.103	6.419	6.722

comparison (see Fig. 1b of [7]) shows that our results are in good agreement with other works. With the $1/N$ expansion method, we have studied the evolution of the ground-state properties of quantum dots in a magnetic field of arbitrary strength.

Appendix

The explicit forms of the parameters γ_1 and γ_2 are given in the following. Here R^* and a^* are used as units of energy and length, respectively.

$$\gamma_1 = c_1 e_2 + 3c_2 e_4 - \bar{\omega}^{-1}[e_1^2 + 6c_1 e_1 e_3 + c_4 e_2^3] \tag{A1}$$

and

$$\gamma_2 = T_7 + T_{12} + T_{16}\,, \tag{A2}$$

where

$$T_7 = T_1 - \bar{\omega}^{-1}[T_2 + T_3 + T_4 + T_5 + T_6]\,, \tag{A3}$$

$$T_{12} = \bar{\omega}^{-2}[T_8 + T_9 + T_{10} + T_{11}]\,, \tag{A4}$$

$$T_{16} = \bar{\omega}^{-2}[T_{13} + T_{14} + T_{15}]\,, \tag{A5}$$

with

$$T_1 = c_1 d_2 + 3c_2 d_4 + c_3 d_6\,, \qquad T_2 = c_1 e_2^2 + 12c_2 e_2 e_4\,,$$
$$T_3 = 2e_1 d_1 + 2c_5 e_4^2\,, \qquad T_4 = 6c_1 e_1 d_3 + 30c_2 e_1 d_5\,,$$
$$T_5 = 6c_1 d_3 e_1 + 2c_4 e_3 d_3\,, \qquad T_6 = 10c_6 e_3 d_5\,,$$
$$T_8 = 4e_1^2 e_2 + 36c_1 e_1 e_2 e_3\,, \qquad T_9 = 8c_4 e_2 e_3^2\,,$$
$$T_{10} = 24ce_1^2 e_4 + 8c_7 e_1 e_3 e_4\,, \qquad T_{11} = 12c_8 e_3^2 e_4\,,$$
$$T_{13} = 8e_1 e_3 + 108c_1 e_1 e_3\,, \qquad T_{14} = 48c_4 e_1 e_3\,,$$
$$T_{15} = 30c_9 e_3\,,$$

where c, d, and e are parameters given as

$$c_1 = 1 + 2n_r\,, \qquad c_2 = 1 + 2n_r + 2n_r^2\,, \qquad c_3 = 3 + 8n_r + 6n_r^2 + 4n_r^3\,,$$
$$c_4 = 11 + 30n_r + 30n_r^2\,, \qquad c_5 = 21 + 59n_r + 51n_r^2 + 34n_r^3\,,$$
$$c_6 = 13 + 40n_r + 42n_r^2 + 28n_r^3\,, \qquad c_7 = 31 + 78n_r^2 + 78n_r^3\,,$$
$$c_8 = 57 + 189n_r + 225n_r^2 + 150n_r^2\,, \qquad c_9 = 31 + 109n_r + 141n_r^2 + 94n_r^3\,,$$
$$e_j = \frac{\varepsilon_j}{\bar{\omega}^{j/2}} \quad \text{and} \quad d_i = \frac{\delta_i}{\omega^{i/2}}\,,$$

where $j = 1, 2, 3, 4$ and $i = 1, 2, 3, 4, 5, 6$.

$$\varepsilon_1 = 2 - a\,, \qquad \varepsilon_2 = -\frac{3(2-a)}{2}\,, \qquad \varepsilon_3 = -1 - \frac{r_0\sqrt{2}}{Q}\,,$$
$$\varepsilon_4 = \frac{5}{4} + \frac{r_0\sqrt{2}}{Q}\,; \qquad \delta_1 = -\frac{(1-a)\,(3-a)}{2}\,,$$

$$\delta_2 = -\frac{3(1-a)\,(3-a)}{4}\,, \qquad \delta_3 = 2(2-a)\,, \qquad \delta_4 = -\frac{5(2-a)}{2}\,,$$

$$\delta_5 = -\frac{3}{2} - \frac{r_0\sqrt{2}}{Q}\,, \qquad \delta_6 = \frac{7}{4} + \frac{r_0\sqrt{2}}{Q}\,.$$

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