Commun. Theor. Phys. (Beijing, China) **31** (1999) pp 321–326

Vol. 31, No. 3, April 30, 1999

The Spectra of Two-Electron Quantum Dot: Shifted $1/N$ Method

Mohammad El-Said

EMU, Physics Department, G. Magosa, Mersin 10, Turkey

(Received May 20, 1997)

Abstract *The spectra of two-electron quantum dot in a magnetic field of arbitrary strength is studied by using the shifted $1/N$ expansion method. The comparisons show that our results are in good agreement with the results of fixed-phase quantum Monte Carlo method and exact ones [Bolton, Phys. Rev.* **B54** *(1996) 4780].*

PACS numbers: 68.65.+g, 73.20.Dx, 85.30.Vw
Key words: quantum dots, interacting electrons, $1/N$ method

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[1–7] and theoretical[8–27] works have been devoted. The spectra of few-electron quantum dot presented in a magnetic field has been intensively studied using different methods.

In this work we have used the shifted $1/N$ expansion method to produce an energy expression and then obtain the spectra of the quantum dot consisting of two electrons. We have shown the crossover of two levels in the calculated spectra. Making use of this energy expression, we have explained this effect as a competition between electron-electron interaction, many-body effect, and the magneto-confinement energy terms. We have compared our results with the results of fixed-phase Monte Carlo method, very recently produced by Bolton, and exact ones.[27]

We have considered electrons of effective masses m^* moving in the xy-plane and confined by a parabolic potential $(1/2)m^*\omega_0 r^2$, $r^2 = x^2 + y^2$, with a characteristic frequency ω_0. The Hamiltonian of two interacting electrons in the presence of a perpendicular magnetic field applied parallel to z-axis is then

$$H = \sum_{i=1}^{2}\Big[-\frac{\hbar^2}{2m^*}\nabla_i^2 + \frac{1}{2}m^*\omega_0^2 r_i^2 + \frac{\hbar\omega_c}{2}L_i^z\Big] + \frac{e}{\epsilon|\vec{r}_2 - \vec{r}_1|} + g^*\mu_B B\sum_i S_{i,z}\,, \tag{1}$$

where L_i^z and $S_{i,z}$ stand for the z-components of the orbital angular momentum and spin for each electron, $\mu_B = e\hbar/2m_e$, g^*, $\omega_c = eB/m^*c$ and ϵ are the Bohr magneton, Lande factor, the cyclotron frequency and the 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

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

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

$$H_R = -\frac{\hbar^2}{2m^*}\nabla_R^2 + \frac{m^*}{2}\omega^2 R^2 + \frac{\hbar\omega_c}{2}L_z^R \tag{3}$$

and the relative motion Hamiltonian

$$H_r = -\frac{\hbar^2}{2m^*}\nabla_r^2 + \frac{m^*}{2}\omega^2 r^2 + \frac{\hbar\omega_c}{2}L_z^r + \frac{e^2}{\sqrt{2}r}\,. \tag{4}$$

Equation (3) describes the Hamiltonian of the harmonic oscillator with the well-known eigen-energies

$$E_{n_{\rm cm},m_{\rm cm}} = (2n_{\rm cm} + |m_{\rm cm}| + 1)\hbar\omega + \frac{\hbar\omega_c}{2} m_{\rm cm} \tag{5}$$

labeled by the radial ($n_{\rm cm} = 0, 1, 2, \cdots$) and the azimuthal ($m_{\rm cm} = 0, \pm 1, \pm 2, \pm 3, \cdots$) quantum numbers. Antisymmetric two-electron wavefunction requires that even m are singlets and odd m triplets with the Zeeman energy term $E_{\rm spin} = g\mu_B^* B S_z$ and total spin $S_z = [1 - (-1)^m]/2$ represents a good quantum number for the system. The total energy states of the Hamiltonian, $E = E_R(n_{\rm cm}, m_{\rm cm}) + E_r(n_r, m) + E_{\rm spin}(S_z)$, are labeled by the cm and relative quantum numbers, $|n_{\rm cm}, m_{\rm cm}; n_r, m\rangle$. The problem is reduced to obtaining eigen-energies $E_{n_r,m}$ of the relative motion Hamiltonian.

The eigen-energies are obtained by the help of the shifted $1/N$ expansion method. In N spatial dimensions the radial Schrödinger equation for the effective potential $V(r) = \sqrt{2}/r + (1/4)\omega^2 r^2$ becomes

$$\left[-\frac{{\rm d}^2}{{\rm d}r^2} + \frac{(\bar{k} + a - 1)(\bar{k} + a - 3)}{4r^2} + V(r)\right]\Psi(r) = E_r \Psi(r)\,, \tag{6}$$

where $\bar{k} = N + 2m - a$ and a is the shift parameter. Following the previous works of the shifted $1/N$ expansion method,[17,28–30] we give here only the energy expression which is needed to produce and explain the spectra of H_r. The energy expression reads as

$$E_{n_r,m} = \frac{\sqrt{2}}{r_0} + \frac{1}{4}\omega^2 r_0^2 + m\frac{\omega_c}{2} + \frac{\bar{k}^2}{4r_0} + \frac{1}{r_0^2}\left[\frac{(1-a)(3-a)}{4} + \gamma_1\right] + \frac{\gamma_2}{\bar{k} r_0^2}\,, \tag{7}$$

$$a = 2 - 2(2n_r + 1)\bar{\omega}\,, \tag{8}$$

$$\bar{\omega} = \left[3 + \frac{r_0 V''(r)}{V'(r_0)}\right]^{1/2}, \tag{9}$$

and the root is determined through the relation

$$(2r_0^3 V'(r_0))^{1/2} = 2 + 2m - a\,. \tag{10}$$

The explicit forms of the parameters γ_1 and γ_2 are given in the Appendix in terms of n_r, $\bar{\omega}$, r_0 and a. Once r_0, for particular quantum state $|n_r, m\rangle$ and confining frequency ω, is determined, the task of computing the energy is relatively simple.

In this work, we have considered QDs made of GaAs/AlGaAs. We have presented our results in Fig. 1 and in Tables 1–3. To show the energy level crossings, we have displayed in Fig. 1a, the energies of the states $|0, 0;\ 0, m\rangle$, $m = 0, -1, -3, \cdots, -7$, for two interacting electrons parabolically confined in the quantum dot with confining energy $\hbar\omega_0 = 3$ meV, as a function of the magnetic field strength B 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 finding of Bolton which was shown in Fig. 1b.[27] The level crossings, which appear in the spectra, can be understood from the dependence of the Coulomb and kinetic energy quantities, for 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, $V(r_0) = \sqrt{2}/r_0 + (1/4)\omega^2 r_0^2$. The roots r_0, which are evaluated for quantum states $|0, 0;\ 0, m\rangle$, $m = 0, -1, -3, \cdots, -7$ at different values of B are shown in Table 1. As clearly seen from the table, the root r_0 increases as $|m|$ increases and in the result the electron-electron interaction term decreases. On the other hand, the magneto-confining term increases. As a result of this competition, the spin and orbital angular momenta of the ground-state of the interacting system change with increasing of the magnetic field. The spin singlet-triplet transition occurs at $B \approx 1.8$ T. Remarkably, these transitions have been observed experimentally.[6] In Table 2, we have listed the energies for quantum states $|0, 0; 0, m\rangle$, $m = 0, -1, -3, \cdots, -7$, calculated at different values of magnetic

field strength B.

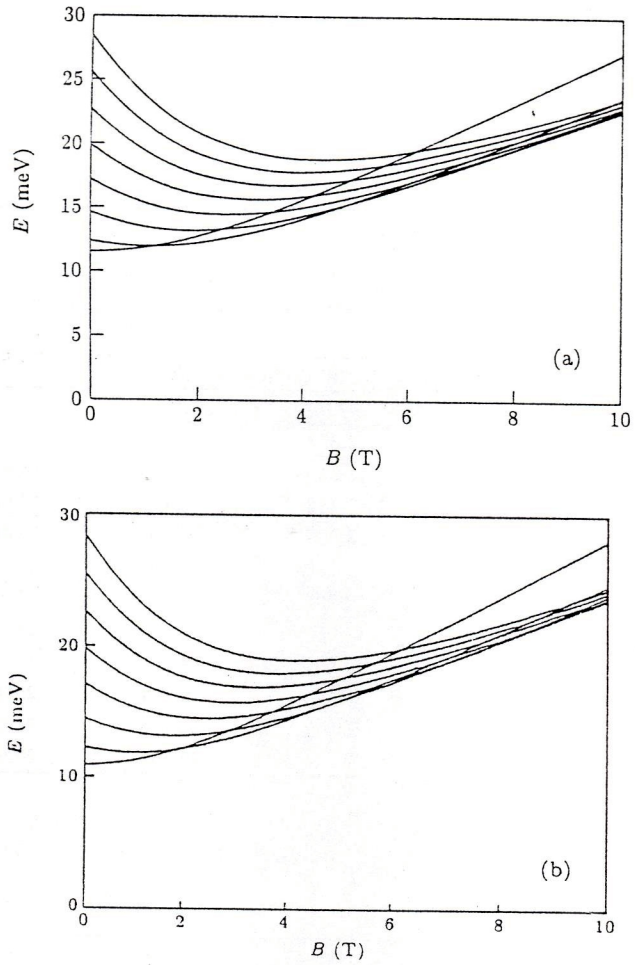

Fig. 1. The eigen-energies of the states $|0,0;\ 0,m\rangle$, $m = 0, -1, -2, \cdots, -7$ for two interacting electrons, of confining energy $\hbar\omega_0 = 3$ meV and $g^* = 0.0$ for (a) present work and (b) Bolton (Ref. [27]).

Table 1. The values of the roots r_0 calculated for the quantum states $|0,0;\ 0,m\rangle$, $m = 0, -1, -3, -5, -7$, at $\hbar\omega_0 = 3$ meV and for different values of magnetic field strength B.

B (T)	m				
	0	−1	−3	−5	−7
0	2.4763	2.9872	3.9530	4.7639	5.4653
1	2.4248	2.9295	3.8805	4.6780	5.3671
2	2.2972	2.7863	3.6998	4.4631	5.1222
3	2.1357	2.6041	3.4691	4.1884	4.8085
4	1.9761	2.4232	3.2386	3.9136	4.4947
5	1.8297	2.2559	3.0246	3.6580	4.2026
6	1.7024	2.1098	2.8366	3.4331	3.9455
7	1.5917	1.9819	2.6714	3.2353	3.7191
8	1.4978	1.8730	2.5299	3.0656	3.5248
9	1.4157	1.7770	2.4052	2.9160	3.3535
10	1.3437	1.6926	2.2950	2.7835	3.2017

Table 2. The energies of the states $|0,0;\ 0,m\rangle$, $m = 0, -1, -3, -5, -7$, for $\hbar\omega_0 = 3$ meV, calculated at different values of magnetic field strength B. The energies are given in meV, ($m^* = 0.067m_0$, $\epsilon = 12.9$).

B (T)	m				
	0	−1	−3	−5	−7
0	11.505	12.372	17.201	22.751	28.497
1	11.833	11.954	15.359	19.498	23.838
2	12.726	12.212	14.525	17.621	20.910
3	14.054	13.009	14.520	16.863	19.431
4	15.643	14.136	15.030	16.821	18.854
5	17.420	15.507	15.919	17.297	18.936
6	19.291	17.015	17.043	18.108	19.451
7	21.239	18.631	18.341	19.159	20.271
8	23.191	20.274	19.704	20.308	21.224
9	25.178	21.977	21.172	21.607	22.371
10	27.187	23.716	22.701	22.990	23.625

Table 3. The energies of the states $|0,0;0,m\rangle$, $m = 0, -1, -3, -5, -7$, for $\hbar\omega_0 = 1.6$ meV, calculated at different values of magnetic field strength B. The energies are given in meV, ($m^* = 0.067m_0$, $\epsilon = 12.9$).

B (T)	m				
	0	−1	−3	−5	−7
0	6.610	7.214	9.588	12.463	15.476
1	7.749	7.128	8.211	9.828	11.593
2	9.310	8.142	8.451	9.374	10.467
3	11.240	9.609	9.389	9.875	10.555
4	13.337	11.329	10.775	11.022	11.486

We have also compared the results produced by the $1/N$ expansion method, displayed in Table 3, against the fixed-phase quantum Monte Carlo method and exact ones, as shown in Fig. 3 of Ref. [27], for $\hbar\omega_0 = 1.6$ meV. The values of the magnetic filed, B_c, at which the first spin singlet-triplet transition occurs for $\hbar\omega_0 = 3$ and 1.6 meV are 1.8 and 0.8 T, respectively. Hence the magnetic field B_c increases as the confining frequency $\hbar\omega_0$ increases. This result is consistent with the work of Pfannkuche *et al.*[10]

In conclusion, we have used the shifted $1/N$ expansion method to calculate and interpret the spectra of two interacting electrons confined in a parabolic quantum dot. We have shown, using this method, that the transition in the angular momentum of the system is due to an electron-electron interaction effect. Based on the results, the shifted $1/N$ expansion method is an effective technique to produce and understand the spectra of two-electron quantum dot presented in an applied 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. The complete discussion of the 1/N method can be found in Refs [17] and [28]–[30].

$$\gamma_1 = c_1e_2 + 3c_2e_4 - \bar{\omega}^{-1}[e_1^2 + 6c_1e_1e_3 + c_4e_2^3] \tag{A1}$$

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

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

where c's, d's and e's are parameters given as

$$c_1 = 1 + 2n_r, \qquad c_6 = 13 + 40n_r + 42n_r^2 + 28n_r^3,$$
$$c_2 = 1 + 2n_r + 2n_r^2, \qquad c_7 = 31 + 78n_r^2 + 78n_r^3,$$
$$c_3 = 3 + 8n_r + 6n_r^2 + 4n_r^3, \qquad c_8 = 57 + 189n_r + 225n_r^2 + 150n_r^2,$$
$$c_4 = 11 + 30n_r + 30n_r^2, \qquad c_9 = 31 + 109n_r + 141n_r^2 + 94n_r^3,$$
$$c_5 = 21 + 59n_r + 51n_r^2 + 34n_r^3,$$
$$e_j = \frac{\varepsilon_j}{\bar{\omega}^{j/2}}, \qquad j = 1 \text{ to } 4,$$
$$2r_0^3 V'(r_0) = Q,$$

and

$$d_i = \frac{\delta_i}{\bar{\omega}^{i/2}}, \quad i = 1 \text{ to } 6,$$

$$\varepsilon_1 = (2-a), \qquad \varepsilon_2 = -\frac{3(2-a)}{2}, \qquad \varepsilon_3 = -1 - \frac{r_0\sqrt{2}}{Q},$$

$$\varepsilon_4 = \frac{5}{4} + \frac{r_0\sqrt{2}}{Q}, \qquad \delta_1 = -\frac{(1-a)(3-a)}{2}, \qquad \delta_2 = -\frac{3(1-a)(3-a)}{4},$$

$$\delta_3 = 2(2-a), \qquad \delta_4 = -\frac{5(2-a)}{2}, \qquad \delta_5 = -\frac{3}{2} - \frac{r_0\sqrt{2}}{Q},$$

$$\delta_6 = \frac{7}{4} + \frac{r_0\sqrt{2}}{Q}.$$

References

[1] H. Drexler, D. Leonard, W. Hansen, J.P. Kothaus and P.M. Petroff, Phys. Rev. Lett. **73** (1994) 2252.

[2] C. Sikorski and U. Merkt, Phys. Rev. Lett. **62** (1989) 2164.

[3] T. Demel, D. Heitmann, P. Grambow and K. Ploog, Phys. Rev. Lett. **64** (1990) 788.

[4] A. Lorke, J.P. Kothaus and K. Ploog, Phys. Rev. Lett. **64** (1990) 2559.

[5] A. Wixforth *et al.*, Semicond. Science and Technol. **9** (1994) 215.

[6] R.C. Ashoori *et al.*, Phys. Rev. Lett. **71** (1993) 613.

[7] P.L. Mc Euen *et al.*, Phys Rev. Lett. **66** (1991) 1926; Phys. Rev. **B45** (1992) 11419.

[8] P.A. Maksym and T.T. Chakraborty, Phys. Rev. Lett. **65** (1990) 108; Phys. Rev. **B45** (1992) 1947.

[9] M. Wagner, U. Merkt and A.V. Chaplik, Phys. Rev. **B45** (1992) 1951.

[10] D. Pfannkuche, V. Gudmundsson and P.A. Maksym, Phys. Rev. **B47** (1993) 2244; D. Pfannkuche, R.R. Gerhardts, P.A. Maksym and V. Gudmundsson, Physica **B189** (1993) 6.

[11] M. Ferconi and G. Vignale, Phys. Rev. **B50** (1994) 14722.

[12] U. Merkt, Physica **B189** (1993) 165.
[13] J.J.S. De Groote, J.E.M. Hornos and A.V. Chaplik, Phys. Rev. **B46** (1992) 12773.
[14] U. Merkt, J. Huser and M. Wagner, Phys. Rev. **B43** (1991) 7320.
[15] K.D. Zhu and S.W. Gu, Phys. Lett. **A172** (1993) 296.
[16] N.F. Johnson and M.C. Payne, Phys. Rev. Lett. **67** (1991) 1157.
[17] M. El-Said, Semicond. Science and Technol. **9** (1994) 272; Physica Status Solidi **B184** (1994) 385.
[18] W. Que, Phys. Rev. **B45** (1992) 11036.
[19] V. Halonen, T. Chakraborty and M. Pietalainen, Phys. Rev. **B45** (1992) 5980.
[20] G.T. Einevoll, Phys. Rev. **B45** (1992) 3410.
[21] Y. Kayanuma, Phys. Rev. **B38** (1990) 9797.
[22] G.W. Bryant, Phys. Rev. Lett. **59** (1987) 1140; Phys. Rev. **B37** (1988) 8763.
[23] V. Halonen, Solid State Commun. **92** (1994) 703.
[24] J.J. Placios, L. Martin-Moreno, G. Chiappe, E. Louis and C. Tejedor, Phys. Rev. **B50** (1994) 5760.
[25] R. Ugajin, Phys. Rev. **B53** (1996) 6963.
[26] F.M. Peeters and V.A. Schweigert, Phys. Rev. **B53** (1996) 1468.
[27] F. Bolton, Phys. Rev. **B54** (1996) 4780.
[28] T. Imbo, A. Pagnamento and U. Sukhatme, Phys. Rev. **D29** (1984) 8763.
[29] T. Imbo, U. Sukhatme, Phys. Rev. **D28** (1983) 418; **31** (1985) 2655.
[30] R. Dutt, U. Mukherji and Y.P. Varshni, J. Phys. **B19** (1986) 3411.