

The Spectral Properties of two Interacting Electrons in a Quantum Dot

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Abstract

The shifted $1/N$ expansion method is used to study the spectral properties of two interacting electrons confined in a QD, under influence of a uniform magnetic field of arbitrary strength. We give explanation to the transitions in the spin and angular momenta of the QD ground state as the magnetic field sweeps. The electron addition energy is also calculated. Based on different comparisons , the shifted $1/N$ expansion method gives very good result against various methods used to study the spectra of a two electron QD.

1. Introduction

Quasi-zero dimensional systems, such as quantum dots (QDs), or artificial atoms, have been the subject of intense research [1-27] in recent years, owing to the nanofabrication techniques that make possible the construction of systems of dimensions very small compared to the de Broglie wavelength of the carriers. In such small structures the electrons are fully quantized into a discrete spectrum of energy levels. Different experimental [1-6] and theoretical methods have been devoted to investigate the electronic structure of the interacting electrons confined in quantum dots under the effect of an applied magnetic field. One of the most interesting features of electrons confined in a quantum dot is the energy level crossings [8-17]. Once the crossings occur the spin and angular momentum quantum numbers of the ground state of the quantum dot changes and this implies a phase transition, i.e., a transition of QD structures. These transitions appear as kinks in the physical properties of the quantum dots, such as optical properties, electronic heat capacity, magnetization and addition energy. Indeed, these kinks have also been experimentally confirmed in the addition energy $\mu(N_e)$ of the quantum dot using single-electron spectroscopy [6] and gate transport methods [7]. The addition energy level $\mu(N_e)$ is the energy required to add one more electron to the QD, raising it from an $(N_e - 1)$ - electron ground state to an N_e - electron ground state:

$$\mu(N_e) = E_G(N_e) - E_G(N_e - 1).$$

In this work we shall use the shifted $1/N$ expansion method [29-32], where N is the spatial dimensions, to study the electronic properties of two interacting electrons confined in a quantum dot, in the presence of an applied magnetic field. In this method, the energy is expanded in inverse power of $\bar{k} = N + 2m - a$, where the shift parameter a is determined by requiring that the first-order energy correction vanish giving exact eigenenergies for the hydrogen and harmonic oscillator potentials. To achieve our aims in this study, we proceed in two steps. First, we produce an eigenenergy expression for two interacting electrons, confined a quantum dot, in a uniform magnetic field of arbitrary strength. Second, using this expression, we give a physical interpretation to the crossing phenomena which occur in the quantum dot spectra. We then

compare our computed QD spectra, in addition to the spin-oscillations, with various theoretical works [9, 14, 23, 27, 28]. The $1/N$ expansion method has advantages over methods such as perturbation theory and numerical calculations. While the $1/N$ expansion method is applicable to the entire range of the magnetic field strength, the perturbation theory is limited to a weak range only. Purely numerical calculations are computationally extensive and hard to follow in the physics of the problem.

The rest of this work is organized as follows. In section 2, we present the Hamiltonian theory for two electrons, confined in a quantum dot, and presented in a uniform magnetic field. In section 3, we describe the shifted $1/N$ expansion method. In section 4, we present our computed results and discussion. We draw our conclusions in the final section.

2. Theory

We consider electrons of effective mass m^* in the xy-plane and confined by a parabolic potential $\frac{1}{2}\omega^2 r^2$, $r^2 = x^2 + y^2$, with a characteristic frequency ω_0 . The Hamiltonian of two interacting electrons in the presence of a perpendicular magnetic field applied along the z-axis is then

$$H = \sum_{i=1}^2 \left[-\frac{\hbar^2}{2m^*} \nabla_i^2 + \frac{1}{2} m^* \omega_0^2 r_i^2 + \frac{\hbar \omega_c}{2} L_z \right] + \frac{e^2}{\varepsilon |\vec{r}_2 - \vec{r}_1|} + g \mu_B^* B \sum_i S_{i,z}, \quad (1)$$

where L_i^z and $S_{i,z}$ are the z-components of the orbital angular momentum and spin for each electron, respectively; and $\mu_B = e\hbar/2m_e$, 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 $\omega = \left[\omega_0^2 + \frac{\omega_c^2}{4} \right]^{\frac{1}{2}}$ depends on both the magnetic field B and the confinement frequency ω_0 . Upon introducing the center-of-mass $\vec{R} = (\vec{r}_1 + \vec{r}_2)/\sqrt{2}$ and the relative coordinates $\vec{r} = (\vec{r}_2 - \vec{r}_1)/\sqrt{2}$ the Hamiltonian in Eq.(1) is decoupled to the center-of-mass motion Hamiltonian

$$H_R = -\frac{\hbar^2}{2m^*} \nabla_R^2 + \frac{m^*}{2} \omega^2 R^2 + \frac{\hbar \omega_c}{2} L_z^R, \quad (2)$$

and the relative motion Hamiltonian

$$H_r = -\frac{\hbar^2}{2m^*} \nabla_r^2 + \frac{m^*}{2} \omega^2 r^2 + \frac{\hbar \omega_c}{2} L_z^r + \frac{e^2}{\sqrt{2}r}. \quad (3)$$

Equation (2) describes the Hamiltonian for the harmonic oscillator with well-known eigenenergies

$$E_{n_{cm}, m_{cm}} = (2n_{cm} + |m_{cm}| + 1) \hbar \omega_c + \frac{\hbar \omega_c}{2} m_{cm}, \quad (4)$$

labeled by the radial ($n_{cm} = 0, 1, 2, \dots$) and the azimuthal ($m_{cm} = 0, \pm 1, \pm 2, \dots$) quantum numbers. Antisymmetric two-electron wave functions require that even m are singlets and odd m triplets with the Zeeman energy term $E_{spin} = g \mu_B^* B S_z$ 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, $E = E_R(n_{cm}, m_{cm}) + E_r(n_r, m) + E_{spin}(S_z)$, 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, Eq. (3).

3. Method of Solution

We shall use the shifted $1/N$ expansion method [29-32] to solve Eq. (3) and obtain the eigenenergies. In N spatial dimension the radial part of schrödinger equation for the effective potential

$$V(r) = \frac{\sqrt{2}}{r} + \frac{1}{4}\omega^2 r^2 + m\frac{\omega_c}{2} \text{ becomes}$$

$$\left[-\frac{d^2}{dr^2} + \frac{(\bar{k} + a - 1)(\bar{k} + a - 3)}{4r^2} + V(r) \right] \Psi(r) = E_r \Psi(r), \quad (5)$$

where $\bar{k} = N + 2m - a$ and a is the shift parameter. Following the previous work of the shifted $1/N$ expansion method [17,29,-32], we give here only the energy expression which is needed to produce and understand the electronic properties of the QD relative Hamiltonian, H_r . The energy expression reads as

$$E_{n_r,m} = \frac{\sqrt{2}}{r_0} + \frac{1}{4}\omega_0^2 r_0^2 + m\frac{\omega_c}{2} + \frac{\bar{k}^2}{4r_0} + \frac{1}{r_0^2} \left[\frac{(1-a)(3-a)}{4} + \gamma_1 \right] + \frac{\gamma_2}{kr_0^2}, \quad (6)$$

$$a = 2 - (2n_r + 1)\bar{\omega}, \quad (7)$$

$$\bar{\omega} = \left[3 + \frac{r_0 V''(r_0)}{V'(r_0)} \right]^{\frac{1}{2}}, \quad (8)$$

and the roots r_0 are determined through the relation

$$[2r_0^3 V'(r_0)]^{\frac{1}{2}} = 2 + 2m - a. \quad (9)$$

The explicit forms of parameter 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 easy.

4. Results and Discussion

We now consider quantum dots made from GaAs/AlGaAs as a practical application of the above modeling, with energies and lengths in Equations 5 to 9 expressed in units of $R^* = 5.83$ meV and $a^* = 98.7$ Å, respectively. Our results are shown in Figures 1-6 and Tables 1 to 6. To show the energy level crossings, we have shown in Figure 1(a) and (b) the energies of the states $|00;0m\rangle$, $m=0, -1, -2, \dots, -10$, for two independent and interacting electrons parabolically confined in a QD of size $\ell_0 = 3a^*$ ($\omega_0 = 1.3$ meV) as a function of the ratio ω_c/ω_0 and B , respectively. As the magnetic field increases the energy of the state $m=0$ increases while the energy of states with non-vanishing angular momentum m decreases, thus leading to a system with different ground states. In Figure 2 we compare our results to the more exact values produced by Wagner et al. [9] for quantum dot states, $m = 0, -1, 2, \dots, -7$, of two interacting electrons computed by shifted $1/N$ expansion method shown in (Figure 2a.) and fixed-phase Monte-Carlo method shown in (Figure 2b) calculated by Bolton [28]. Further computed results for QD spectra with confining frequencies $\hbar\omega_0 = 3meV$ and 1.6 meV are listed in Tables 1 and 2 for comparison. Comparison shows that our QD spectra computed by $1/N$ method is in very good agreement against the more exact and fixed phase Monte-Carlo methods. The level crossings, which appear in the spectra, can be understood from the dependence of the Coulomb and kinetic energy terms on the azimuthal quantum number $|m|$. The dominant contribution to the relative energy $E_{n_r,m}$ of the system comes from the first term, namely, $V(r_0) = \frac{\sqrt{2}}{r_0} + \frac{1}{4}\omega^2 r_0^2$. We calculated the roots (r_0) for different quantum dot states $|00,0m\rangle$, $m = 0, -1, -2, \dots, -10$ and various frequency ratios ω_c/ω_0 . These roots are listed in Table 3 and Figure 3. As can be seen clearly from Table 3 and Figure 3, the roots

(r_0) increase with $|m|$ while the electron-electron interaction energy term $V_{e-e}(r_0) = \frac{\sqrt{2}}{r_0}$, decreases. On the other hand, the magneto-confining term, $\frac{1}{4}\omega^2 r_0^2$, increases.

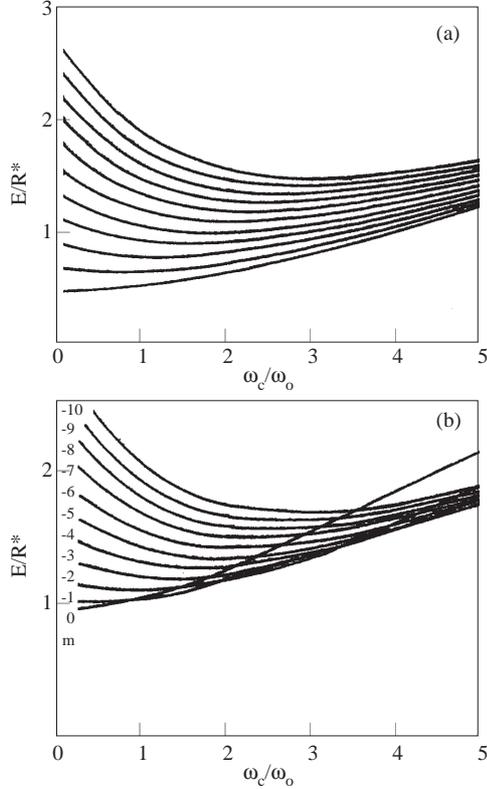


Figure 1. The total eigenenergies of the states $|00; 0m\rangle$, $m = 0, -1, -2, \dots, -10$, (states are from bottom to top) for two (a) independent and (b) interacting electrons, parabolically confined in the quantum dot with $\hbar\omega_0 = 1.3$ meV, as a function of the ratio ω_c/ω_0 .

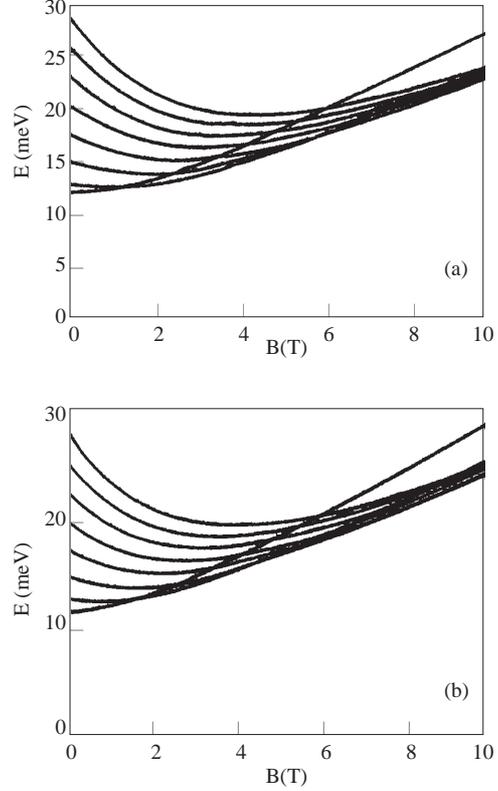


Figure 2. The eigenenergies of the states $|00; 0m\rangle$ $m = 0, -1, -2, \dots, -7$ (states are from bottom to top) for two interacting electrons of confining frequency $\hbar\omega_0 = 3$ meV and $g^* = 0$ for (a) the present work ($1/N$) and (b) Bolton [28].

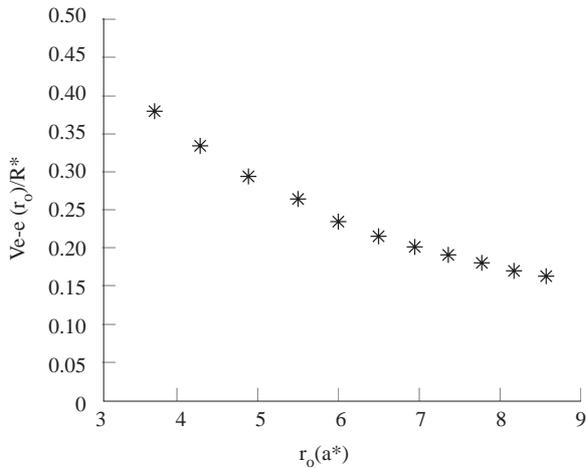


Figure 3. The Coulomb interaction energy as a function of the roots for quantum states $|0m\rangle$, $m = 0, -1, -2, \dots, -10$, $\omega_c/\omega_0 = 2$ and $\ell_0 = 3a^*$. $\omega_0 = 2$ and $\ell_0 = 3a^*$.

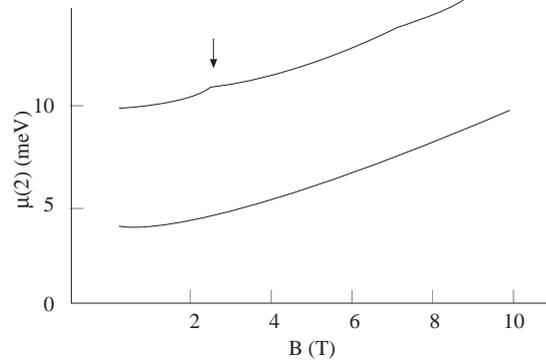


Figure 4. Addition energy spectra for two independent (bottom spectra) and interacting (top spectra) electrons in a quantum dot with confining frequency $\hbar\omega_0 = 4$ meV. The arrow indicates the singlet-triplet transition.

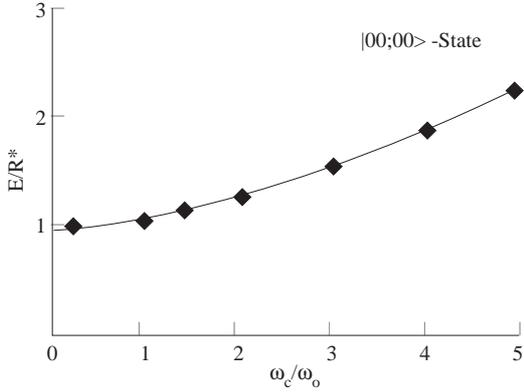


Figure 5. The total ground-state energy $|00,00 \rangle$ for two interacting electrons in a quantum dot of size $\ell_0 = 3a^*$ against the ratio ω_c/ω_o . (●●●) present results, (—) Ref [9].

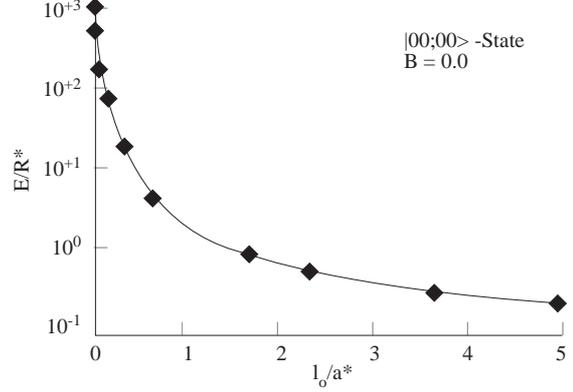


Figure 6 The relative ground state energy $|00\rangle$ for two interacting electrons in a quantum dot as a function of confinement length $\ell_0 = \left[\frac{\hbar}{m^*\omega_0}\right]^{\frac{1}{2}}$ for $B = 0$: (—) Ref [14], (●●●) present work $(1/N)$.

Table 1. 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, ($m^* = 0.067m_0, \varepsilon = 12.9$)

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	14.436	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	25.187	21.977	21.172	21.607	22.371
10	27.187	23.716	22.701	22.990	23.625

Table 2. 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, ($m^* = 0.067m_0, \varepsilon = 12.9$)

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

The reduction in the electron-electron interaction energy does not completely consume the enhancement in the kinetic energy. Instead the electron jumps to a new state with a higher angular momentum m to decrease further the Coulomb interaction energy. This transition in the angular momentum of the QD ground state is accompanied by a flip in the spin to keep the wavefunction of the ground state totally antisymmetric in accordance with Pauli exclusion principle. Increasing more the strength of the magnetic field B , the ground state of the QD changes discontinuously. These spin transitions and the singlet-triplet oscillations have been reported experimentally [6,7]. To characterize further the effect of electron-electron interaction on the QD spectra we list in Table 4, the relative energies for the QD $|0, m\rangle$ $0, -1, -2, \dots, -10$,

calculated for various values of frequency ratio ω_c/ω_0 . The change in the level ordering of the QD spectra due to the e-e interaction are clearly seen at $\omega_c/\omega_0 = 3.0$ and 5.0 comparable with the levels at $\omega_c/\omega_0 = 0.2$ in Table 4. For example, the order of the states at $\omega_c/\omega_0 = 0.2$ labelled by $a_0, a_1, a_2, \dots, a_{10}$ changed to $a_4, a_3, a_5, a_6, a_2, a_7, a_8, a_9, a_{10}, a_1, a_0$ at $\omega_c/\omega_0 = 5.0$. This level ordering has also been reported by Zhu et.al, [27]. In addition to this qualitative agreement, we have compared in Table 5 our computed results with Zhu et al [27] calculated at $\gamma = \omega_c/2 = 1$. These tabulated results show very good quantitative agreement. Figure 4 shows the calculated electron addition energies $\mu(N_e)$ as a function of the applied magnetic field B for a quantum dot with two electrons. The electron addition energy spectra $\mu(2)$, displayed in Figure 4, is in very good agreement compared with that calculated by Halonen [23] using the more exact diagonalization method. The spin and angular momenta transitions appear as a kink in the electron addition energy (see Figure 4) and is indicated by an arrow.

Table 3. The values of the roots r_0 calculated for quantum states with non-vanishing azimuthal quantum numbers (m) at $\hbar\omega_0 = 1.3$ meV and for $\omega_c/\omega_o = 0.2$ and 5 .

$ 0\ m\rangle$	$\omega_c/\omega_o = 0.2$	$\omega_c/\omega_o = 5$
$ 00\rangle$	4.332	2.504
$ 01\rangle$	5.130	2.943
$ 02\rangle$	5.784	3.398
$ 03\rangle$	6.429	3.825
$ 04\rangle$	7.041	4.220
$ 05\rangle$	7.618	4.586
$ 06\rangle$	8.162	4.929
$ 07\rangle$	8.676	5.250
$ 08\rangle$	9.165	5.555
$ 09\rangle$	9.631	5.844
$ 10\rangle$	10.077	6.120

Table 4. Quantum levels ($|n\ m\rangle$) of two electrons in QD with $\omega_0 = 1.3$ meV and different ω_c . The enegies are expressed in units of effective Rydberg (R) .

$ 0\ m\rangle$	$\omega_c/\omega_o = 0.2$	$\omega_c/\omega_o = 3.0$	$\omega_c/\omega_o = 5.0$
$ 00\rangle$	a_0 0.953	a_1 1.323	a_4 1.734
$ 0-1\rangle$	a_1 1.013	a_2 1.335	a_3 1.740
$ 0-2\rangle$	a_2 1.143	a_3 1.341	a_5 1.741
$ 0-3\rangle$	a_3 1.302	a_4 1.367	a_6 1.757
$ 0-4\rangle$	a_4 1.474	a_5 1.405	a_2 1.774
$ 0-5\rangle$	a_5 1.655	a_6 1.450	a_7 1.778
$ 0-6\rangle$	a_6 1.840	a_7 1.500	a_8 1.803
$ 0-7\rangle$	a_7 2.029	a_0 1.531	a_9 1.830
$ 0-8\rangle$	a_8 2.219	a_8 1.552	a_{10} 1.860
$ 0-9\rangle$	a_9 2.412	a_9 1.606	a_1 1.865
$ 0-10\rangle$	a_{10} 2.606	a_{10} 1.663	a_0 2.130

To test further the accuracy of our results, we have compared, in Figures 5 and 6, our results produced by $1/N$ method against exact results produced by Wagner et al. [9] and Merkt et al. [14]. The computed data, used to plot Figure 5, are also given in Table 6. It is obvious from both figures that the $1/N$ expansion method gives very good results comparable with various methods.

Table 5. The energies of the relative states $|0\ m\rangle$, $m = 0, -1, -2 \dots, -10$, calculated, at $\gamma = 1.0 = \omega_c/2$ by different methods (For GaAs material $\gamma=1$ corresponds to $B = 6.75$ T, Ref. 27). The energies are given in R^* .

$n_r, m; n_{cm}m_{cm}S \rangle$	Zhu et al. [27]	Present work ($1/N$)
00;000 \rangle	3.3196	3.2703
01;001 \rangle	3.8278	3.7953
00;010 \rangle	4.3196	4.2408
02;000 \rangle	4.6436	4.6432
01;011 \rangle	4.8278	4.7953
10;000 \rangle	5.1472	4.9292
00;100 \rangle	5.3196	5.2703
03;001 \rangle	5.5174	5.5136
02;010 \rangle	5.6436	5.6432
11;001 \rangle	5.7438	5.6769
01;101 \rangle	5.8278	5.7953
10;010 \rangle	6.1472	5.9294
00;110 \rangle	6.3196	6.2703
04;000 \rangle	6.4693	6.4782
12;000 \rangle	6.5956	6.5844
02;100 \rangle	6.6436	6.6432

Table 6. The ground state energy $|00; 00 \rangle$ of two interacting electrons calculated $1/N$ expansion for quantum dot of size $\ell_o = 3 a^*$

ω_c/ω_o	0.2	1.0	1.4	2	3	4	5
E / R^*	0.953	1.040	1.115	1.256	1.531	1.827	2.130

5. Conclusion

We have used the shifted $1/N$ expansion method to produce an expression for the spectra of the quantum dot presented in a magnetic field of arbitrary strength. We have used this expression to calculate the excited states of the QD spectra and also understand the spin singlet-triplet and angular momenta transitions which occur in the spectra. These transitions appear as a kink in calculated electron addition energy $\mu(2)$ for a two electron quantum dot. Based on comparisons with different methods, the shifted $1/N$ expansion method is an effective technique to produce and understand the electronic spectra of a quantum dot presented in a magnetic field of arbitrary strength.

Appendix

The parameters γ_1 and γ_2 , appeared in Eq.6 are given as follows:

$$\gamma_1 = [(1 + 2n_r) e_2 + 3(1 + 2n_r + 2n_r^2) e_4] - \varpi^{-1} [e_1^2 + 6(1 + 2n_r) e_1 e_3 + (11 + 30n_r + 30n_r^2) e_3^2]$$

$$\gamma_2 = (1 + 2n_r) d_2 + 3(1 + 2n_r + 2n_r^2) d_4 + 5(3 + 8n_r + 6n_r^2 + 4n_r^3) d_6$$

$$\begin{aligned}
 & -\varpi^{-1} \left[\begin{aligned} & (1 + 2n_r) e_2^2 + 12 (1 + 2n_r + 2n_r^2) e_2 e_4 + 2e_1 d_1 + 2 (21 + 59n_r + 51n_r^2 + 34n_r^3) e_4^2 \\ & + 6 (1 + 2n_r) e_1 d_3 + 30 (1 + 2n_r + 2n_r^2) e_1 d_5 + 6 (1 + 2n_r) e_3 d_1 + \\ & 2 (11 + 30n_r + 30n_r^2) e_3 d_3 + 10 (13 + 40n_r + 42n_r^2 + 28n_r^3) e_3 d_5 \end{aligned} \right] \\
 & + \varpi^{-2} \left[\begin{aligned} & 4e_1^2 e_2 + 36 (1 + 2n_r) e_1 e_2 e_3 + 8 (11 + 30n_r + 30n_r^2) e_2 e_3^2 + 24 (1 + n_r) e_1^2 e_4 \\ & + 8 (31 + 78n_r + 78n_r^2) e_1 e_3 e_4 + 12 (57 + 189n_r + 225n_r^2 + 150n_r^3) e_3^2 e_4 \end{aligned} \right] \\
 & - \varpi^{-3} [8e_1^3 + 108 (1 + 2n_r) e_1^2 e_3^2 + 48 (11 + 30n_r + 30n_r^2) e_1 e_3^3 + 30 (31 + 109n_r + 141n_r^2 + 94n_r^3) e_3^4]
 \end{aligned}$$

with

$$e_j = \varepsilon_j / \varpi^{j/2} \text{ and } d_i = \delta_i / \varpi^{j/2}$$

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

The definition of ε_j and δ_i quantities are

$$\varepsilon_1 = (2 - a) \quad \varepsilon_2 = -3(2 - a)/2$$

$$\varepsilon_3 = -1 + r_0^5 V^{(3)}(r_0) / 6Q \quad \varepsilon_4 = \frac{5}{4} + \frac{r_0^6 V^{(4)}(r_0)}{24Q}$$

$$\delta_1 = -(1 - a)(3 - a)/2 \quad \delta_2 = 3(1 - a)(3 - a)/4$$

$$\delta_3 = 2(2 - a) \quad \delta_4 = -5(2 - a)/2$$

$$\delta_5 = -\frac{3}{2} + r_0^7 V^{(5)}(r_0) / 120Q \quad \delta_6 = \frac{7}{4} + r_0^8 V^{(6)}(r_0) / 720Q.$$

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