

ELECTRONIC SPECTRA OF TWO INTERACTING ELECTRONS CONFINED IN A QUANTUM DOT IN A MAGNETIC FIELD

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الخلاصة :

حصلنا على الطيف الإلكتروني لزوج من الإلكترونات متشادة ومحصورة في نقطة كمية ذات قطع مكافئ موجودة في مجال مغناطيسي. كما تمت دراسة كل من التشاد الإلكتروني وحجم النقطة الكمية على مستويات الطاقة لهذه النقطة الكمية. وقمنا أيضاً بإعطاء تفسير للخواص البارزة لهذه النقطة الكمية مثل تقاطع مستويات الطاقة وإزالة التطابق (Degeneracy) فيها. أظهرت نتائجنا الحسابية تطابقاً إلى درجة جيد جداً مع مثيلاتها من الأعمال الحسابية الأخرى.

ABSTRACT

The energy spectrum of two interacting electrons, confined in a parabolic quantum dot, presented in a magnetic field, is obtained by using the shifted $1/D$ expansion method. The effects of electron-electron interaction and quantum dot size on the energy levels are studied. Interesting features of the quantum dot spectra such as the energy level crossings and the removal of the degeneracy are explained. Based on comparisons, our calculated results are in very good agreement with numerical ones.

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1. INTRODUCTION

Quasi-zero-dimensional systems, such as quantum dots (QDs), have been the subject of intense research in recent years, owing to the nanofabrication techniques that make possible the realization of systems of very small dimensions comparable to the de Broglie wavelength of carriers. In such small structures the electrons are fully quantized into a discrete spectrum of energy levels. The confinement in the z -direction, which is the growth direction, is assumed to be stronger than in the xy -plane, so that the dot can be viewed as a two-dimensional disk. Different experimental [1–7] and theoretical [8–20] methods have been used to investigate the energy spectrum and correlation effects of the interacting electrons confined in quantum dots under the effect of an applied magnetic field. One of the most interesting features of the electron correlation is the change of the spin and angular momentum structures in the ground state of those systems in the presence of the magnetic field. The singlet–triplet transitions which occur in the two-electron parabolic quantum dot, as a simple case but not trivial one, have recently received great attention [14–17].

In this work we shall study the spectroscopic properties of a quantum dot by using different approach, namely, the shifted $1/D$ expansion method where D is the number of spatial dimensions. We proceed in two steps: first, we used the shifted $1/D$ expansion method to produce an analytical expression for two interacting electrons confined in a quantum dot in the presence of a magnetic field of arbitrary strength. Second, we focus on the effects of electron–electron interaction and quantum dot size on the spectra in addition to the spin and angular momentum transitions. We give explanation to these salient features, which occur in the spectra by making use of the energy expression we have obtained. The rest of this work is outlined as follows. In Section 2 we have presented the Hamiltonian theory for two interacting electrons parabolically confined in quantum dot. We have described, in Section 3, the shifted $1/D$ expansion technique. The final section is devoted to results and discussions.

2. MODEL

The effective-mass Hamiltonian for two interacting electrons, parabolically confined in a quantum dot, in the presence of a perpendicular magnetic field applied parallel to the z -axis is given as:

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

where L_i^z and $S_{i,z}$ stand for the z -components of the orbital angular momentum and spin of each electron,

$\mu_B = \frac{e\hbar}{2m_e}$, g^* , $\gamma = \omega_c = \frac{eB}{m_c^*}$, and ϵ are the Bohr magneton, Lande factor, the cyclotron frequency, and the dielectric constant of the medium, respectively.

The frequency ω , depends on the magnetic field B and the confinement frequency $\Gamma_d = \omega_0$, and is given as:

$$\Gamma = \omega = \left(\omega_0^2 + \frac{\omega_c^2}{4} \right)^{1/2} \quad (2)$$

Upon introducing the center of mass (cm) $\vec{R} = \frac{\vec{r}_1 + \vec{r}_2}{\sqrt{2}}$ and the relative coordinates $\vec{r} = \frac{\vec{r}_1 - \vec{r}_2}{\sqrt{2}}$, the Hamiltonian in

Equation (1) decoupled to the cm motion Hamiltonian:

$$H_R = -\frac{\hbar^2}{2m^*} \nabla_R^2 + \frac{1}{2} m^* \omega^2 R^2 + \frac{\hbar \omega_c}{2} L_z^R \quad (3)$$

and the relative motion Hamiltonian:

$$H_r = -\frac{\hbar^2}{2m^*} \nabla_r^2 + \frac{1}{2} m^* \omega^2 r^2 + \frac{\hbar \omega_c}{2} L_z + \frac{e^2}{\sqrt{2}r} \quad (4)$$

Equation (3) describes the Hamiltonian of the harmonic oscillator with well-known eigenenergies:

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

labeled by the radial $n_{cm} = 0, 1, 2, \dots$ and the azimuthal $m_{cm} = 0, \pm 1, \pm 2, \dots$ quantum numbers. Antisymmetrization of the two-electron wave function requires that even m states are singlets and m states are triplets with the Zeeman spin energy term $E_{spin} = g^* \mu_B B S_z$ and the total spin $S_z = [1 - (-1)^m]/2$ each representing 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 $|n_{cm}, m_{cm}, n_r, m\rangle$. Quantitatively, the spin Zeeman energy term will not change significantly the spectra of the QD while the spin oscillations make the spectra very rich. The problem is reduced to obtaining the eigenenergies $E_{n_r, m}$ of the relative motion Hamiltonian. The eigenenergies are obtained by the help of $1/D$ expansion method [21–24]. In D spatial dimensions the radial Schrödinger equation for the effective potential

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

$$\left[-\frac{d^2}{dr^2} + \frac{\bar{k}^2 \left[1 - \frac{(1-a)}{\bar{k}} \right] \left[1 - \frac{(3-a)}{\bar{k}} \right]}{4r^2} + \frac{V(r)}{Q} \right] \Psi(r) = E_{n_r, m} \Psi(r), \quad (6)$$

where $\bar{k} = D + 2m - a$ and a is the shift parameter. Q is a scaling constant to be determined later from Equation 11. In order to get useful results from $1/\bar{k}$ expansion, the large \bar{k} limit of the potential must be suitably defined [21]. Since the angular momentum barrier term in Equation 6 behaves like \bar{k}^2 at large \bar{k} , the potential should therefore 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. Following the previous work of the shifted $1/D$ expansion method [21–24], we give here only the energy expression which is needed to calculate the spectra of H_r . The energy expression reads as,

$$E_{n_r, m} = E_{n_r, m}^{(0)} + \frac{\bar{k}^{-2}}{4r_0^2} + \frac{1}{r_0^2} \left[\frac{(1-a)(3-a)}{4} + \alpha_1 \right] + \frac{\alpha_2}{\bar{k}r_0^2} \quad (7)$$

$$E_{n_r, m}^{(0)} = \frac{\sqrt{2}}{r_0} + \frac{1}{4} \omega^2 r_0^2 + m \frac{\omega_c}{2} \quad (8)$$

$$a = 2 - (2n_r + 1)\bar{\omega} \quad (9)$$

$$\bar{\omega} = \left[3 + r_0 \frac{V''(r_0)}{V'(r_0)} \right]^{1/2} \quad (10)$$

and the root is determined through the relation:

$$(2r_0^3 V'(r_0))^{1/2} = 2 + 2|m| - a = Q^{1/2} \quad (11)$$

The explicit forms of the parameters α_1 and α_2 are given in the appendix in the terms of n_r , $\bar{\omega}$, r_0 , and a . Once r_0 , for particular quantum states $|n_r, m\rangle$ and confining frequency ω , is calculated, the task of computing the energy using Equation 7 is relatively simple.

3. RESULTS AND CONCLUSIONS

Our numerical results are computed for a QD made of GaAs/AlGaAs and are presented in Figures 1 and 2 and Tables 1–5. We compared our calculated results with the work of Zhu *et al.* [15] upon replacing the quantities: $\omega_0, \omega_c, \omega$ with Γ_d, γ , and Γ , respectively. Zhu *et al.* [15] had used the method of series expansion to calculate the one-electron and two-electron spectra in QDs and to investigate the singlet–spin–triplet oscillations as the magnetic field strength changes. In Figure 1 we have shown the energies of the states $|0, m; 00, s\rangle$, $m = 0, -1, -2, \dots, -9$ for two interacting electrons parabolically confined in the quantum dot of characteristic confinement frequency $\Gamma_d = 0.2$ as a function of γ . As γ increases, the energy of the state $m = 0$ increases while the energies of the states with non-vanishing quantum number m decreases, thus leading to a sequence of different ground states. The transition in the m -quantum number is accompanied by a flip in the spin of the state to keep the wave function of the electron state totally antisymmetric in accordance with Pauli exclusion principle. The transition phenomena can be understood from the competition between Coulomb and magneto-confinement energies which appear in Equation (8). The major contribution (~50%) to the relative energy is due to this term: $E_{n_r, m}^{(0)} = \frac{\sqrt{2}}{r_0} + \frac{1}{4}\Gamma^2 r_0^2 + m\gamma$. The roots r_0 are calculated for all the quantum states $|0, m\rangle$, $m = 0, -1, -2, \dots$

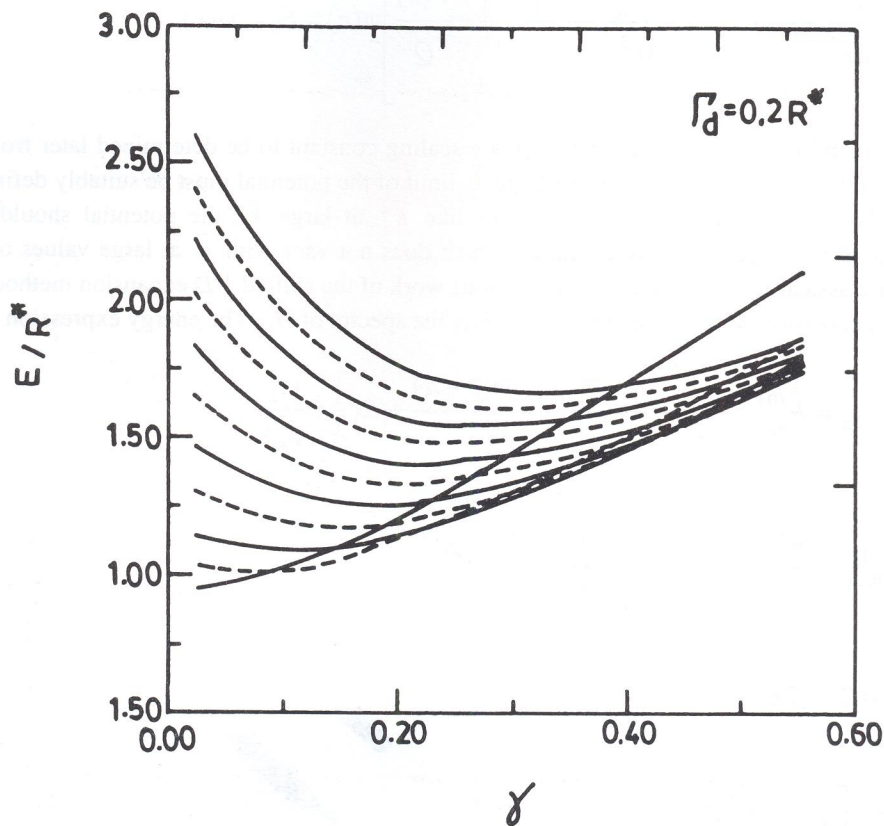


Figure 1. The total eigenenergies of the states $|0, m; 00, s\rangle$ for two interacting electrons, parabolically confined in a quantum dot of confining frequency $\Gamma_d = 0.2R^*$ and $g^* = -0.44$. For GaAs $a^* = 10\text{nm}$ and $R^* = 5.8\text{meV}$, (— singlet states; - - - triplet states).

at different values of γ and various values of these roots are given in Table 1. These roots r_0 show dependence on m , both numerically (Table 1) and analytically (Equation 2). As clearly seen from Table 1, the root r_0 increases as $|m|$ decreases and thus the electron–electron interaction energy $E_{e-e}^{(0)}(r_0, m) = \frac{\sqrt{2}}{r_0(m)}$ decreases showing a dependence on the angular quantum number. On the other hand, the magneto-confinement energy term $E_c^{(0)}(r_0, m) = \frac{1}{4}\Gamma_d^2 r_0^2$ increases. This

Table 1. The Values of the Roots r_0 Calculated for Quantum Relative States at $\Gamma_d = 0.5$ and for Various Values of γ .

λ	r_0	
	$ 0, -1 \rangle$	$ 0, -5 \rangle$
0.022	5.130	7.618
0.056	5.056	7.517
0.111	4.827	7.209
0.156	4.591	6.889
0.200	4.344	6.551
0.222	4.222	6.384
0.334	3.682	6.635
0.445	3.263	5.044
0.556	2.943	4.586

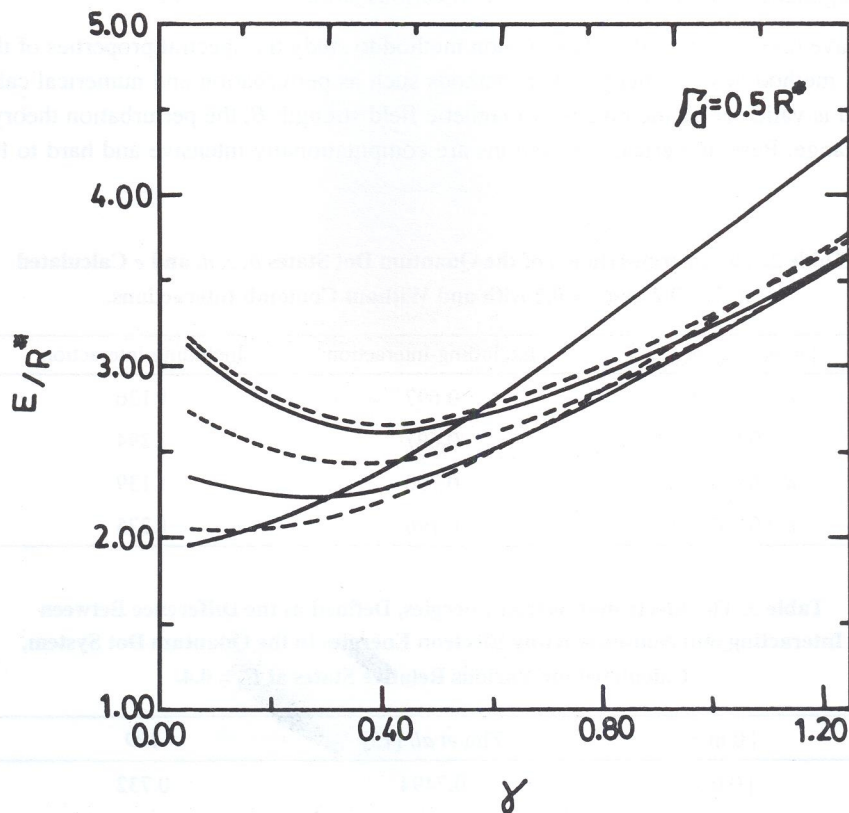


Figure 2. The total eigenenergies of the states $|0, m; 00, s \rangle$ for two interacting electrons, parabolically confined in quantum dots of confining frequency $\Gamma_d = 0.5R^*$ and $g^* = -0.44$. (--- $m = -1$, — $m = -2$).

coulomb–confinement competition removes the level degeneracy, which appears in the spectra of independent electrons. We have given, in Table 2, the energies of the states: *b* and *c*; *d* and *e* for non-interacting and interacting electron cases. It is obvious that the electron–electron interaction energy, and its dependence on the quantum number *m* through r_0 ,

$V_{e-e} = \frac{\sqrt{2}}{r_0(m)}$ splits each pairs of degenerate states in two independent states with higher and lower energies. For

example: the states *b* and *c* with equal energies $0.697 R^*$ at $\gamma = \Gamma_d = 0.2$ are now splitted in two different states with 1.126 and 1.294 R^* upon including the Coulomb interacting energy. The amount of the electron–electron energies of two interacting electrons confined in quantum dot calculated at $\Gamma = 0.4$ are compared, in Table 3, with the results of Zhu *et al.* [15]. For particular relative state $|0, m\rangle$ and fixed confinement frequency Γ_d , the roots r_0 decreases as we increase the magnetic field γ_c and so the coulomb electron interaction energy $\sim \frac{1}{r_0}$, for this state, enhances. Increasing

the magnetic field further, the electron–electron interaction energy enhances and thus the electron jumps to next state with higher angular momentum $|m|$, equivalently larger r_0 . By doing this the electron–electron energy in the new states tends to decrease. As a result of this electron jumping, the transition occurs and the ground state of the interacting electron, confined in a quantum dot, changes its angular momentum (*m*) and spin (*S*) quantum numbers. These transitions appear as kinks in the energy addition spectra of the QD. Indeed, these transitions had been observed experimentally by Ashoori *et al.* [5] using single–electron spectroscopy (SES) technique.

To study the effect of varying the confinement frequency Γ_d on the spectra we have plotted, in Figure 2 and also listed in Table 4, the energies of the states $m = 0, -1, -2, \dots, -5$ as a function of confinement frequency $\Gamma_d = 0.5$. Figures 1 and 2 clearly show the influence of the confinement frequency on the level ordering to these quantum dot spectra. In addition to these qualitative agreement, we have compared in Table 5, our computed quantum dot spectra with those of Zhu *et al.* [15], calculated at $\gamma = 1$. We have also obtained good agreement when we compared our results with those calculated by exact diagonalization methods as reported in various works [7, 8, 10, 11].

In conclusion, we have used the shifted $1/D$ expansion method to study the spectral properties of the quantum dot. The shifted $1/D$ expansion method has advantages over methods such as perturbation and numerical calculations. While the $1/D$ expansion method is valid for all the ranges of magnetic field strength *B*, the perturbation theory is limited only to a weak magnetic field range. Pure numerical calculations are computationally intensive and hard to follow in the physics

Table 2. The Energies (in R^*) of the Quantum Dot States *b, c, d, and e* Calculated at $\Gamma_d = 0.2$ and $\gamma = 0.2$ with and Without Coulomb Interactions.

$ n, m; n_{cm}, m_{cm}, s\rangle$	Excluding Interaction	Including Interaction
<i>b</i> : $ 0, 1; 00; 0\rangle$	0.697	1.126
<i>c</i> : $ 00; 0, 1; 0\rangle$	0.697	1.294
<i>d</i> : $ 02; 0, 0; 0\rangle$	0.796	1.139
<i>e</i> : $ 01; 0, 1; 1\rangle$	0.796	1.225

Table 3. The Electron–Electron Energies, Defined as the Difference Between Interacting and Non-interacting Electron Energies in the Quantum Dot System, Calculated for Various Relative States at $\Gamma_d = 0.4$.

$ 0 m\rangle$	Zhu <i>et al.</i> [15]	$1/D$
$ 0 0\rangle$	0.7494	0.732
$ 0 1\rangle$	0.5066	0.425
$ 0 2\rangle$	0.3998	0.400

Table 4. The Energies of the State $|0, -1; 0, 0; 1\rangle$ Calculated at $\Gamma_d = 0.2$ and 0.5 for Various Values of γ .

$\Gamma_d = 0.2$		$\Gamma_d = 0.5$	
γ	energy	γ	Energy
0.022	1.013	0.05	2.046
0.056	1.002	0.125	2.018
0.111	1.002	0.250	2.050
0.156	1.065	0.375	2.160
0.200	1.126	0.5	2.326
0.222	1.62	0.75	2.754
0.334	1.324	1.0	3.248
0.445	1.613	1.25	3.774

Table 5. The Energies of the States $|n_r, m; n_{cm}, m_{cm}, s\rangle$ Calculated at $\gamma = 1$ by Present Work (1/D Method) and Numerical Results [15].

$ n_r, m; n_{cm}, m_{cm}, s\rangle$	Zhu <i>et al.</i> [15]	Present work (1/D method)
$ 0 1; 0 0; 1\rangle$	3.8278	3.7953
$ 0 2; 0 0; 0\rangle$	4.6436	4.6432
$ 0 3; 0 0; 1\rangle$	5.5174	5.5136
$ 0 2; 0 1; 0\rangle$	5.6436	5.6432
$ 0 4; 0 0; 0\rangle$	6.4693	6.4782
$ 1 2; 0 0; 0\rangle$	6.5956	6.5844
$ 0 2; 1 0; 0\rangle$	6.6436	6.6432

of the problem. We study the effect of electron–electron interaction and confinement frequency on the energy levels of the quantum dot spectra. We give an explanation for the energy level crossings and for the removal of the level degeneracy. Based on calculated results, the shifted 1/D expansion method is an effective technique of producing and understanding the spectral properties of the two-electron quantum dot presented in a magnetic field of arbitrary strength.

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APPENDIX

The parameters α_1 and α_2 , appeared in Equation 7 are given as follows:

$$\alpha_1 = [(1 + 2n_r)e_2 + 3(1 + 2n_r + 2n_r^2)e_4] - \varpi^{-1} [e_1^2 + 6(1 + 2n_r)e_1e_3 + (11 + 30n_r + 30n_r^2)e_3^2]$$

$$\alpha_2 = (1 + 2n_r)d_2 + 3(1 + 2n_r + 2n_r^2)d_4 + 5(3 + 8n_r + 6n_r^2 + 4n_r^3)d_6$$

$$- \varpi^{-1} \left[\begin{aligned} &(1 + 2n_r)e_2^2 + 12(1 + 2n_r + 2n_r^2)e_2e_4 + 2e_1d_1 + 2(21 + 59n_r + 51n_r^2 + 34n_r^3)e_4^2 \\ &+ 6(1 + 2n_r)e_1d_3 + 30(1 + 2n_r + 2n_r^2)e_1d_5 + 6(1 + 2n_r)e_3d_1 + \\ &2(11 + 30n_r + 30n_r^2)e_3d_3 + 10(13 + 40n_r + 42n_r^2 + 28n_r^3)e_3d_5 \end{aligned} \right]$$

$$+ \varpi^{-2} \left[\begin{aligned} &4e_1^2e_2 + 36(1 + 2n_r)e_1e_2e_3 + 8(11 + 30n_r + 30n_r^2)e_2e_3^2 + 24(1 + n_r)e_1^2e_4 \\ &+ 8(31 + 78n_r + 78n_r^2)e_1e_3e_4 + 12(57 + 189n_r + 225n_r^2 + 150n_r^3)e_3^2e_4 \end{aligned} \right]$$

$$- \varpi^{-3} [8e_1^3 + 108(1 + 2n_r)e_1^2e_3^2 + 48(11 + 30n_r + 30n_r^2)e_1e_3^3 + 30(31 + 109n_r + 141n_r^2 + 94n_r^3)e_3^4]$$

with

$$e_j = \frac{\epsilon_j}{\varpi^{j/2}} \quad \text{and} \quad d_i = \frac{\delta_i}{\varpi^{i/2}}$$

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

The definition of ε_j and δ_i quantities are:

$$\varepsilon_1 = (2 - a)$$

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

$$\varepsilon_3 = -1 + r_0^5 V^{(3)}(r_0)/6Q$$

$$\varepsilon_4 = \frac{5}{4} + \frac{r_0^6 V^{(4)}(r_0)}{24Q}$$

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

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

$$\delta_3 = 2(2 - a)$$

$$\delta_4 = -5(2 - a)/2.$$