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The spectral properties of two-electron quantum dot

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Abstract

The spectra of two interacting electrons, confined in a quantum dot, is studied for any ratio of coulomb to confinement energy by using the shifted $1/N$ expansion method. An explanation is given to the energy-level crossings which occur in the quantum dot spectra. The oscillation of the spin of the ground state as the magnetic field varies is studied. Based on comparisons, the method shows very good agreement with very recent results produced by using WKB-approximation and exact numerical methods. © 2002 Elsevier Science B.V. All rights reserved.

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 a system of very small dimension 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 z -direction, which is the growth direction, is assumed to be stronger than that in xy -plane, so the dots can be viewed as two-dimensional disks. Different experimental [1–5] and theoretical [6–13] methods have been devoted to the investigation of the energy spectrum and correlation effects of the interacting electrons confined in quantum dots under the effect of applied magnetic field. In particular, the spectral properties of the two-electron quantum dot for any

ratio of the coulomb strength to the harmonic confinement recently received great attention [14–20]. In this work, we will also study the same case using another approach namely, the shifted $1/N$ expansion method. To achieve our aim we proceed in two steps. First, we use the shifted $1/N$ expansion method, as a non-perturbative technique, to produce an analytical energy expression for two interacting electrons confined in a quantum dot for any ratio of the coulomb strength to the harmonic confinement. Second, we give an explanation of the energy-level crossings which occur in the spectra of the quantum dot by making use of the energy expression we have obtained.

The rest of this work is organized as follows. In Section 2, we have presented the Hamiltonian theory for two interacting electrons confined in a harmonic QD in magnetic field. We have described, in Section 3, the shifted $1/N$ expansion technique. Section 4 is devoted to results and conclusions.

2. The Hamiltonian theory

The effective-mass Hamiltonian for two interacting electrons, confined by a harmonic potential of characteristic length $l_0 = (\hbar/m^*\omega_0)^{1/2}$ in the xy -plane, can be decoupled to center-of-mass and relative motion as follows:

$$H_R = \frac{1}{2M} \left(\mathbf{P} + \frac{Q}{c} \mathbf{A}(R) \right)^2 + \frac{1}{2} M \omega_0^2 R^2, \quad (1)$$

$$H_r = \frac{1}{2\mu} \left(\mathbf{p} + \frac{q}{c} \mathbf{A}(r) \right)^2 + \frac{1}{2} \mu \omega_0^2 r^2 + \frac{e^2}{\varepsilon} \frac{1}{|r|}. \quad (2)$$

For the center-of-mass $M = 2m^*$, $Q = 2e$, $P = p_1 + p_2$ and its coordinate $\vec{\mathbf{r}}_{\text{cm}} = (\vec{\mathbf{r}}_1 + \vec{\mathbf{r}}_2)/2$. Similarly, for the relative part we have reduced mass $\mu = m^*/2$, $q = e/2$, $\vec{\mathbf{p}} = (\vec{\mathbf{p}}_1 - \vec{\mathbf{p}}_2)/2$ and its coordinate $\vec{\mathbf{r}} = \vec{\mathbf{r}}_1 - \vec{\mathbf{r}}_2$.

The magnetic field B is taken to be uniform and is applied along z -axis, perpendicular to the plane of the interacting electrons. The relative Hamiltonian, Eq. (2), can be written as

$$H_r = -\frac{1}{2\mu} \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2}{\partial \varphi^2} \right] + \frac{1}{2} \mu \Omega^2 r^2 - \frac{i}{2} \omega_c \frac{\partial}{\partial \varphi} + \frac{e^2}{\varepsilon r} \quad (3)$$

with the cyclotron frequency given by $\omega_c = eB/m^*c$ and the effective confinement $\Omega^2 = \omega_0^2 + \omega_c^2/4$. The Zeeman energy term $E_{\text{spin}} = g\mu_B^* S_z$, where $S_z = [(1 - (-1)^m)/2]$ is the total spin, can be included directly in the total Hamiltonian state where even m quantum numbers are singlets ($S_z = 0$) and states with odd m are triplets ($S_z = 1$). Quantitatively, the Zeeman energy is very small and is not going to add a significant contribution to the total energy of the QD spectra. For example, the Zeeman energy is almost ~ 0.1 meV for QD made from GaAs ($g = -0.44$, $m^* = 0.067m_e$) in an applied magnetic field of strength 5 T. However, the oscillations of the spin make the physics of the QD spectra more rich and thus this issue deserves more analysis. By making the substitution

$$\phi(r) = r^{-1/2} \chi(r) e^{im\phi},$$

we obtain

$$\frac{d^2 \chi(r)}{dr^2} + \left(2\mu E - m\mu\omega_c - \frac{m^2 - 1/4}{r^2} - \mu\Omega^2 r^2 - \frac{2\mu e^2}{\varepsilon} \frac{1}{r} \right) \chi(r) = 0, \quad (4)$$

where $m = 0, \pm 1, \pm 2, \dots$ is the azimuthal quantum number. The eigenenergies for the center-of-mass motion can be exactly obtained as

$$E_{\text{cm}} = (2N_{\text{cm}} + |M_{\text{cm}}| + 1)\Omega + 1/2 M_{\text{cm}} \omega_c,$$

$$N_{\text{cm}} = 0, 1, 2, \dots, \quad M_{\text{cm}} = 0, \pm 1, \pm 2, \dots \quad (5)$$

The problem is reduced to solving the Hamiltonian of the relative motion, Eq. (2). By making the substitution $r = \sqrt{2}lx$, where $l^2 = (\hbar/m^*\Omega)$, we write Eq. (2) as

$$\frac{d^2 \chi(x)}{dx^2} + \left(\varepsilon - x^2 - \frac{\beta}{x} - \frac{m^2 - 1/4}{x^2} \right) \chi(x) = 0 \quad (6)$$

with

$$\varepsilon = (2E - m\omega_c)/\Omega \quad \text{and} \quad \beta = \sqrt{2}l/a_B, \quad a_B = \frac{1}{m^*e^2}, \quad (7)$$

where β is a tuning parameter and it measures the ratio of the coulomb interaction to the harmonic confinement,

$$\beta = \frac{\sqrt{2}l}{a^*} = 2\sqrt{\frac{R^*}{\hbar\Omega}} \quad (8)$$

with an effective Bohr radius $a^* = \hbar^2 \varepsilon / m^* e^2$.

We can adjust both the confinement energy through the frequency parameter ω_0 and the coulomb interaction energy by changing the dielectric constant ε of the medium leading to their relative change in β .

Since Eq. (6) represents the problem of relative motion confined in a harmonic potential coupled with a coulomb potential, $V(x) = x^2 + \beta/x$, which cannot be solved exactly by any analytical method, it is clear that we are going to resort to approximation methods.

3. Method of solution

The shifted $1/N$ expansion method, N being the spatial dimension is a pseudoperperturbative technique in the sense that it proposes a perturbation parameter that is not related to the coupling constant [22–26]. The

method starts by writing the radial Schrödinger equation, for an arbitrary cylindrical symmetric potential, in N -dimension space, as

$$\left[-\frac{d^2}{dr^2} + \frac{\bar{k}^2 [1 - (1-a)/\bar{k}] [1 - (3-a)/\bar{k}]}{4r^2} + \frac{V(r)}{Q} \right] \psi(r) = \varepsilon_{n_r, m} \psi(r), \tag{9}$$

where

$$V(r) = r^2 + \frac{\beta}{r} \tag{10}$$

and $\bar{k} = N + 2m - a$, a is a shifted parameter and Q is a scaling constant to be determined. The shifted $1/N$ expansion method consists of solving Eq. (9) in terms of the expansion parameter $1/\bar{k}$. It is convenient to shift the origin to r_0 by the definition

$$y = \bar{k}^{1/2} (r - r_0) / r_0 \tag{11}$$

and to expand Eq. (9) about $y = 0$ in powers of y . We obtain a one-dimensional Schrödinger equation with anharmonic oscillator potential as follows:

$$\left[-\frac{d^2}{dy^2} + \frac{1}{4} \bar{\omega}^2 y^2 + \varepsilon_0 + V(y) \right] \psi(y) = \varepsilon_{n_r, m} \psi(y), \tag{12}$$

where $V(y)$ is the perturbation potential,

$$\begin{aligned} V(y) = & g^{1/2} (\varepsilon_1 y + \varepsilon_3 y^3) + g (\varepsilon_2 y^2 + \varepsilon_4 y^4) \\ & + g^{3/2} (\delta_1 y + \delta_3 y^3 + \delta_5 y^5) \\ & + g^2 (\delta_2 y^2 + \delta_4 y^4 + \delta_6 y^6) \end{aligned} \tag{13}$$

and $g = 1/\bar{k}$.

The eigenenergies $\varepsilon_{n_r, m}$ for anharmonic oscillator can be analytically calculated in terms of its parameters using the perturbation techniques. Now, cutting the series obtained in Eq. (9) (after $1/\bar{k}$ expansion) to the same order in y and \bar{k} as Eq. (12), we can compare both equations term by term to identify all the parameters: anharmonic frequency $\bar{\omega}$, energy eigenvalues $\varepsilon_{n_r, m}$ and the shift parameter a , in terms of \bar{k} , r_0 and the potential derivatives. The harmonic frequency

$$\bar{\omega} = \left[3 + \frac{V''(r_0)}{V'(r_0)} \right]^{1/2} \tag{14}$$

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

$$\begin{aligned} \varepsilon_{n_r, m} = & \frac{\beta}{r_0} + r_0^2 + \frac{\bar{k}^2}{4r_0^2} + \frac{1}{r_0^2} \left[\frac{(1-a)(3-a)}{4} + \alpha_1 \right] \\ & + \frac{\alpha_2}{\bar{k}r_0^2} \end{aligned} \tag{15}$$

α_1 and α_2 are parameters expressed in terms of $Q, \bar{\omega}, n_r$ and given in the appendix. The shift parameter a is fixed by making the second contribution term to the energy series vanish, namely,

$$\frac{\bar{k}}{r_0} \left[\left(n_r + \frac{1}{2} \right) \bar{\omega} - \frac{(2-a)}{2} \right] = 0 \tag{16}$$

which gives

$$a = 2 - (2n_r + 1)\bar{\omega}. \tag{17}$$

This choice was physically motivated by the requirement that the eigenenergies produced by $1/\bar{k}$ expansion method agree with the analytic results for the harmonic oscillator and coulomb potential [23].

Q is a scaling constant which is introduced in order to get useful results from $1/\bar{k}$ expansion in large \bar{k} limit. Since the angular momentum barrier term goes like \bar{k}^2 at large \bar{k} (see Eq. (9)), it is essential to properly define the potential. For this reason, Q is introduced with the purpose of rescaling the potential in \bar{k}^2 , that is the order of magnitude of the centrifugal barrier to yield an effective potential V_{eff} which does not vary with \bar{k} at large values of \bar{k} . Q is determined by making the effective potential,

$$\bar{k}^2 V_{\text{eff}}(r) = \bar{k}^2 \left[\frac{1}{4r^2} + \frac{V(r)}{Q} \right] \tag{18}$$

having a minimum at $r_0 (\frac{dV_{\text{eff}}}{dr} |_{r_0} = 0)$, where the system has well-defined bound states. The roots r_0 are determined, for a particular quantum state (n_r, m) and confining frequency ω , through the following relation:

$$[2r_0^3 V'(r_0)]^{1/2} = Q^{1/2} = \bar{k} = (2 + 2m - a). \tag{19}$$

After obtaining the roots r_0 through Eqs. (17) and (19), the task of computing the energy from Eq. (15) is relatively easy. n_r is the radial quantum number related to the principle (n) quantum number by the relation $n_r = n - |m| - 1$.

4. Results and conclusions

Our results for QDs of two interacting electrons are presented in Figs. 1 and 2 and Tables 1–3. Fig. 1 shows the energy spectrum of two interacting electrons confined in QD produced with $1/N$ expansion technique for $n_r = 0$ and $m = 0, -1, -2, -3, -4$ and for finite electron–electron interaction, $\beta = 3$, against the ratio ω_c/ω_0 . It is obvious from the figure that the ground state shifts to the states with higher angular momentum as the magnetic field increases. The spin also changes to keep the wave function of the quantum electron state totally antisymmetric in accordance with the Pauli exclusion principle. For example, the first level crossing occurs at $\omega_c/\omega_0 \approx 0.9$. At this crossing, the ground state of the QD changes from $m = 0, S_z = 0$ to $m = -1$ and $S_z = 1$. The second crossing occurs at $\omega_c/\omega_0 \approx 1.5$ and the state (m, S_z) quantum numbers changes from $(-1, 1)$ to $(-1, 0)$. These spin (S_z) changes, from $S_z = 0$ to 1 and from 1 to 0, which occur in the QD spectra of interacting electrons are known as spin oscillations. Thus, the spin of the quantum dot states oscillates between singlet ($S_z = 0$) and triplet ($S_z = 1$) states as the applied magnetic field B increases. Our numerical results are in very good agreement with the ones of Ref. [14] produced very recently with WKB-approximation method. The level crossings which occur in the QD spectra are due to the dependence of the electron–electron interaction on the azimuthal quantum number $m, V_{e-e}(m)$, and can be physically understood from the analytical expression we obtained, Eq. (15), namely $V(r_0) = \beta/r_0 + r_0^2$. For this purpose we have listed, in Table 1, the roots r_0 which correspond to different quantum states $|0, m\rangle$ and for particular finite interaction strength $\beta = 1$, say. The table shows the following behavior: as the azimuthal quantum number m increases, the roots r_0 increases and thus the electron–electron coulomb energy, $V_{e-e}(m), (\sim 1/r_0(m))$ decreases leading to a reduction in the energy of the state. These results have been obtained for electron–electron interaction energy and are in quantitative agreement with the one obtained by Zhu et al. [15]. In this work [15], they have used the perturbation theory to calculate the analytic expression for the interaction energy matrix element, namely, $E_r(0, m) = \langle \phi_{0m} | 2/r | \phi_{0m} \rangle$. The expression gives the dependence of the coulomb energy, $E_r(0, m)$ on the quantum number m and clearly

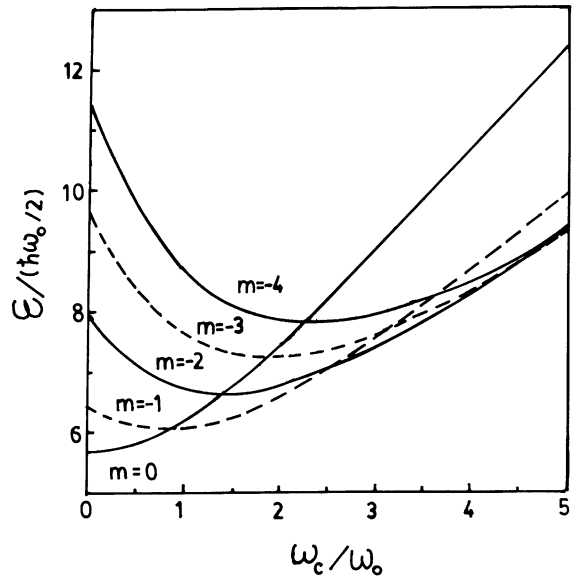


Fig. 1. The energy spectrum of a two interacting electrons, confined in a quantum dot, calculated by $1/N$ expansion method for quantum state $|0, m\rangle, m = 0, -1, -2, -3, -4$ and for finite electron–electron interaction parameter $\beta = 3$ (— singlet ($S_z = 0$) and - - - triplet ($S_z = 1$) states).

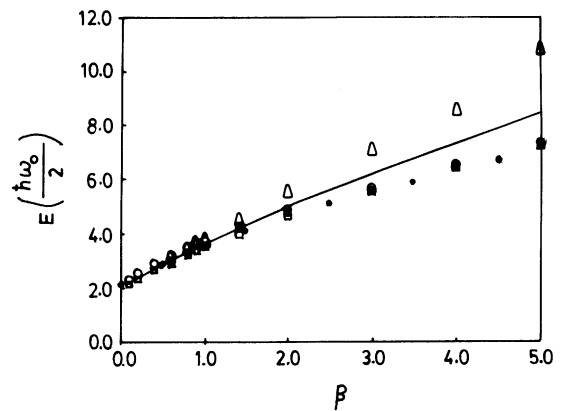


Fig. 2. The energies of the ground state $|0, 0\rangle$ as function of β calculated by: $1/N$ (●●●●●), variational (— — —), WKB (○ ○ ○ ○ ○), perturbation ($\Delta \Delta \Delta \Delta \Delta$) and exact numerical ($\square \square \square \square \square$) methods.

shows that this interaction coulomb energy (for fixed Ω and nodeless states $n_r = 0$) decreases as the azimuthal quantum number m increases, which again supports our results. On the other hand, the confinement energy ($\sim r_0^2$) is enhanced. The reduction in the

Table 1

The values of the roots r_0 for quantum dots states with different angular momentum $m = 0, -1, -2, \dots, -9$, calculated at $\beta = 1.0$

$ n, m\rangle$	r_0
$ 0, 0\rangle$	1.176
$ 0, -1\rangle$	1.495
$ 0, -2\rangle$	1.782
$ 0, -3\rangle$	2.203
$ 0, -4\rangle$	2.264
$ 0, -5\rangle$	2.472
$ 0, -6\rangle$	2.665
$ 0, -7\rangle$	2.845
$ 0, -8\rangle$	3.015
$ 0, -9\rangle$	3.175

Table 2

The spectra of two interacting electrons confined in a quantum dot calculated by different methods [16]; exact numerical (shooting) method, $1/N$ expansion method and WKB approximation for different quantum states, $|n, m\rangle^a$

$ n, m\rangle$	Exact	$1/N$	WKB
$\beta = 10.0$			
$ 0, 0\rangle$	10.4816	10.4398	10.5220
$ 0, -1\rangle$	10.8495	10.8341	10.8797
$ 0, -2\rangle$	11.7903	11.7860	11.8078
$ 0, -3\rangle$	13.0720	13.0717	13.0823
$ 0, -4\rangle$	14.5546	14.5544	14.5611
$ 0, -5\rangle$	16.1628	16.1629	16.1672
$ 0, -6\rangle$	17.8543	17.8541	17.8573
$ 0, -7\rangle$	19.6037	19.6037	19.6059
$ 0, -8\rangle$	21.3954	21.3954	21.5342
$ 0, -9\rangle$	23.2188	23.2188	23.2200
$\beta = 1.0$			
$ 0, 0\rangle$	3.4952	3.4234	3.6898
$ 0, -1\rangle$	4.8553	4.8524	4.8720
$ 0, -2\rangle$	6.6538	6.6535	6.6583
$ 0, -3\rangle$	8.5485	8.5484	8.5503
$ 0, -4\rangle$	10.4814	10.4814	10.4824
$ 0, -5\rangle$	12.4340	12.4340	12.4346
$ 0, -6\rangle$	14.3983	14.3983	14.3986
$ 0, -7\rangle$	16.3701	16.3701	16.3704
$ 0, -8\rangle$	18.3472	18.3472	18.3473
$ 0, -9\rangle$	20.3280	20.3280	20.3282

^aEnergies are expressed in units of $\hbar\omega_0/2$ for $\beta = 10$ and 1.

e–e interaction energy does not consume completely the enhancement energy. This competition between e–e interaction energy and confinement energy leads to a system with different ground states. In addition to this agreement with Refs. [14,15], we numerically test our results against the ones produced by

Table 3

The energies of the ground state $|0, 0\rangle$, expressed in units of $\hbar\omega_0/2$, for different values of parameter β produced by $1/N$ expansion method

β	$\epsilon_{0,0}$
0.5	2.7654
1.0	3.4234
1.5	4.0088
2.0	4.5421
2.5	5.0360
3.0	5.4998
3.5	5.9361
4.0	6.3544
4.5	6.7527
5.0	7.1343

WKB-approximation also in Ref. [16]. For $\beta = 1$ and 10, we compare, in Table 2, the eigenenergy spectrum produced by $1/N$ expansion technique against the numerical results produced by WKB-approximation and exact ones. The table clearly shows excellent agreement between both works. To test further the accuracy of our method, for different ranges of parameter β , against various methods used to study the same case, we plot, in Fig. 2, the energies in units of $(\hbar\omega_0/2)$ for the ground stage $n_r = n, m = 0$ against β . Fig. 2 shows that our results ($\bullet \bullet \bullet$) are in very good agreement with WKB-double parabola ($\circ \circ \circ$) and the exact numerical ($\diamond \diamond \diamond$) results. The energies produced by $1/N$ method for a large range of β are also given in Table 3. On the other hand, the results produced by perturbation theory and variational methods show a significant deviation from the ones produced by $1/N$, WKB and exact methods. This comparison indicates that the perturbation theory and variational methods are not reliable methods for all ranges of parameter β .

In conclusion, we have studied the spectral properties of two interacting electrons confined in a QD using the shifted $1/N$ expansion technique. The method provides us with an analytical energy expression that we use to understand the energy-level crossing and the transitions in the ground state of the interacting system. In addition to this, the method gives us very accurate energy spectra. Based on comparisons with different methods, WKB-approximation, perturbation, variational method and exact method, the shifted $1/N$ expansion technique gives accurate results for any degree of the coulomb to confinement ratio.

Appendix

The parameters α_1 and α_2 , appearing in Eq. (15) are given as follows:

$$\alpha_1 = [(1 + 2n_r)e_2 + 3(1 + 2n_r + 2n_r^2)e_4] - \bar{\omega}^{-1}[e_1^2 + 6(1 + 2n_r)e_1e_3 + (11 + 30n_r + 30n_r^2)e_3^2], \quad (\text{A.1})$$

$$\begin{aligned} \alpha_2 = & (1 + 2n_r)d_2 + 3(1 + 2n_r + 2n_r^2)d_4 \\ & + 5(3 + 8n_r + 6n_r^2 + 4n_r^3)d_6 \\ & - \bar{\omega}^{-1}[(1 + 2n_r)e_2^2 + 12(1 + 2n_r + 2n_r^2)e_2e_4 \\ & + 2e_1d_1 + 2(21 + 59n_r + 51n_r^2 + 34n_r^3)e_4^2 \\ & + 6(1 + 2n_r)e_1d_3 + 30(1 + 2n_r + 2n_r^2)e_1d_5 \\ & + 6(1 + 2n_r)e_3d_1 + 2(11 + 30n_r + 30n_r^2)e_3d_3 \\ & + 10(13 + 40n_r + 42n_r^2 + 28n_r^3)e_3d_5] \\ & + \bar{\omega}^{-2}[4e_1^2e_2 + 36(1 + 2n_r)e_1e_2e_3 \\ & + 8(11 + 30n_r + 30n_r^2)e_2e_3^2 + 24(1 + n_r)e_1^2e_4 \\ & + 8(31 + 78n_r + 78n_r^2)e_1e_3e_4 \\ & + 12(57 + 189n_r + 225n_r^2 + 150n_r^3)e_3^2e_4] \\ & - \bar{\omega}^{-3}[8e_1^3e_3 + 108(1 + 2n_r)e_1^2e_3^2 \\ & + 48(11 + 30n_r + 30n_r^2)e_1e_3^3 \\ & + 30(31 + 109n_r + 141n_r^2 + 94n_r^3)e_3^4] \quad (\text{A.2}) \end{aligned}$$

with

$$e_j = \varepsilon_j / \bar{\omega}^{j/2} \quad \text{and} \quad d_i = \delta_i / \bar{\omega}^{i/2} \quad (\text{A.3})$$

where

$$j = 1, 2, 3, 4; \quad i = 1, 2, 3, 4, 5, 6.$$

The definitions of ε_j and δ_i quantities are

$$\varepsilon_1 = (2 - a), \quad \varepsilon_2 = -3(2 - a)/2, \quad (\text{A.4})$$

$$\begin{aligned} \varepsilon_3 = & -1 + r_0^5 V^{(3)}(r_0)/6Q, \\ \varepsilon_4 = & 5/4 + r_0^6 V^{(4)}(r_0)/24Q, \end{aligned} \quad (\text{A.5})$$

$$\begin{aligned} \delta_1 = & -(1 - a)(3 - a)/2, \\ \delta_2 = & 3(1 - a)(3 - a)/4, \end{aligned} \quad (\text{A.6})$$

$$\delta_3 = 2(2 - a), \quad \delta_4 = -5(2 - a)/2, \quad (\text{A.7})$$

$$\begin{aligned} \delta_5 = & -3/2 + r_0^7 V^{(5)}(r_0)/120Q, \\ \delta_6 = & 7/4 + r_0^8 V^{(6)}(r_0)/720Q. \end{aligned} \quad (\text{A.8})$$

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