Energy States of Two Electrons in a Parabolic Quantum Dot in a Magnetic Field

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Abstract. — The energy spectra of two interacting electrons in a quantum dot confined by a parabolic potential in an applied magnetic field of arbitrary strength are obtained. The shifted $1/N$ expansion method is used to solve the effective-mass Hamiltonian. The influence of the electron-electron interaction on the ground-state energy and its significant effect on the energy level-crossings in states with different angular momenta is shown. The dependence of the ground-state energy on the magnetic field strength for various confinement energies is presented. *Comparisons show that our calculated spectra of the quantum dot states are in good agreement with different works.*

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 far infrared (FIR) experiments on gated and etched GaAs/AlGaAs and InSb structures have reported discrete states in these microstructures [1–3]. The growing interest in this field is motivated by the physical effects and the potential device applications of the QDs, to which many experimental [2,3] and theoretical [4–18] works have been devoted. The magnetic field dependence plays a useful role in identifying the absorption features. The effects of the magnetic field on the state of the impurity [8] and excitons [11–15] confined in QD have been extensively studied. Kumar, Laux and Stern [4] have self-consistently solved the Poisson and Schrödinger equations and obtained the electron states in GaAs/AlGaAs for both cases: in zero and for magnetic fields applied perpendicular to the heterojunctions. The results of their work [4] indicated that the confinement potential can be approximated by a simple one-parameter adjustable parabolic potential. Merkt, Huser and Wagner [5] have presented a study of quantum dots in which both the magnetic field and the electron-electron interaction terms were taken into account. Pfannkuche and Gerhardts [6] have devoted a theoretical study to the magneto-optical response to far-infrared radiation (FIR) of quantum-dot helium, accounting for deviations from the parabolic confinement. More recently, De Groote, Hornos and Chaplik [7]

have investigated the thermodynamic properties of quantum dots taking into consideration the spin effect, in addition to the electron-electron interaction and magnetic field terms. The purpose of this study is to show the effect of the electron-electron interaction on the spectra of the quantum dot states with non-vanishing azimuthal quantum numbers and the transitions in the ground state of the system as the magnetic field strength increases.

In this work, we shall use the shifted $1/N$ expansion method to obtain an energy expression for the spectra of two confined electrons in a quantum dot by solving the effective-mass Hamiltonian including the following terms: the electron-electron interaction, applied field and the parabolic confinement potential. The work is organized as follows. In Section 2, we present the Hamiltonian of the two interacting electrons, parabolically confined in the QD, subjected to a magnetic field. The shifted $1/N$ expansion method is described in Section 3. Results and conclusions are given in the final section.

2. Theory

Within the effective-mass approximation (EMA), the Hamiltonian for an interacting pair of electrons confined in a quantum dot by 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 where the electrons are restricted to move) in the symmetric gauge is written as follows,

$$H = \sum_{i=1}^{2} \left[-\frac{\hbar^2 \nabla_i^2}{2m^*} + \frac{1}{2} m^* \omega^2 r_i^2 + \frac{\hbar \omega_c}{2} L_i^z \right] + \frac{e^2}{\in |\mathbf{r}_1 - \mathbf{r}_2|}, \tag{1}$$

where the two-dimensional vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ describe the positions of the first and the second electron in the (x,y) plane, respectively. L_i^z stands for the z-component of the orbital angular momentum for each electron and $\omega_c = eB/m^*c$, m^* and $\in$ are 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

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

The natural units of length and energy to be used are the effective Bohr radius $a^* = \dfrac{\in \hbar^2}{m^* e^2}$ and effective Rydberg $R^* = \dfrac{\hbar^2}{2m^* a^{*2}}$. The dimensionless constant $\gamma = \dfrac{\hbar \omega_c}{2R^*}$ plays the role of an effective magnetic field strength.

Upon introducing the center-of-mass $\mathbf{R} = \dfrac{\mathbf{r}_1 + \mathbf{r}_2}{\sqrt{2}}$ and the relative coordinates $\mathbf{r} = \dfrac{\mathbf{r}_1 - \mathbf{r}_2}{\sqrt{2}}$, the Hamiltonian [7] in equation (1) can be written as a sum of two separable parts that represent the center-of-mass motion Hamiltonian,

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

and the relative motion Hamiltonian,

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

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

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

labelled by the radial ($n_{cm} = 0, 1, 2, ...$) and azimuthal ($m_{cm} = 0, \pm 1, \pm 2, \pm 3, ...$) quantum numbers. The problem is reduced to obtaining eigenenergies $E_{n_r,m}$ of the relative motion Hamiltonian. The energy states of the total Hamiltonian are labelled by the CM and relative quantum numbers, $|n_{cm}m_{cm}, n_r m >$. The coexistence of the electron-electron and the oscillator terms make the exact analytic solution with the present special functions not possible.

3. The Shifted 1/N Expansion Method

The shifted $1/N$ expansion method, N being 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 [20–22]. The aspect of this method has been clearly stated by Imbo et al. [20,21] who had displayed step-by-step calculations relevant to this method. Following their work, we present here only the analytic expressions which are required to determine the energy states.

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

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

where $k = N + 2m$.

In order to get useful results from $1/\bar{k}$ 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 [16]. 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, equation (6) in terms of the shift parameter becomes,

$$\left[-\frac{d^2}{dr^2} + \frac{\bar{k}^2 \left[1 - (1-a)/\bar{k}\right] \left[1 - (3-a)/\bar{k}\right]}{4r^2} + \frac{V(r)}{Q} \right] \Psi(r) = E_r \Psi(r) \tag{7}$$

where

$$V(r) = \frac{2}{r} + \frac{1}{4}\omega^2 r^2 + m\frac{\omega_c}{2} \tag{8}$$

and Q is a scaling constant to be specified from equation (10). The shifted $1/N$ expansion method consists in solving equation (7) systematically in terms of the expansion parameter $1/\bar{k}$. The leading contribution term to the energy comes from

$$\bar{k}^2 V_{\text{eff}}(r) = \frac{\bar{k}^2}{r_0^2} \left(\frac{1}{4} + \frac{r_0^2 V(r_0)}{Q} \right) \tag{9}$$

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

$$2r_0^3 V'(r_0) = Q \tag{10}$$

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

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

and expanding equation (7) 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 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

$$\bar{\omega} = \left[3 + \frac{V''(r_0)}{V'(r_0)} \right]^{1/2} \tag{12}$$

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

$$E_{n_r,m} = V(r_0) + \frac{\bar{k}^2}{4r_0} + \frac{1}{r_0^3} \left[\frac{(1-a)(3-a)}{4} + \gamma_1 \right] + \frac{\gamma_2}{\bar{k}r_0^2} \tag{13}$$

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 $\bar{k}$ to vanish, namely,

$$\frac{\bar{k}}{r_0^2} \left[\left(n_r + \frac{1}{2} \right) \bar{\omega} - \frac{(2-a)}{2} \right] = 0. \tag{14}$$

By requiring an agreement between $1/\bar{k}$ expansion and the exact analytic results for the harmonic and Coulomb potentials. From equation (14) we obtain

$$a = 2 - (2n_r + 1)\bar{\omega} \tag{15}$$

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 equations (6-15) are expressed in units of R^* and a^*, respectively.

For the two-dimensional case, $N = 2$, equation (10) takes the following form,

$$\sqrt{2r_0 V'(r_0)} = 2 + 2m - a = Q^{1/2} \tag{16}$$

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

4. Results and Conclusions

Our results are presented in Figures 1-5 and Tables I and II. The relative ground-state energy $|00>$ of the relative motion, for zero-magnetic field case, against the confinement length is displayed in Figure 1. The present results (dotted line) clearly show an excellent agreement with the numerical results of reference [5] (solid line). In Figure 2, the first low-energy levels, $|00>$, $|10>$ and $|20>$ of the relative Hamiltonian are presented as a function of the effective confinement frequency ω, using parameters appropriate to InSb, where the dielectric constant $\epsilon = 17.88$, electron effective mass $m^* = 0.014m_e$ and confinement energy $\hbar\omega_0 = 7.5$ meV [7]. The energy levels obviously show a linear dependence on the effective frequency. As the effective frequency w increases the confining energy term dominates the interaction energy term and thus the linear relationship between the energy and the frequency is maintained. This result is consistent with reference [7].

To investigate the effect of the electron-electron interaction on the energy spectra of the quantum dot, we have plotted in Figure 3 the total ground-state energy $|00;00>$ of the full
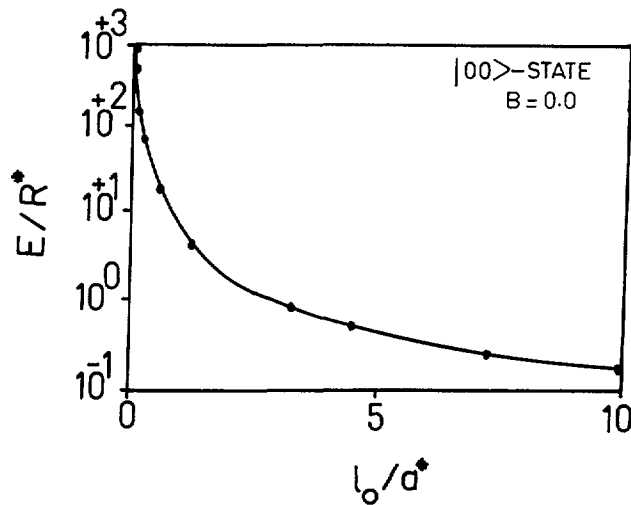
Fig. 1. — The relative ground state energy $|00>$ for the electrons in a quantum dot as a function of confinement length $\ell_0 = \left(\dfrac{\hbar}{m^*\omega_0}\right)^{1/2}$ for zero magnetic field: (——) reference [5]; (...) present calculations.
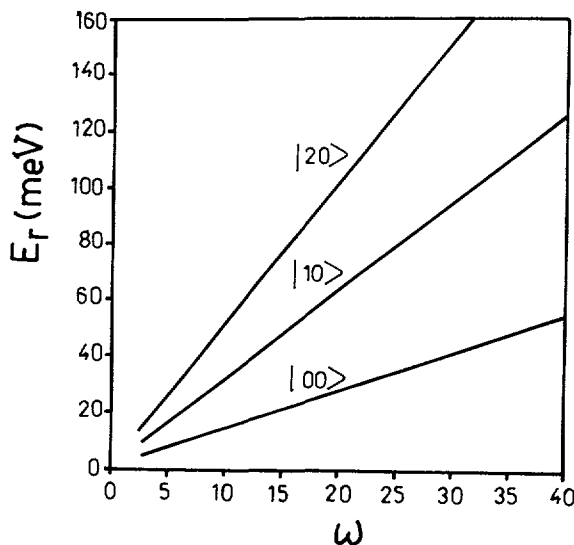

Fig. 2. — The low-lying relative states $|00>, |10>$ and $|20>$ for two electrons in a quantum dot made of InSb as a function of confinement frequency ω.

Hamiltonian for independent (——) and interacting (– – –) electrons as a function of the ratio ω_c/ω_0. The figure shows, as we expect, a significant energy enhancement when the electron-electron coulombic interaction term is turned on. Furthermore, as the magnetic field increases, the electrons are further squeezed in the QD, resulting in an increase of the repulsive electron-electron coulombic energy, and in effect the energy levels.

The energy level-crossings are shown in Figure 4. We have displayed the eigenenergies of
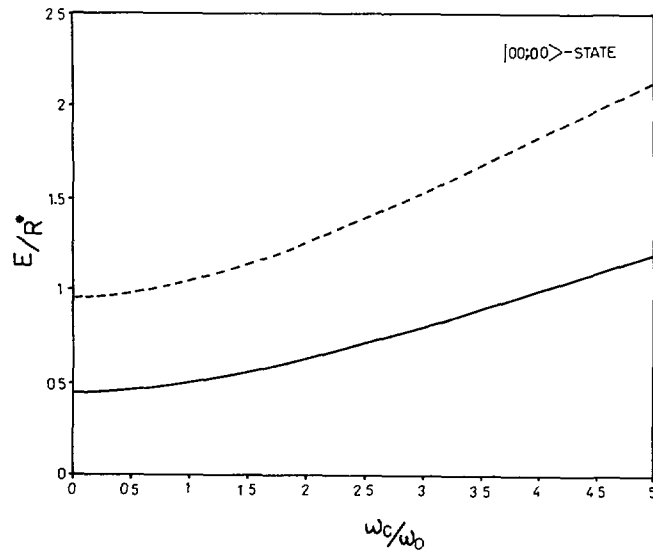
Fig. 3. — The total ground-state energy $|00;00>$ for two-electrons in a quantum dot as a function of the ratio ω_c/ω_0. For independent (——) and interacting (– – –) electrons.
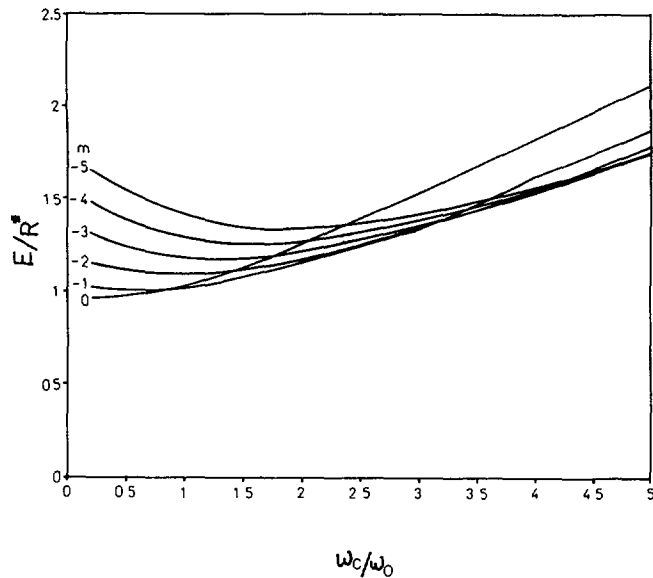

Fig. 4. — The total eigenenergies of the states $|00;0m>, m = 0, -1, -2, \ldots, 5$, for two interacting electrons parabolically confined in the quantum dot of size $\ell_0 = 3a^*$ as a function of the ratio ω_c/ω_0.

the states $|00;0m>; m = 0, -1, -2, . \quad -5$, for two interacting electrons parabolically confined in the quantum dot of size $\ell_0 = 3a^*$ as a function of the ratio ω_c/ω_0. As the magnetic field strength increases the energy of the state $m = 0$ increases while the energy of the states with non-vanishing quantum number m decreases, thus leading to a sequence of different

Table I. — *The roots r_0 determined by equation (16) for quantum dot states with non-vanishing azimuthal quantum numbers (m) against the ratio ω_c/ω_0.*

m ω_c/ω_0	0	-1	-2	-3	-4	-5
1	4.262	4.827	5.457	6.075	6.659	7.209
2	3.692	3.682	4.212	4.719	5.193	5.635
3	3.188	2.943	3.398	3.825	4.229	4.586

ground states, as reported in reference [16]. In the interacting system, the interaction energy is the lower the higher the angular momentum of the relative motion. This is caused by the structure of the relative wave function : The larger the angular momentum the larger the spatial extent and therefore, the larger is the distance between the electrons [17]. To confirm this numerically, we list in Table I the roots r_0 of the potential for the interacting electrons in the QD for states with different angular momentum. At particular values of the ratio ω_c/ω_0, as the azimuthal quantum number $|m|$ increases, the root r_0 also increases and thus the electron-electron interaction $V_{e-e}(r) = 2/r_0$, in the leading term of the energy series expression, decreases.

In Figure 5, we have shown the dependence of the ground-state energy on the magnetic field strength for confinement energies: $\hbar\omega_0 = 6$ and 12 meV. For constant value of the magnetic field, the larger the confinement energy, the greater the energy of the interacting electrons in the QD. The spin effect can be included in the Hamiltonian equation (1) added to the centre-of-mass part as a space-independent term, and equation (3) is still an analytically solvable harmonic oscillator Hamiltonian [7].

We have compared, in Table II, our calculated results for the ground state energies $|00>$ of the relative Hamiltonian at different confining frequencies with the results of Taut [18]. In a very recent work, Taut has reported a particular analytical solution of the Schrödinger equation for two interacting electrons in an external harmonic potential. The Table shows as $1/\omega$ increases the difference between both results noticeably decreases until it becomes $\approx 1.4 \times 10^{-3}$ at $1/\omega = 1419.47$.

Quantum dots with more than two electrons can also be studied. The Hamiltonian for n_e-interacting electrons, provided that the electron-electron interaction term depends only on the relative coordinates between electrons $V(|\mathbf{r}_i - \mathbf{r}_j|) = \dfrac{e^2}{\in |\mathbf{r}_{ij}|}$, and parabolically confined in the quantum dot, is separable into a CM and a relative Hamiltonians. The parabolic potential form $V(r_i) = m_i\omega_0^2 r_i^2/2$, $i = 1, 2, 3, \quad$, n_e is the only potential which leads to a separable Hamiltonian. The CM motion part is described by the one-particle Hamiltonian, equation (3), with the electron mass replaced by the total mass $M = n_e m^*$ and the electron charge replaced by the total charge $Q = n_e e$. The relative Hamiltonian part, which involves only the relative coordinates and momenta, has a cylindrically symmetric potential and can be handled by the $1/N$-expansion technique. When the confining potential is quadratic, FIR spectroscopy
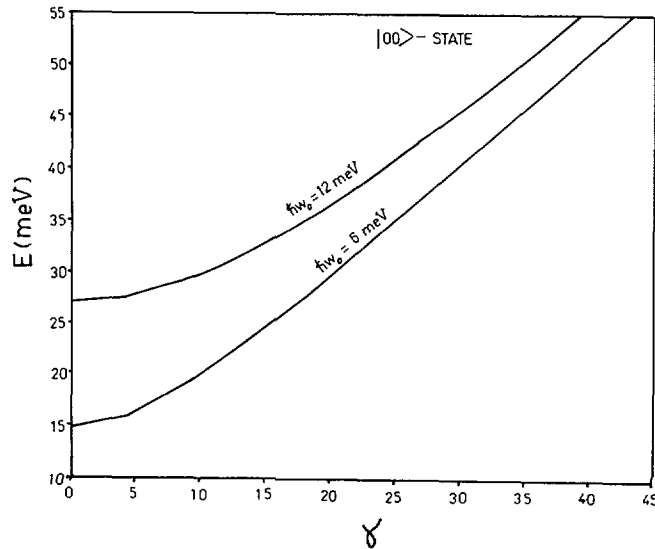
Fig. 5. — The relative ground-state energy $|00>$ against the magnetic field strength for two different confinement energies.

is insensitive to the interaction effects because of the CM and relative motions. The radiation dipole operator $\sum_i e_i \mathbf{r}_i = Q\mathbf{R}$, being a pure CM variable, then it does not couple to H_r which contains all the electron-electron interactions. The dipole operator then induces transitions between the states of the CM but does not affect the states of the relative Hamiltonian. The eigenenergies for the CM Hamiltonian, equation (5), does not change because ω_c in the energy expression remains the same, namely, $\dfrac{QB}{Mc} = \dfrac{eB}{m^*c}$. Consequently, the FIR absorption experiments see only the feature of the single-electron energies. There are only two allowed dipole transitions ($\Delta m = \pm 1$) and the FIR resonance occurs at frequencies

$$\omega_\pm = \sqrt{\left(\frac{(\omega_c)}{2}\right)^2 + \omega_0^2} \pm \frac{\omega_c}{2} \qquad (17)$$

Many different experiments on quantum dots have proved the validity of Kohn's theorem and that the observed resonance frequency of an electron system in a parabolic potential is independent of electron-electron interactions and thus the actual number of electrons in the well, as reported by Wixforth in a very recent review article [19].

In conclusion, we have obtained the energy spectra of two interacting electrons as a function of confinement energies and magnetic field strength. The method has shown good agreement with the numerical results of Merkt et al. [5], Taut [18] and Wagner et al. [16]. Our calculations have also shown the effect of the electron-electron interaction term on the ground state energy and its significance on the energy level-crossings in states with different azimuthal quantum numbers. The shifted $1/N$ expansion method yields quick results without putting restrictions on the Hamiltonian of the system.

Table II. — *The ground-state energies (in atomic units) of the relative Hamiltonian calculated by $1/N$ expansion at different frequencies, compared with the results of Taut [18].*

$1/\omega$	$1/N$ Expansion	Taut
4	0.4220	0.6250
20	0.1305	0.1750
54.7386	0.0635	0.0822
115.299	0.0375	0.0477
523.102	0.0131	0.0162
1054.54	0.0081	0.0100
1419.47	0.0067	0.0081

Acknowledgments

Appendix A

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

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

and

$$\gamma_2 = T_7 + T_{12} + T_{16} \tag{A.2}$$

where

$$T_7 = T_1 - \bar{\omega}^{-1} \left[T_2 + T_3 + T_4 + T_5 + T_6 \right] \tag{A.3}$$

$$T_{12} = \bar{\omega}^{-2} \left[T_8 + T_9 + T_{10} + T_{11} \right] \tag{A.4}$$

$$T_{16} = \bar{\omega}^{-2} \left[T_{13} + T_{14} + T_{15} \right] \tag{A.5}$$

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

$$c_1 = 1 + 2n_r \qquad c_4 = 11 + 30n_r + 30n_r^2 \qquad c_7 = 31 + 78n_r^2 + 78_r^3$$
$$c_2 = 1 + 2n_r + 2n_r^2 \qquad c_5 = 21 + 59n_r + 51n_r^2 + 34n_r^3 \qquad c_8 = 57 + 189n_r + 225n_r^2 + 150n_r^2$$
$$c_3 = 3 + 8n_r + 6n_r^2 + 4n_r^3 \qquad c_6 = 13 + 40n_r + 42n_r^2 + 28n_r^3 \qquad c_9 = 31 + 109n_r + 141n_r^2 + 94 + n_r^3$$

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

$$\text{where} \quad j = 1, 2, 3, 4 \quad \text{and} \quad i = 1, 2, 3, 4, 5, 6.$$

$$\epsilon_1 = (2 - a) \quad \epsilon_2 = -\frac{3(2-a)}{2} \quad \epsilon_3 = -1 - \frac{2r_0}{Q}$$

$$\epsilon_4 = \frac{5}{4} + \frac{2r_0}{Q} \quad \delta_1 = -\frac{(1-a)(3-a)}{2}$$

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

$$\delta_5 = -\frac{3}{2} - \frac{2r_0}{Q} \quad \delta_6 = \frac{7}{4} + \frac{2r_0}{Q}$$

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