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The energy level structure of two interacting electrons in a quantum dot

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ABSTRACT

The energy level structure of the relative motion of two electrons confined in a quantum dot is studied using the 1/N expansion method for any ratio of Coulomb to confinement energies.

Keywords: Interacting electrons, quantum dots, shifted 1/N expansion method.

I. 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 z-direction, which is the growth direction, is assumed to be stronger than that in the xy-plane, so that the dot can be viewed as two-dimensional disks. Different experimental (Drexler *et al.* 1994, Sikorski & Merkt 1989, Demel *et al.* 1990, Lorke *et al.* 1990, Wixforth *et al.* 1994, Ashhori 1996, Tarucha *et al.* 1996), and theoretical (Maksym & Chakraborty 1990, Wagner *et al.* 1992, Pfannkuche & Gerhardts 1993, De Groote *et al.* 1992, Merkt *et al.* 1991, Pfannkuche & Gerhardts 1991, Zhu & Gu 1993, Klama & Mishchenko 1998, Jhonson Payne 1991), methods have been devoted to investigating the energy spectrum and correlation effects of the interacting electrons confined in quantum dots under the effect of an applied magnetic field. In particular, the spectral properties of two-electron quantum dot for any ratio of the Coulomb strength to the harmonic confinement recently received great attention (Klama & Mishehenko 1998, Garcia-Castelan *et al.* 1998, A nisimovas & Matulis 1998, Matulis & Peeters 1994, Blanter *et al.* 1996, Peeters & Schweigert 1996, Oh *et al.* 1996). In this work we will also study the same case using a different 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 Coulomb strength to the harmonic confinement. Second, we give an explanation of the energy shifts and level-crossing, 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 outlined as follows. In section II, we present the Hamiltonian theory for two interacting electrons parabolically confined in a quantum dot. We describe, in section III, the shifted 1/N expansion technique. The final section is devoted to results and conclusions.

II. THE HAMILTONIAN THEORY

The effective-mass Hamiltonian for two interacting electrons, confined by a parabolic potential of characteristic length $\ell_0 = \left(\hbar/m^*\omega_0\right)^{1/2}$ in the xy-plane, can be decoupled to center-of-mass and relative motion as follows:

$$H_r = \frac{P^2}{2M} + \frac{1}{2}M\omega_0^2 R^2 \tag{1}$$

$$H_r = \frac{p^2}{2\mu} + \frac{1}{2}\mu\omega_0^2 r^2 + \frac{e^2}{\varepsilon\left|\overrightarrow{r}\right|} \tag{2}$$

for the center-of-mass $M = 2m^*$, $Q = 2e$, $\overrightarrow{P} = \overrightarrow{P_1} + \overrightarrow{P_2}$ and its coordinate $\overrightarrow{r_{cm}} = \frac{(\overrightarrow{r_1}+\overrightarrow{r_2})}{2}$. Similarly, for the relative part we have the reduced mass $\mu = m^*/2$, $q = e/2$, its momentum $\overrightarrow{p^2} = \frac{(\overrightarrow{p_1}-\overrightarrow{p_2})}{2}$ and its coordinate $\overrightarrow{r} = \overrightarrow{r_1} - \overrightarrow{r_2}$. The relative motion Hamiltonian in Eq.2 can be written in an operator form as,

$$H_r = \frac{\hbar^2}{2\mu}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2}\right] + \frac{1}{2}\mu\omega_0^2 r^2 + \frac{e^2}{\varepsilon r} \tag{3}$$

Acting with H_r on the wavefunction $\Phi(r,\varphi) = r^{-1/2}\chi(r)e^{im\varphi}$, we obtain the following radial equation,

$$\frac{d^2\chi(r)}{dr^2} + \left(\frac{2\mu}{\hbar^2}E - \frac{m^2-1/4}{r^2} - \frac{\mu^2\omega_0^2}{\hbar^2}r^2 - \frac{2\mu e^2}{\hbar^2\varepsilon}\frac{1}{r}\right)\chi(r) = 0 \tag{4}$$

where $m = 0,\ \pm1,\ \pm2,\ \ldots$ the azimuthal quantum number.

The eigenenergies for the center-of-mass motion can be exactly obtained as

$$E_{cm} = (2N_{cm} + |M_{cm}| + 1)\,\omega_0 \tag{5}$$

$$N_{cm} = 0, 1, 2 \ldots \quad , \; M_{cm} = 0, \pm 1, \pm 2, \ldots$$

The problem is reduced to solving the Hamiltonian of the relative motion. By making the substitution $r = \sqrt{2}\,\ell_0 x$, we write Eq.2 as

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

with

$$\varepsilon = \frac{E}{\frac{\hbar\omega_0}{2}} \tag{7}$$

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

$$\lambda = \frac{\sqrt{2}\,\ell_0}{a^*} = 2\sqrt{\frac{R^*}{\hbar\omega_0}} \tag{8}$$

with an effective Bohr radius $a^* = \dfrac{\hbar^2\varepsilon}{m^* e^2}$. We can adjust both the confinement energy through the frequency parameter ω_0 and the Coulomb energy by changing the dielectric constant, ε, of the medium leading to their relative change in λ.

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

III. METHOD OF SOLUTION

The shifted 1/N expansion method N being the spatial dimension, is a pseudoperturbative technique in the sense that it proposes a perturbation parameter that is not related to the coupling constant (Imbo *et al.* 1984, Imbo & Sukhatme 1985, Imbo & Sukhatme 1983. Dutt *et al.* 1986, El-Said 1995).

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

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

where

$$V(r)=r^2+\frac{\lambda}{r} \qquad (10)$$

$\bar{k}=N+2m-a$, a is a shift parameter and Q is a scaling constant to be determined. It is convenient to shift the origin to r_0 by the definition

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

and to expand Eq.10 about $y=0$ in powers of y. Comparing the coefficients of powers of y in the series with the corresponding ones of the same order in the Schrödinger equation for a one-dimensional anharmonic oscillator, we determine the anharmonic frequency, the energy eigenvalue, the scaling constant and the shift parameter, in terms of $\bar{k}$, r_0 and the potential derivatives. The anharmonic frequency parameter is

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

The energy eigenvalues in powers of $\frac{1}{\bar{k}}$ (including second order) read as

$$\varepsilon_{n_r,m}=\frac{\lambda}{r_0}+r_0^2+\frac{\bar{k}^{-2}}{4r_0}+\frac{1}{r_0^3}\left[\frac{(1-a)(3-a)}{4}+\alpha_1\right]+\frac{\alpha_2}{\bar{k}^{-2}r_0^2} \qquad (13)$$

$$a=2-(2n_r+1)\bar{\omega} \qquad (14)$$

$$\sqrt{2r_0^3V'(r_0)}=2+2m-a=Q^{1/2} \qquad (15)$$

where α_1 and α_2 are parameters expressed in terms of Q, $\bar{\omega}$, a and n_r and given in the appendix. The roots r_0 (for particular quantum state $|n_r\ ,\ m>$ and confining frequency, ω_0) can be determined through Eq.14 and Eq.15, and thus the task of computing the energies, from Eq.13, is relatively easy. n_r is the radial

quantum number related to the principle (n) and magnetic (m) quantum number by the relation, $n_r = n - |m| - 1$.

IV. RESULTS AND CONCUSIONS

Our results for QD of two interacting electrons are presented in Figs.(1-3) and Tables (I-III). Figure.1 compares the energy spectra of two independent $(\lambda = 0)$

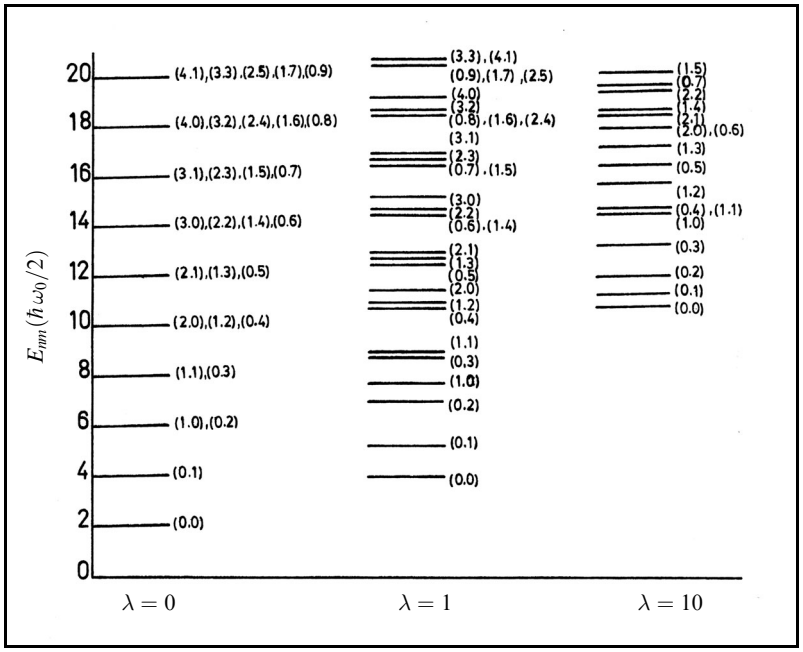

Fig.1. The spectra of the relative motion of two confined electrons in a quantum dot for $\lambda = 0$, 1 and 10 produced by 1/N method. Different numerical values for common spectra produced by various methods are given in Table III.

and interacting ($\lambda = 1$ and 10) electrons confined in a quantum dot. Experimental works report that the range of ratio λ is approximately 2, $(\hbar\omega_0 \approx 5meV)$. The comparison shows that the spectra of the quantum dot is influenced by the Coulomb interaction energy in two ways. First, the states of the spectra are shifted to higher energies. In particular, the states with low quantum numbers. (0 , 0), (0, 1), (1, 0) and (0, 2) are significantly shifted. Second, the degeneracy of the states, which appears for the independent case, is now lifted. To understand both effects, particular attention should be paid to the first term in the energy series expression, namely, $V(r_0) = \dfrac{\lambda}{r_0} + r_0^2$. The contribution of this term to the total

energy of each quantum state is noticebly large, almost 50%. In addition to this significant amount of energy contribution, this term represents the competition between Coulomb interaction and confinement energies. We list, in Table I, the root r_0 which corresponds to each quantum state $|0,\ m>$, $m = 0,\ +1,\ +2,\ \ldots,$ $+9$ for $\lambda = 1$ and 10. It is clear from the table that, as the azimuthal quantum number m increases, the corresponding roots (r_0) also increase. Thus the electron-electron interaction term $(\sim \dfrac{1}{r_0})$ decreases leading to a reduction in the energy of the state. In this behaviour, the Coulomb interaction energy, $V_{e-e}(r_0) = \dfrac{\lambda}{r_0}$ shows a dependence on the azimuthal quantum number (m) and λ, displayed in Figs.2 (a & b). This Coulomb interaction dependence on m and λ, namely, $V_{e-e}(m, \lambda)$ is

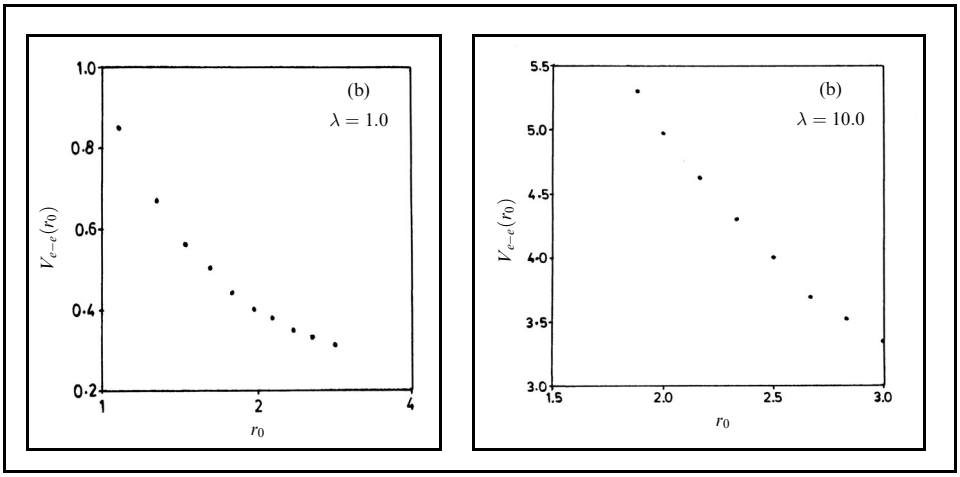

Fig.2. The Coulomb interaction energy as a function of the roots r_0 corresponding to quantum states $|0,\ m>= 0,\ -1,\ \ldots,\ -9$; for a) $\lambda = 1$ and b) $\lambda = 10$

significant since it eliminates the possibility of having different quantum states $(n, |m|)$ but the same energy and in this way the Coulomb energy removes the state degeneracy. For example, the states with different values of m which are degenerate for the independent case $(\lambda = 0)$ like; $|2,\ 1>$, $|1,\ 3>$ and $|0,\ 5>$ are split for $\lambda = 1$ with the corresponding different energies: 6.56318, 6.53910 and 6.51522. These energies are calculated by using the first energy term only (see Table II). Figure.1 shows that the energy of the state with high m-values reduced and thus shifted to lower states upon degeneracy removal by finite electron interaction $(\lambda = 1)$. The physical reason for this is the following: states with high m-values correspond to large roots (r_0): 2.48199, 2.47697 and 2.47198 and eventually more electron separation which in turn reduces the Coulomb

interaction contribution. On the other hand, the confinement energy ($\sim r_0^2$) is enhanced. The reduction in the electron-electron interaction energy does not consume completely the enhancement in the confinement energy. This competition between electron-electron interaction energy and confinement energy shifts the energy of the spectra and leads to a system with different ground states. For this purpose, we have calculated and listed explicitly, in Table II, the roots r_0 and the dominant energy contribution $V(r_0)$ which corresponds to each quantum state of the spectra. Using the leading energy term, namely $V(r_0) = \frac{\lambda}{r_0} + r_0^2$ we successfully placed all the non-degenerate quantum states in their correct spectral order, calculated exactly. The result calculated by 1/N and exact methods are displayed in Fig.3.

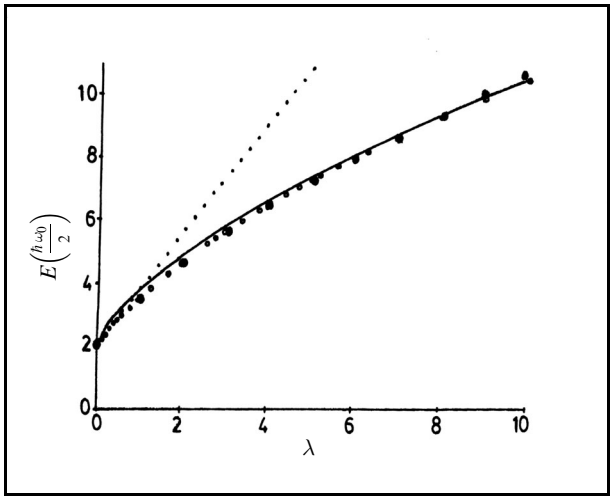

Fig.3. The ground state ($n = 0,\ m = 0$) eigen energies calculated by 1/N (●●●), WKB-double parabola (———), exact numerical (○ ○ ○) and perturbation (◇ ◇ ◇) methods

In addition to this qualitative explanation of the spectral properties of the quantum dots, we numerically test our results produced by 1/N expansion method against the ones produced by exact and WKB results, given in Garcia-Castelan, Choe & LEE (1998). Our computed results are in very good agreement, comparable with both methods for various values of λ. For comparison purposes, we listed in Table III the eigenenergies of the frequent dot states given in different works. We test further the accuracy of our method against various ones used to study the same case. In Fig.3, we show the energies of the ground state ($n_r = 0,\ m = 0$) against the finite interaction parameter λ. The plot shows that our result (●●●) using the shifted 1/N expansion method are in very good agreement with the WKB-double parabola (———) and exact

($\circ\circ\circ$) results. On the other hand, the results produced by perturbation theory ($\diamond\diamond\diamond$) show a significant deviation from all: exact, WKB-double parbola and 1/N expansion methods. This comparison shows that the perturbation theory is not a reliable method for all ranges of the finite parameter λ.

Table I. The roots (r_0) corresponding to quantum states $|n,\ m>,\ m = 0,\ 1,\ 2,\ \ldots,\ 9$ for $\lambda = 1$ and 10.

	r_0	
$\|\mathbf{0},\ \boldsymbol{m}>$	$\lambda = \mathbf{1.0}$	$\lambda = \mathbf{10.0}$
$\|0,\ 0>$	1.17600	1.88500
$\|0,\ 1>$	1.49502	2.00700
$\|0,\ 2>$	1.78202	2.16099
$\|0,\ 3>$	2.03601	2.32899
$\|0,\ 4>$	2.26398	2.50099
$\|0,\ 5>$	2.47198	2.66999
$\|0,\ 6>$	2.66499	2.83499
$\|0,\ 7>$	2.84499	2.99299
$\|0,\ 8>$	3.01499	3.14599
$\|0,\ 9>$	3.17499	3.29299

Table II. The energy contribution of the dominant energy term, $V(r_0) = r_0^2 + \dfrac{\lambda}{r_0}$, calculated for the quantum states shown in Fig.1 for $\lambda = 1$.

$\|\mathbf{0},\ \boldsymbol{m}>$	$\boldsymbol{r_0}$	$\boldsymbol{V(r_0) = r_0^2 + \dfrac{\lambda}{r_0}}$
$\|1,\ 7>$	3.17694	10.40772
$\|0,\ 9>$	3.17499	10.39552
$\|4,\ 0>$	3.02397	9.47085
$\|3,\ 2>$	3.02195	9.46309
$\|2,\ 4>$	3.01897	9.44542
$\|1,\ 6>$	3.01697	9.43357
$\|0,\ 8>$	3.01499	9.42184
$\|3,\ 1>$	2.85398	8.49559
$\|2,\ 3>$	2.85095	8.47868
$\|1,\ 5>$	2.84795	8.46195
$\|0,\ 7>$	2.84499	8.44546
$\|3,\ 0>$	2.67596	7.53446
$\|2,\ 2>$	2.67296	7.51883

Table II. The energy contribution of the dominant energy term, $V(r_0) = r_0^2 + \dfrac{\lambda}{r_0}$, calculated for the quantum states shown in Fig.1 for $\lambda = 1$. (cont'd.)

$\|\mathbf{0},\ m>$	r_0	$V(r_0) = r_0^2 + \dfrac{\lambda}{r_0}$
$\|0,\ 7>$	2.84499	8.44546
$\|3,\ 0>$	2.67596	7.53446
$\|2,\ 2>$	2.67296	7.51883
$\|0,\ 6>$	2.66499	7.47741
$\|2,\ 1>$	2.48199	6.56318
$\|1,\ 3>$	2.47697	6.53910
$\|0,\ 5>$	2.47198	6.51522
$\|2,\ 0>$	2.27799	5.62822
$\|1,\ 2>$	2.27099	5.59773
$\|0,\ 4>$	2.26398	5.56731
$\|1,\ 1>$	2.04702	4.67881
$\|0,\ 3>$	2.03601	4.63649
$\|1,\ 0>$	1.80101	3.79885
$\|0,\ 2>$	1.78202	3.73676
$\|0,\ 1>$	1.49502	2.90397
$\|0,\ 0>$	1.17600	2.33332

Table III. The spectra of the quantum dot produced by different methods for various values of parameter λ.

$\|\mathbf{0},\ m>$	$\lambda = \mathbf{1.0}$			$\lambda = \mathbf{10.0}$		
	1/N	**Exact**	**WKB**	**1/N**	**Exact**	**WKB**
$\|0,\ 0>$	3.4234	3.4952	3.6898	10.4398	10.4816	10.5220
$\|0,\ 1>$	4.8524	4.8553	4.8720	10.8341	10.8495	10.8797
$\|0,\ 2>$	6.6535	6.6538	6.6583	11.7860	11.7903	11.8078
$\|0,\ 3>$	8.5484	8.5485	8.5503	13.0717	13.0720	13.0823
$\|0,\ 4>$	10.4814	10.4814	10.4824	14.5544	14.5546	14.5611
$\|0,\ 5>$	12.4340	12.4340	12.4346	16.1629	16.1628	16.1672
$\|0,\ 6>$	14.3983	14.3983	14.3986	17.8541	17.8543	17.8573
$\|0,\ 7>$	16.3701	16.3701	16.3704	19.6037	19.6037	19.6059
$\|0,\ 8>$	18.3472	18.3472	18.3473	21.3954	21.3954	21.3970
$\|0,\ 9>$	20.3280	20.3280	20.3282	23.2188	23.2188	23.2200

In conclusion, we have studied the spectral properties of two interacting electrons confined in a quantum dot using the shifted 1/N expansion technique. With this method, we are able to produce an energy expression that we use to understand the physical properties of the quantum dot spectra. In addition to this, the method shows good accuracy. Based on comparison with different methods: exact WKB-approximation and perturbation methods, the shifted 1/N expansion technique gives us the energies with very good accuracy for any degree of Coulomb to confinement ratio.

APPENDIX

The parameters α_1 and α_2, which appeared in Eq.13 are given as follows:

$$\alpha_1 = \left\lfloor (1+2n_r)e_2 + 3(1+2n_r+2n_r^2)e_4 \right\rfloor - \bar{\omega}^{-1}\left[e_1^2 + 6(1+2n_r)e_1e_3 + (11+30n_r+30n_r^2)e_3^2\right]$$

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

$$-\bar{\omega}^{-1}\begin{bmatrix} (1+2n_r)e_2^2 + 12(1+2n_r+2n_r^2)e_2e_4 + 2e_1d_1 + 2(21+59n_r+51n_r^2+34n_r^3)e_4^2 \\ +6(1+2n_r)e_1d_3 + 30(1+2n_r+2n_r^2)e_1d_5 + 6(1+2n_r)e_3d_1 + \\ 2(11+30n_r+30n_r^2)e_3d_3 + 10(13+40n_r+42n_r^2+28n_r^3)e_3d_5 \end{bmatrix}$$

$$+\bar{\omega}^{-2}\begin{bmatrix} 4e_1^2e_2 + 36(1+2n_r)e_1e_2e_3 + *(11+30n_r+30n_r^2)e_2e_3^2 + 24(1+n_r)e_1^2e_4 \\ +8(31+78n_r+78n_r^2)e_1e_3e_4 + 12(57+189n_r+225n_r^2+150n_r^3)e_3^2e_4 \end{bmatrix}$$

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

with

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

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

The definition of ε_j and δ_i quantities are

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

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

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

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

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

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بنية مستوى طاقة ألكترونين متفاعلين في نقطة كمية

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ص.ب: 2440 – هيل – المملكة العربية السعودية

خلاصة

تمت دراسة مستوى الطاقة للحركة النسبية لألكترونين مدخلين في نقطة كمية وذلك باستخدام طريقة مفكوك الـ 1/N لأي نسبة من طاقات الكولوم للمدخلات.