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The ground state of two-electron quantum dot in a magnetic field: the 1/N expansion method

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ABSTRACT

The ground-state properties of a two-dimensional quantum-dot are studied. We have used the shifted 1/N expansion method to solve the relative part of the Hamiltonian of two electrons confined in a quantum dot in the presence of an applied uniform magnetic field. The spin singlet-triplet transition in the ground state of the QD is shown. We have also displayed the singlet-triplet energy gap against the strength of the magnetic field for a two electron quantum dot. Based on comparisons, the eigenenergies obtained by the 1/N shifted method are in excellent agreement with exact numerical diagonalization and variational methods.

Keywords: Quantum Dots , Magnetic Field, Eigenenergies , 1/N method.

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INTRODUCTION

Quantum dots (QDs), or artificial atoms, have been the subject of intense research over the last few years. The growing interest is motivated by the new physical effects and potential device applications. Different analytical and numerical methods (Burkard *et al.*, 1999, Ciftja *et al.*, 2005, Ciftja *et al.*, 2004, Dyblaski *et al.*, 2005, Elsaid 2003, Elsaid 1995, Helle *et al.*, 2005, Kyriakidis *et al.*, 2005, Kyriakidis *et al.*, 2002, Loss *et al.*, 1998, Matulis *et al.*, 2001, Matulis *et al.*, 1994, Merkt et al., 1991, Peeters *et al.*, 1996 , Szafran *et al.*, 2004, Taut 1994, Taut 1993, Wagner *et al.,* 1992, Xu *et al.*, 2005) have been used to investigate the energy spectrum and the correlation effects of the interacting electrons confined in a quantum dot for zero and finite magnetic fields. The QD has the potential to serve as a qubit for a quantum computer since the magnetic field can be used to tune the transition in the spin of the ground state of the quantum dot from the singlet ($S = 0$) to the triplet ($S = 1$) state (Ciftja, 2005, Ciftja, 2004). Szafran and his collaborators (Szafran *et al.*, 2004) used the exact diagonalization method to study laterally coupled quantum dots occupied by two electrons. They considered two-dimensional double quantum dots in a perpendicular magnetic field along the z-axis with a confinement potential

considering V(x,y) of two Gaussian dots, where V_ℓ and V_R are the depths of the left and right potential wells, respectively. They showed that the asymmetry ($V_\ell > V_R$) gives rise to an enhancement of the tunable exchange energy, the triple-singlet energy difference, J, for a finite magnetic field. One of the most interesting features of electron correlation is the change of the spin and angular momentum structure in the ground state of the QD system in the presence of a magnetic field. In this work we shall test the applicability of the shifted 1/N expansion method by solving the relative part Hamiltonian of two interacting electrons that are confined in a quantum dot and study its electronic ground state properties. The singlet-triplet energy splitting J is also calculated. We have compared our computed results with the corresponding ones obtained by exact numerical diagonolization techniques, variational and Laughlin-type variational wavefunction methods (Ciftja *et al.*, 2005) .

THE STUDY

The effective-mass Hamiltonian for an interacting pair of electrons confined in a quantum-dot by a parabolic potential in a uniform magnetic field of strength B is given by,

$$H = \sum_{i=1}^{2} \left\{ \frac{P_i^2}{2m^*} + \frac{1}{2} m \left[\omega_0^2 + \frac{\omega_c^2}{4} \right] \rho_i^2 + \frac{\omega_c}{2} L_i \right\} + \frac{e^2}{\kappa |\vec{\rho}_2 - \vec{\rho}_1|} + g \mu_B B S_z, \quad (1)$$

where ω_0 is the confinement frequency, μ_B is the Bohr magneton and κ is the dielectric constant. The energy E is measured in units of $\hbar\omega_0$. λ is the dimensionless parameter defined as the ratio of the coulomb strength to the confining energy, $\lambda = e^2\alpha/\hbar\omega_0$, where $\alpha = \sqrt{\frac{m\omega_0}{\hbar}}$ has the dimension of inverse length and $\gamma = \frac{\omega_c}{\omega_0}$. Upon introducing the standard coordinates and momenta transformation, the Hamiltonian (H) can be decoupled to center-of-mass (H_R) and relative H_r parts. The Hamiltonian H_R is of a harmonic oscillator type with well-known eigenenergies $E_{n_{cm}m_{cm}} = (2n_{cm} + |m_{cm}| + 1)\hbar\omega_0$, and quantum numbers $n_{cm} = 0, 1, 2, ...$, and $m_{cm} = 0 \pm 1, \pm 2, ...$ The main issue in the present work is to solve the relative-part Hamiltonian H_r,

$$H_r = \frac{p^2}{2\mu} + \frac{1}{2}\mu \left[\omega_0^2 + \frac{\omega_c^2}{4} \right] \rho^2 + m\frac{\hbar\omega_c}{2} + \frac{e^2}{k\rho} + g\mu_B B S_z \quad , \quad (2)$$

by using the shifted 1/N expansion method. The steps to produce the eigenenergies by the shifted method are presented in previous works (Elsaid 1995, Imbo *et al.,* 1983, Imbo *et al.,* 1984, Imbo *et al.,* 1985) and will not be

repeated here. Only the necessary expressions to compute the energies will be given. The method starts by writing the radial Schrödinger equation for an arbitrary cylindrically symmetric potential in a N-dimensional space as

$$\left(-\frac{d^2}{d\rho^2}+\frac{(k-1)(k-3)}{4\rho^2}+V(\rho)\right)\psi(\rho)=E_\rho\psi(\rho) \tag{3}$$

where k = N + 2|*m*|. 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. Since the angular momentum barrier term 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 $\bar{k}$, resulting in a sensible zeroth-order classical result. Hence Equation (3) in terms of the shift parameter becomes

$$\left[-\frac{d^2}{d\rho^2}+\frac{\bar{k}^2\left[1-(1-a)/\bar{k}\right]\left[(1-(3-a)/\bar{k}\right]}{4\rho^2}+\frac{V(\rho)}{Q}\right]\psi(\rho)=E_\rho\psi(\rho), \tag{4}$$

where Q is a scaling constant to be determined from (7), and V(ρ) is the potential given in the relative Hamiltonian equation (2) as

$$V(\rho)=\frac{\lambda}{\rho}+\frac{1}{4}\left[1+\frac{\lambda^2}{4}\right]\rho^2+\frac{m\gamma}{2}+g\mu_B BS_z \quad . \tag{5}$$

The dimensionless parameter λ is defined as the ratio of the coulomb strength to the confining energy, $\lambda = e2\alpha/\hbar\omega 0$, where $\alpha=\sqrt{\frac{m^*\omega_0}{\hbar}}$ has the dimension of inverse length and $\gamma=\frac{\omega_c}{\omega_0}$. The shifted 1/N expansion method consists of solving equation (4) systematically in terms of the expansion parameter $1/\bar{k}$. The term making the leading contribution to the energy comes from the effective potential,

$$V_{eff}(\rho)=\frac{1}{4\rho^2}+\frac{V(\rho)}{Q}, \tag{6}$$

whose minimum ρ_0 of the effective potential ($\frac{dV_{eff}}{d\rho}=0$) is given by

$$2\rho_0^3V'(\rho_0)=Q. \tag{7}$$

It is convenient to shift the origin to $\rho_0$by the definition

$$x=k^{-}\frac{1}{2}(\rho-\rho_0)/\rho_0 \quad , \tag{8}$$

and expanding equation (4) 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 a one dimensional anharmonic oscillator, we determine the anharmonic oscillator frequency, the shift parameter, and the scaling constant.

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

$$E_{n,m}=\frac{\lambda}{\rho_0}+\frac{1}{4}\left[1+\frac{\gamma^2}{4}\right]\rho_0^2+\frac{1}{2}\gamma|m_z|+g\mu_B\ BS_z+\frac{\bar{k}^2}{4\rho_0^2}+\frac{1}{\rho_0^2}\left[\frac{(1-a)(3-a)}{4}+\alpha_1\right]+\frac{\alpha_2}{\bar{k}\rho_0^2}\quad , \quad (9)$$

where α_1 and α_2 are parameters expressed in terms of Q, ϖ, ρ_0, a , and quantum numbers n_r and m, are given in the Appendix . $\bar{k}=N+2|m|-a$, where N = 2 is the spatial dimension, shift parameter $a=2-(2n_r+1)\varpi$ and $\varpi=\left[3+\rho_0\frac{V''(\rho_0)}{V'(\rho_0)}\right]^{1/2}$. The roots ρ_0 are determined for a particular quantum state $|n_r m\rangle$, through the relation:

$$\left[2\rho_0^3V'(\rho_o)\right]^{\frac{1}{2}}=Q^{\frac{1}{2}}=\bar{k}=(2+2|m|-a) \quad (10)$$

After obtaining the roots, ρ_0, from Eq.(\ref{eq8}), the eigenenergies can be computed using Eq.(3). n_r is the radial quantum number related to the principle (n) one by the standard relation $n_r=n-|m|-1$. Our computed results for a quantum dot in a magnetic field are presented in Tables I and II and Figures 1 and 2. We have listed, in Table I, the ground state energies, in units of $\hbar\omega_0$, calculated by the exact numerical digonalization technique, variation, Laughlin-type variational wavefunction and shifted methods for various values of magnetic field strength ($\gamma=0,1,...,5$) and ratio parameter ($\lambda=0,1,...,5$). The angular momentum quantum number $(m)m_z$ is also mentioned. The energy results produced by 1/N method are given against various methods: exact, variational and Laughlin-type variation wavefunction. For the variational calculations, Ciftja and his collaborators (Ciftja *et al.*, 2004) have used a trial wave function with a spacial part as follows:

$$\Psi(\vec{\rho}_1,\vec{\rho}_2)=exp[-\frac{a^2}{2}(\rho_1^2+\rho_2^2)-\frac{b^2}{2}(\vec{\rho}_1-\vec{\rho}_2)^2]exp[cb|\vec{\rho}_1-\vec{\rho}_2|]. \quad (12)$$

Table I.

The ground eigenenergies, in units of $\hbar\omega_0$, of the 2D quantum-dot helium as a function of the magnetic field strength γ and various Coulomb to confining ratio parameter λ calculated by the shifted 1/N method against: exact numerical diagonalization technique, variational and Laughlin-type trial wave function methods (Ciftja *et al.*, 2004) .

$m_z=0$ $\lambda=1$ $\gamma=0$	$m_z=1$ $\lambda=2$ $\gamma=1$	$m_z=1\lambda=3$ $\gamma=1$
Exact 3.0009	4.0668	4.6059
Var. 3.0017	4.0670	4.6063
1/N 2.9562	4.0626	4.6002
Laughlin 3.5331	4.17932	4.8419
$m_z=1$ $\lambda=1$ $\gamma=2$	$m_z=1$ $\lambda=2$ $\gamma=2$	$m_z=2$ $\lambda=4$ $\gamma=2$
Exact 3.9573	4.6188	5.7364
Var. 3.9573	4.6190	5.7366
1/N 3.9549	4.6138	5.7349
Laughlin 3.9879	4.7331	5.8925
$m_z=1$ $\lambda=1$ $\gamma=3$	$m_z=2$ $\lambda=2$ $\gamma=3$	$m_z=3$ $\lambda=4$ $\gamma=3$ $m_z=4$ $\lambda=6$ $\gamma=3$
Exact 4.7189	5.4312	6.5352 7.4678
Var. 4.7190	5.4313	6.5353 7.4679
1/N 4.7162	5.4305	6.5350 7.4901
Laughlin 4.7497	5.4732	6.6174 7.5775
$m_z=1$ $\lambda=1$ $\gamma=4$	$m_z=2$ $\lambda=2$ $\gamma=4$	$m_z=3$ $\lambda=3$ $\gamma=4$ $m_z=4$ $\lambda=4$ $\gamma=4$
Exact 5.6143	6.3071	6.8900 7.4160
Var. 5.6144	6.3077	6.8900 7.4160
1/N 5.6122	6.3068	6.8898 7.4159
Laughlin 5.6453	6.3499	6.9374 7.4663
$m_z=5$ $\lambda=6$ $\gamma=4$	$m_z=0$ $\lambda=0$ $\gamma=5$	$m_z=2$ $\lambda=1$ $\gamma=5$ $m_z=3$ $\lambda=2$ $\gamma=5$
Exact 8.3453	5.3852	6.5307 7.2268
Var. 8.3453	5.3851	6.5307 7.2268
1/N 8.3833	5.3852	6.5303 7.2267
Laughlin 8.4198	5.3852	6.5416 7.2483
$m_z=4$ $\lambda=3$ $\gamma=5$	$m_z=5$ $\lambda=4$ $\gamma=5$	$m_z=6$ $\lambda=5$ $\gamma=5$
Exact 7.8138	8.3387	8.8228
Var. 7.8139	8.3388	8.8228
1/N 7.8139	8.3387	8.8228
Laughlin 7.8425	8.3725	8.8603

The three parameters: a, b and c are considered to be non-negative. In fact the choice of this wave function is very important and the eigenenergies calculated by this trial wavefunction are in excellent agreement with the corresponding ones produced by the exact numerical diagonalization method. On the other hand, the authors have used a trial wave function of Laughlin-type with the following form:

$$\Psi(\vec{\rho}_1, \vec{\rho}_2) = J(\rho_{12})(z_1 - z_2)^{|m_z|} exp[-\frac{\rho_1^2 + \rho_2^2}{4\ell_\Omega^2}], \tag{13}$$

where the Jastrow factor $J(\rho_{12})$is

$$J(\rho_{12}) = \exp[-\frac{b^2}{2}\rho_{12}^2 + cb\rho_{12}], \tag{14}$$

Where $z_j = x_j - iy_j$ is the position coordinate given in complex notation, b and c are non-negative variational parameters to be optimized, and the effective magnetic length $\ell_\Omega = (\frac{\hbar}{2m\Omega})^{1/2}$ and $\Omega^2 = \omega_0^2 + (\omega_c/2)^2$.

Our calculated results show that the ground state energy of the system for $\gamma = 0$ and $\lambda = 0$ has, as usual, zero angular momentum, $m_z = 0$. As we sweep the parameters γ and/or λ the angular momentum changes from $m_z = 0$ to higher values indicating a spin singlet-triplet transition in the ground state of the quantum dot. For example, when $\lambda = 1$, the angular momentum changes from $m_z = 0$ to $m_z = 1$ as γ changes from 1 to 2. In the high magnetic field range the angular momentum of the ground state jumps to higher values: $|m_z| = 6$ at $\lambda = \gamma = 5$. To make a comparison between our results and the recent ones given by Ciftja and Kumar (Ciftja *et al.*, 2004), we have displayed in Fig.1 the roots (ρ_0) of the QD-ground state as a function of λ for $\gamma = 0$ and 1. They also plotted (but not shown here) the mean square distance between the electrons in the QD against λ for the same values of γ. In fact, both figures showed the same crossing behavior. This type of crossing between the $\gamma = 0$ and $\gamma = 1$ curves can be attributed to the transitions in the QD ground state and thus to jumps in the corresponding angular momentum quantum number. For example, at the overlapping value $\lambda \approx 2$ in our curve the transition occurs, and the angular momentum of the QD-ground state jumps from $m_z = 0$ at $\gamma = 0$ to $m_z = 1$ at $\gamma = 1$. The exact values of the roots are 1.9720 at $\gamma = 0$ and 2.1610 at $\gamma = 1$. Thus, the roots in our calculations give information on the angular momentum transitions of the QD ground state like the mean-square values given by (Ciftja *et al.*, 2004). The computed values of the roots (ρ_0) for large range of λ (from 0 to 10), and $\gamma$are given in Table II.

Table II:

The energy difference between the ground state energies of the 2D quantum-dot helium calculated by exact diagonalization and 1/N methods, $\Delta E = E_{exact} - E_{1/N}$.

$\lambda = 1, m_z = 1$		$\gamma = 1, m_z = 1$	
γ	ΔE	λ	ΔE
2	0.0024	2	0.0042
3	0.0027	3	0.0057
4	0.0021		

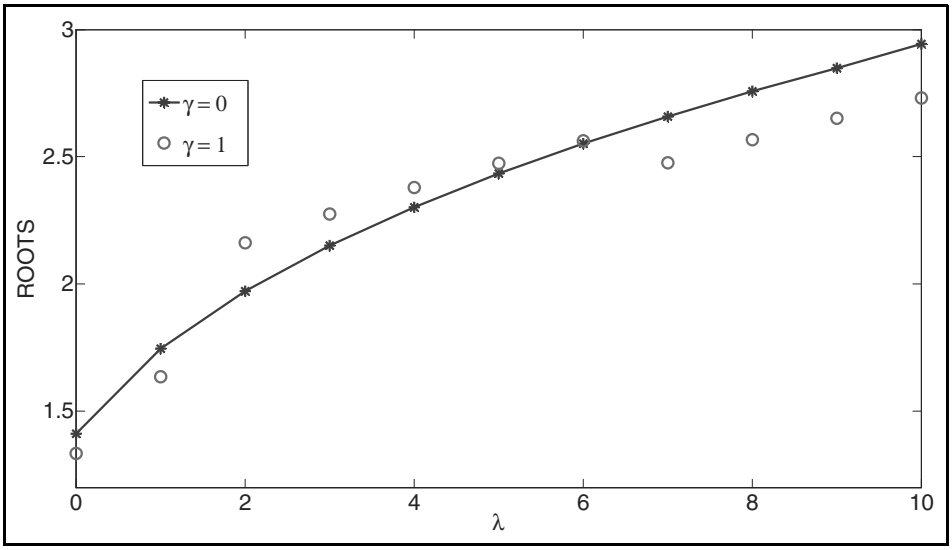

Fig.1 The roots (ρ_0) of the ground state energies against Coulomb ratio λ for $\gamma = 0$ (***) and for $\gamma = 1$ (ooo)

In Fig.2 we have also calculated, the singlet-triplet splitting $J = E_T - E_S$ as a function of magnetic field strength B for a quantum dot system and for confinement energy $\hbar\omega_0 = 3meV$. We can obviously see the changes in the sign of J at different values of B. The change in the sign of J is an indication that J can be manipulated by an external magnetic field. As the magnetic field strength (B) increases, the magnetic length $\ell_B = \left(\frac{\hbar c}{eB}\right)^{1/2}$ decreases and thus the ratio$\chi = (\frac{a_0}{a_B})^{1/3}(\frac{a_0}{\ell_B})$, which is the electron density in the quantum dot, enhances also and the Wigner crystal state becomes

more pronounced (Matulis et al., 2001). Thus, both a strong magnetic field and strong interaction favors Wigner crystallization in a different way. The electron interaction makes the system less dense by enlarging the interparticle distance. The magnetic field also makes the system effectively less dense by compressing the single electron wave packages. The same behavior of the electron-electron interaction and the magnetic field quantities also can be seen in our work by making use of the computed data for the quantities: λ, γ and ρ_0. For fixed values of the coulomb interaction parameter λ, the root (ρ_0) or the average electron separation distance decreases as the strength of the magnetic field (γ) increases leading to a compression in the electron wavefunction. For example, when $\lambda = 1$, the value of the root ρ_o decreases from 1.7450 to 1.6360 for $\gamma = 0$ and $\gamma = 1$, respectively. On the other hand, if we fix the strength of the magnetic field parameter λ and enhance the Coulomb strength λ, the value of the root ρ_0, or the separation between the electrons, increases and thus makes the electron system less dense. For example, when $\gamma = 1$ the value of the root ρ_0 increases from 1.6360 to 2.1610 for $\lambda = 1$ and 2, respectively. Table II shows the accuracy of the 1/N shifted method tested against various methods by calculating the energy difference between the exact results produced by diagonalization and the 1/N shifted results as $\Delta E = E_{exact} - E_{1/N}$ for different values of γ, λ and m_z. The comparison shows an excellent agreement while the results produced by the Laughlin--type wavefunction show a clear deviation from the results calculated by the aforementioned methods. Furthermore, as $|m_z|$ increases, the expansion parameter $1/\bar{k}$, $\bar{k} = \mathrm{N} + 2|m|$-a, decreases leading to a rapid convergence of the energy eigenvalues series (Eq.(9)). This is quite clear from the calculated results given in Table I. For example, the energies calculated by the exact and 1/N methods for states $\mathrm{m}_z = 6$, $\lambda = 5$, $\gamma = 5$ and $m_z = 5$, $\lambda = 4$ and $\gamma = 5$ are exactly the same and in this case the value of ΔE is zero. In addition to this agreement, we had also tested the 1/N expansion technique against different earlier results (Merkt *et al.*, 1991, Taut 1993, Wagner *et al.,* 1992) as reported in a previous work by the author, (Elsaid, 1995).

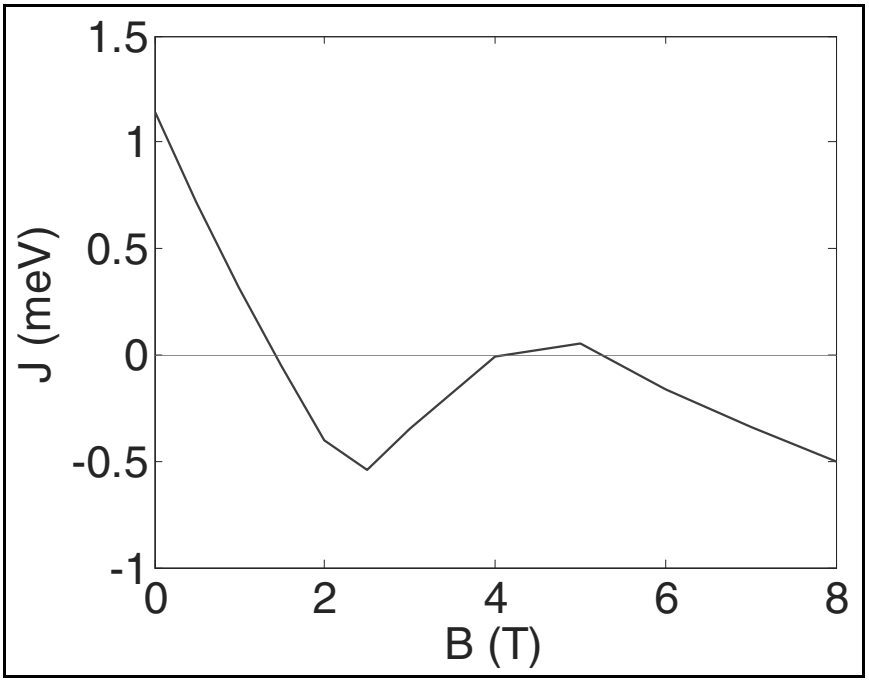

Fig.2 The dependence of singlet-triplet energy splitting J (in meV) on the strength of the magnetic field B (in T) for a two-electron quantum dot for confinement energy $\hbar\omega_0 = 3meV$

CONCLUSION

In conclusion, we have studied the spectral properties of a $2e$ QD-system in the presence of an applied uniform magnetic field using the shifted 1/N expansion method. The ground state energies of the QD-helium are calculated for various values of the magnetic field, γ, and a wide range of the ratio parameter, λ. The spin singlet-triplet transition in the ground state of the QD system is also investigated. We have also computed the singlet-triplet energy as a function of the magnetic field strength. Based on comparisons with exact diagonalization and variational methods, the shifted 1/N expansion method gives excellent results for all ranges of magnetic field strength (γ) and ratio parameter (λ) of the QD system.

Appendix

The parameters α_1 and α_2, appeared in Eq.(9)) are given as follows:

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

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

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

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

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

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 are

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

$$\varepsilon_3 = -1 + \rho_0^5 V^{(3)}(\rho_0)/6Q \qquad \varepsilon_4 = \frac{5}{4} + \frac{\rho_0^6 V^{(4)}(\rho_0)}{24Q}$$

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الحالة الأرضية لنقطة كمية ذات إلكترونين موجودة في مجال مغناطيسي: مفكوك طريقة 1/N

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ص.ب 2440 – حائل – المملكة العربية السعودية

خلاصة

لقد تمت دراسة الحالة الأرضية لنقطة كمية ذات بعدين. قمنا باستعمال طريقة مفكوك 1/N لحل الهاملتونين (دالة الطاقة) لزوج من الإلكترونيات محصورة في نقطة كمية وموجودة في مجال مغناطيسي. كما تم أيضاً إظهار الانتقال بين مستويات الطاقة الأحادية والثلاثية في الحالة الأرضية للنقطة الكمية، بالإضافة إلى ذلك حسبنا فجوة الطاقة بين هذين المستويين الأحادي والثلاثي والمعتمدة على شدة المجال المغناطيسي لزوج من الإلكترونيات في هذه النقطة الكمية.

تبين الدراسة بأن نتائج قيم الطاقة المميزة والمحسوبة بواسطة مفكوك 1/N بأنها على درجة ممتازة من الاتفاق مقارنة مع مثيلاتها من النتائج العددية والمحسوبة بطرق المتغير والطرق الدقيقة.