

Study of Energy and some atomic properties for electronic shells at ground state of three electron systems by analysis Hartree-Fock-Roothaan wavefunction

Rukia Jaber Dosh Qassim Shamkhi AL-Khafaji,
Department of physics ,college of science ,Kufa University

E-mail :rukiadosh@yahoo.com

Abstract:

Ground state energies and other properties of the atomic systems at open shell of three electron systems for N^{+4} and O^{+5} are given by Hartree-Fock-Roothaan wavefunction published by Clementi and Roetti(see ref.41) (1974). The radial expectation values for one electron $\langle r_1^m \rangle$ and for inter electrons $\langle r_{12}^m \rangle$ where $m=(-2,-1,0,1,2)$, repulsion energies $\langle V_{ee} \rangle$, attraction energies $\langle V_{en} \rangle$, potential energies $\langle V \rangle$, kinetic energies $\langle T \rangle$, and Hartree-Fock energies are tabulated by using partitioning technique, wherever in this series there are three shells K-shell, $K\alpha L\alpha$ -shell, $K\beta L\alpha$ -shell. with analysis the one electron radial density function $D(r_1)$ and inter electron density function $f(r_{12})$ for each shell.

Keywords: Hartree-Fock-Roothaan method, ion N^{+4} and ion O^{+5} .

دراسة الطاقة وبعض الخواص الذرية للقشرات الذرية للحالة الأرضية للأنظمة ثلاثية الإلكترون من تحليل الدالة الموجية لهارتري-فوك-روثان

رقية جابر دوش قسم الفيزياء/كلية العلوم /جامعة الكوفة قاسم شمخي الخفاجي قسم الفيزياء/كلية العلوم /جامعة الكوفة
الخلاصة :

طاقة الحالة الأرضية وخواص أخرى للأنظمة الذرية ذات الأغلفة المفتوحة للحالة الأرضية للأيونات الشبيهة بالليثيوم لاينون النروجين N^{+4} وايون الاوكسجين O^{+5} اعطيت باستعمال الدالة الموجية لهارتري-فوك-روثان المنشورة بواسطة Clementi and Roetti (1974) (مصدر 41). القيم المتوقعة القطرية للإلكترون واحد $\langle r_1^m \rangle$ ولإلكترونين $\langle r_{12}^m \rangle$ حيث $m=-2,-1,0,1,2$ طاقات التنافر $\langle V_{ee} \rangle$, طاقات التجاذب $\langle V_{en} \rangle$, طاقات الجهد $\langle V \rangle$, الطاقات الحركية $\langle T \rangle$, وطاقات هارتري فوك $\langle E \rangle$ قد حسبت باستعمال تقنية التجزئة حيث يوجد في هذه السلسلة ثلاثة أغلفة هي الغلاف K, والغلاف $K\alpha L\alpha$ والغلاف $K\beta L\alpha$. تم تحليل الدالة القطرية للإلكترون واحد $D(r_1)$ والدالة القطرية للمسافة البينية بين الإلكترونين $f(r_{12})$ لكل غلاف من الأغلفة.

الكلمات المفتاحية: طريقة هارتري-فوك-روثان، ايون النروجين N^{+4} وايون الاوكسجين O^{+5}

Introduction

The formulation and development of quantum theory in the first half of the 20th century has led to a revolution in our understanding of fundamental physics. Quantum theory has demonstrated surprising accuracy and predictive power, and the importance of quantum theory is unchallenged. The Schrodinger equation, which is the fundamental equation of quantum mechanics, cannot be solved analytically for any but the most trivial of systems. Numerical many-body approaches provide powerful tools for solving this equation. In electronic structure calculations the treatment of electron-electron interactions is the main source of difficulty. These interactions cannot easily be separated out or treated without approximation [1]. we must be content with approximate solutions to the Schrodinger equation. The underlying difficulty is that many particles are interacting with one another simultaneously. This is the many-body problem. For all such systems, approximate rather than exact solutions to their respective equations of motion must be sought [2]. The most widely used computational techniques are based on the Hartree-Fock HF method, these calculations are begin with the central-field approximation in which the electrons are uncorrelated [3]. This method is based on the mean-field approximation. This approximation implies that interelectron coulomb repulsion is accounted for by means of an average integration of the repulsion term, i.e. the interaction of one electron with the others are accounted for as the interaction of this electron with an

average field induced by other electrons. The electron correlation (interaction between electrons) for the electrons of opposite spin is completely neglected. A certain amount of electron correlation is already considered within the HF approximation, found in the electron exchange term describing the correlation between electrons with parallel spin [4].

The Theory

the Hartree-Fock method is one of the simplest approximations of the electronic structure of atoms and molecules. By assuming minimal correlation between the N electrons, it reduces Schrödinger's equation, a linear partial differential equation, to the Hartree-Fock equations, a system of N coupled nonlinear equations [5]. The aim of this approximation is to replace the original wave-function dependent on coordinates of all electrons by the system of equations dependent only on coordinates of one-electron, in which this electron moves in an average electric field of the other electrons and nuclei. The main defect of the HF method is that it does not treat electron correlation properly [6]. The fundamental principle of condensed matter physics and chemistry is given in the many body schrodinger equation, which is

$$\hat{\mathcal{H}}\psi(x_1, x_2, \dots, x_N) = E\psi(x_1, x_2, \dots, x_N) \quad \dots(1)$$

This is a schrodinger equation of N electrons under the Born-Oppenheimer approximation, $\hat{\mathcal{H}}$ is the electronic Hamiltonian operator describing kinetic and potential electronic

energy, and E is the energy of the system, The electronic wave function $\psi(x_1, x_2, \dots, x_N)$ is a quantity directly related to the electronic distribution in an atomic, whose absolute square represents an electronic density. The electron wave function $\psi(x_1, x_2, \dots, x_N)$ must be antisymmetric in the exchange of arbitrary two spin coordinates x_i and x_j . One of the central problem in condensed matter physics and chemistry is to find the solution of (1) and the ground state energy E_0 of the given system [7]. We consider the Hamiltonian of the atome with N non-relativistic electrons and fixed nuclei of (positive) charges Z in atomic unit , given by [8],

$$\hat{\mathcal{H}} = \frac{1}{2} \sum_{i=1}^N \nabla_i^2 + \sum_{i=1}^N \frac{Z}{r_i} + \frac{1}{2} \sum_{i=1}^N \sum_{j \neq i}^N \frac{1}{r_{ij}} \quad \dots(2)$$

Where ∇^2 Laplace operator and it is a differential operator , Z is the atomic number , r_i the position of the i th electron, r_{ij} the distance between i th and j th electrons, N is the number of electrons . The interpretation of this Hamiltonian is as follows: the first term corresponds to the kinetic energy of the electrons, the second term is the one-particle attractive interaction between the electrons and the nuclei, and the third term is the standard two-particle

repulsive interaction between the electrons [9]. the electron wavefunction $\psi(x_1, x_2 \dots x_N)$ must be antisymmetric in the exchange of arbitrary two spin coordinates x_i and x_j according to Pauli exclusion principle [10,11],

$$\hat{p}\psi(x_1, \dots, x_i, x_j, \dots x_N) = -\psi(x_1, \dots, x_j, x_i, \dots x_N) \quad \dots(3)$$

Where $\hat{p}$ is an operator which performs one of the $N!$ possible permutations of the N electrons. The total antisymmetry of a wavefunction can thus be written compactly:

$$\hat{p}\psi = (-1)^p \psi \quad \dots(4)$$

with $(-1)^p$ the parity of this permutation, $(-1)^p = 1$ for even permutations and $(-1)^p = -1$ for odd permutations. From a given wavefunction ψ , we can project out a totally antisymmetric part using the antisymmetrizer as :

$$\mathcal{A} = \frac{1}{\sqrt{N!}} \sum_p (-1)^p \hat{p} \quad \dots(5)$$

in the Hatree-Fock approximation, the many body wavefunction $\psi(x_1, x_2 \dots x_N)$ is approximated by a single slater determinant

We can write wavefunction as [12,13,14],

$$\Psi_{\text{HF}} = \det(\phi_1(x_1)\phi_2(x_2) \dots \phi_N(x_N)) \dots (6)$$

$$\Psi_{\text{HF}} = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(x_1) & \phi_1(x_2) \cdots & \phi_1(x_N) \\ \phi_2(x_1) & \phi_2(x_2) \cdots & \phi_2(x_N) \\ \vdots & \vdots & \vdots \\ \phi_3(x_1) & \phi_3(x_2) \cdots & \phi_3(x_N) \end{vmatrix} \dots (7)$$

The factor $\frac{1}{\sqrt{N!}}$ ensures the normalization condition on the wavefunction. Here the variables x_i include the coordinates of spin and space, $\phi_i(x_j)$ terms are called spin orbitals and these spin orbitals are orthonormal functions, which are spatial orbitals times a spin functions. The wavefunction Ψ_{HF} in equation (7) is clearly antisymmetric because interchanging any pair of particles is equivalent to interchanging two columns and hence changes the sign of the determinant. Moreover, if any pair of particles are in the same single-particle state, then two rows of the Slater determinant are identical and the determinant vanishes, in agreement with the Pauli exclusion principle.

we can write the wave function Ψ_{HF} as [15],

$$\Psi_{\text{HF}} = \frac{1}{\sqrt{N!}} \sum_{p=1}^{N!} (-1)^p p(\phi_1, \phi_2, \dots, \phi_N) \dots (8)$$

(ϕ_i) being a set of spin-orbitals (one electron function).

The one-electron orbitals used to construct the ϕ_i each consist of a radial function $R_{nl}(r)$, a spherical harmonic $Y_{lm}(\theta, \phi)$ and a spin function $\sigma_{m_s}(s)$ as [16,17,18],

$$\phi = R_{nl}(r)Y_{lm}(\theta, \phi)\sigma_{m_s}(s) \dots (9)$$

The spatial part of one-electron spin orbital may be expressed as linear combination of Slater type orbital called basis functions,

$$\Phi_{nlm}(r, \theta, \phi) = \sum_i c_i \mathcal{X}_i \dots (10)$$

Where c_i the expansion coefficient determined by minimizing the energy using one of several procedures and this process is continued until $\hat{H}_{\text{HF}}$ and Ψ_{HF} converge, at which point a self-consistent field (SCF) has been achieved. This usually yields the lowest-energy single determinant within the basis. $\mathcal{X}_i$ is a Slater type orbital.

The Hartree–Fock–Roothaan (HFR) or basis-set expansion method is a convenient and powerful tool for the study of electronic structure of atoms and molecules. It is well

known that the choice of the basis functions is very important when the algebraic approximation is employed, because it determines both the computational efficiency and accuracy of the results obtained within a given approach. The most frequently used basis functions for atomic calculations are Slater type orbitals (STO) defined as [19],

$$\chi_{nlm}(\xi, r) = \sum_i \frac{(2\xi_i)^{n_i + \frac{1}{2}}}{[(2n)!]^{\frac{1}{2}}} r^{n_i - 1} \exp(-\xi_i r) Y_{lm}(\theta, \phi) \quad \dots(11)$$

Here, $Y_{lm}(\theta, \phi)$ a spherical harmonics, $\xi_i > 0$ is the orbital exponent. The quantity n occurring in eq. (11) is a positive principal quantum number of (STO). The determination of nonlinear parameters n and ξ is very important for describing the atomic orbitals.

3. Atomic properties

3.1: second-order reduced density matrix $\Gamma(r_1, r_2)$

Most of the physically interesting properties of a quantum mechanical system can be calculated from the two-particle reduced density matrix for the system $\Gamma(x_1, x_2)$, without reference to the full wavefunction. If we can determine it, the wavefunction

can be eliminated from the quantum mechanics and the $\Gamma(x_1, x_2)$ take over its role [20,21]. The two electron reduced density matrix contains all of the information necessary to calculate the energy and many properties of the atom. It is obtained by integrating the spin and spatial coordinates of all electrons except two (1,2) from the N -particle density matrix [22].

so the two-electron reduced density matrix $\Gamma(x_1, x_2)$ is then given by [23,24],

$$\Gamma(x_1, x_2) = \frac{N(N-1)}{2} \int \dots \int |\psi(x_1, x_2, \dots, x_N)|^2 dx_3 \dots dx_N \quad \dots(12).$$

Where $x_i = (r_i, s_i)$ combined space and spin variable [25]. $\frac{N(N-1)}{2}$ represents the number of electron pairs which can be obtained by integrating the second-order reduced density matrix, so $\Gamma(x_1, x_2)$ is normalized to the number of independent electron pairs within the system as [26,27].

$$\int \int \Gamma(x_1, x_2) dx_1 dx_2 = \frac{N(N-1)}{2} \quad \dots(13)$$

3.2 : two-electron radial density function $D_2(r_1, r_2)$ and one-electron radial density function $D(r_1)$:

The two-electron radial density function $D(r_1, r_2)$ is given by [28],

$$D(r_1, r_2) = \frac{N(N-1)}{2} r_1^2 r_2^2 \int |\psi(x_1, x_2, \dots, x_N)|^2 dx_3, \dots, dx_N d\Omega_1 d\Omega_2 \dots (14)$$

$$d\Omega_i = \sin \theta_i d\theta_i d\phi_i \dots (15)$$

where (r_i, Ω_i) is the polar coordinate of the vector r_i . The two-electron radial density function represents the probability density that, one electron is located at a radius r_1 and the other electron at a radius r_2 simultaneously. The two-electron radial density $D(r_1, r_2)$ can be written as [29].

$$D(r_1, r_2) = \iint \Gamma(r_1, r_2) r_1^2 r_2^2 d\Omega_1 d\Omega_2 \dots (16)$$

While the one-electron radial density function $D(r_1)$ represents the probability density function of finding an electron at a distance between r_1 and $r_1 + dr_1$ from the coordinate origin i.e nucleus and defined as [30].

$$D(r_1) = \int_0^\infty D(r_1, r_2) dr_2 \dots (17)$$

3.3 :Inter –particle distribution function $f(r_{12})$

The radial electron-electron distribution function $f(r_{12})$, which describes the probability of locating two electrons separated by distance r_{12} from each other

, was first introduced by Coulson and Neilson in their study of electron correlation for $\text{He}(^1\text{S})$ in the ground state. [31,32]. Pair distribution function can be written as [33].

$$f(r_{12}) = 8\pi^2 r_{12} \left[\int_0^{r_{12}} r_1 dr_1 \int_{r_1-r_{12}}^{r_1+r_{12}} \Gamma(r_1, r_2) r_2 dr_2 + \int_{r_{12}}^\infty r_1 dr_1 \int_{r_{12}-r_1}^{r_{12}+r_1} \Gamma(r_1, r_2) r_2 dr_2 \right] \dots (18)$$

3.4 one –electron expectation value and inter-electron expectation value:

The one-electron expectation value $\langle r_1^m \rangle$ is determined from the expression as [34],

$$\langle r_1^m \rangle = \int_0^\infty D(r_1) r_1^m dr_1 \dots (19)$$

Where m integer number ($-2 \leq m \leq 2$).

The inter-electron expectation values $\langle r_{12}^m \rangle$ for each shell is given by the relation [31].

$$\langle r_{12}^m \rangle = \int_0^\infty f(r_{12}) r_{12}^m dr_{12} \dots (20)$$

where r_{12} represents the distance between two-electrons.

3.5 energy expectation value $\langle E \rangle$:

the average values of the energy for the wavefunction ψ , takes the formula [35].

$$\langle E \rangle = \frac{\langle \psi | \hat{H} | \psi \rangle}{\langle \psi | \psi \rangle} \dots (21)$$

Since our wavefunction ψ is normalized, the denominator of Eq. (21) is unity then, the energy thus is given by the expression [36,37].

$$\langle E \rangle = \int \psi^* \left[-\frac{1}{2} \sum_{i=1}^N \nabla_i^2 + \sum_{i=1}^N \frac{Z}{r_i} + \frac{1}{2} \sum_{j \neq i}^N \frac{1}{r_{ij}} \right] \psi d\tau \dots (22)$$

Hartree-Fock method satisfied the virial theorem. The virial theorem is necessary condition for the stationary state, the condition of the virial theorem is [38],

$$\langle T \rangle + 2\langle V \rangle = 0 \dots (23)$$

Where $\langle V \rangle$ is the total expectation value of potential energy and $\langle T \rangle$ is the expectation value of kinetic energy. From the theorem, we are led to

$$\langle E \rangle = \langle T \rangle + \langle V \rangle \dots (24)$$

$$\langle E \rangle = -\langle T \rangle = \langle V \rangle / 2 \dots (25)$$

Expectation value of potential energy proportional to the expectation values of $\langle r_1^{-1} \rangle$ and $\langle r_{12}^{-1} \rangle$ respectively, where [39,40].

$$\langle V \rangle = -Z\langle r_1^{-1} \rangle + \langle r_{12}^{-1} \rangle \dots (26)$$

4.Result and discussion

In this research we are using the atomic data for Hartree-fock wavefunction for Li(²S) isoelectronic series for Clementi and Roetti

[41]. The atomic properties such as inter-particle distribution function $f(r_{12})$, one-particle radial distribution function $D(r_1)$, two-particle radial density function $D(r_1, r_2)$, all expectation values $\langle r_1^m \rangle$, $\langle r_{12}^m \rangle$, $\langle V \rangle$, $\langle V_{ee} \rangle$, $\langle V_{en} \rangle$, $\langle T \rangle$, $\langle E \rangle$, are obtained numerically by using Mathcad 2001i. Each plot in this work is normalized to unity and all the result of the expectation values checked according to the normalization condition. Also we used the atomic units in calculations in this work. Table (1) shows the calculated one electron expectation values for the elements $Z=7,8$ (N^{+4}, O^{+5}) for Li-isoelectronic series and table (2) presented the inter-electron expectation values for these systems, while in this series there are three shells K-shell, $K\alpha L\alpha$ -shell and $K\beta L\alpha$ -shell. We noted for each electronic individual shell and for total system the expectation value for one electron and inter electrons when m is negative increases as atomic number Z , increases and vice-versa when m takes positive values, also we can note the expectation values for one and inter electrons for K-shell are greater than those for $K\alpha L\alpha$ -shell and $K\beta L\alpha$ -shell when m is negative and vice-versa when m is positive values.

Plot (1) represented the relation between one electron radial density function $D(r_1)$ and r_1 , we can note the maximum values of $D(r_1)$ increase as Z increases and decrease their positions towards the nucleus as Z increases according to Coulomb law, we can find also there is one peak in the K-shell which represented the probability of finding the electron in the K-shell, while in the $K\alpha L\alpha$ -shell and $K\beta L\alpha$ -shell it is found there are two peaks for $K\alpha L\alpha$ and $K\beta L\alpha$ Shells. The first peak represented the probability of finding the electron in the K-shell, the second peak represented the probability of finding the electron in the L-shell and we can see also the probability of finding an electron in the K-shell is larger than that in the L-shell because K-shell is closer to the nucleus than L-shell, so that attraction force between the nucleus and the electron is larger for K-shell than for L-shell According to coulomb law.

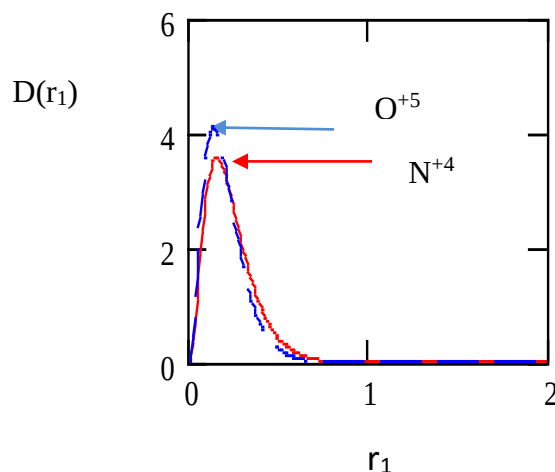
Table(1) values of one-electron expectation values for three electron systems.

Ion	shell	$\langle r_1^{-2} \rangle$	$\langle r_1^{-1} \rangle$	$\langle r_1^0 \rangle$	$\langle r_1^1 \rangle$	$\langle r_1^2 \rangle$
N^{+4}	K	90.3772	6.6784	1	0.2269	0.0692
	$K\alpha L\alpha \equiv k\beta L\alpha$	48.9737	4.0240	1	0.6398	0.6810
	total	62.7748	4.9088	1	0.5022	0.4771
O^{+5}	K	119.2467	7.6778	1	0.1971	0.0522
	$K\alpha L\alpha \equiv k\beta L\alpha$	64.9274	4.6494	1	0.5457	0.4925
	total	83.0338	5.6589	1	0.4295	0.3457

Table(2) values of inter-electron expectation values for three electron systems.

Ion	shell	$\langle r_{12}^{-2} \rangle$	$\langle r_{12}^{-1} \rangle$	$\langle r_{12}^0 \rangle$	$\langle r_{12}^1 \rangle$	$\langle r_{12}^2 \rangle$
N^{+4}	K	29.5082	4.1455	1	0.3316	0.1385
	$K\alpha L\alpha$	1.4657	1.0906	1	1.0859	1.3619
	$k\beta L\alpha$	2.8725	1.1925	1	1.0807	1.3619
	total	11.2821	2.1429	1	0.8327	0.9541
O^{+5}	K	39.0375	4.7701	1	0.2880	0.1044
	$K\alpha L\alpha$	2.0180	1.2804	1	0.9239	0.9849
	$k\beta L\alpha$	3.9947	1.4044	1	0.9192	0.9850
	total	15.0167	2.4849	1	0.7104	0.6914

Figure (2) represent the relation between inter electron density function and inter distance r_{12} for three shells. We noted the maximum probability of pair distribution function $f(r_{12})$ increases as atomic number increases and their locations decreasing because the influence of increasing in attraction nuclear force. We can see from plot (2) there is one peak in the K-shell and $K\alpha L\alpha$ -shell which represented the probability of finding two electrons in the small distance between them while there are two peak in the $K\beta L\alpha$ -shell. First peak indicates the probability of finding two electrons simultaneous in small distance r_{12} and the second peak represented the probability of finding two electrons in the big distance r_{12} . in table (3) we are present the expectation values of energies $\langle V_{en} \rangle$, $\langle V_{ee} \rangle$, $\langle V \rangle$, $\langle T \rangle$ and $\langle E_{HF} \rangle$. It is clear when Z increases the expectation values of all energies increase too, we can note also the expectation values of all energies in the K-shell larger than those in the $K\alpha L\alpha$ and $K\beta L\alpha$ -shells because K-shell closer to the nucleus than other shells.



Fig(1.a) one- particle radial density function for K-shell of N^{+4} and O^{+5} for three electron systems

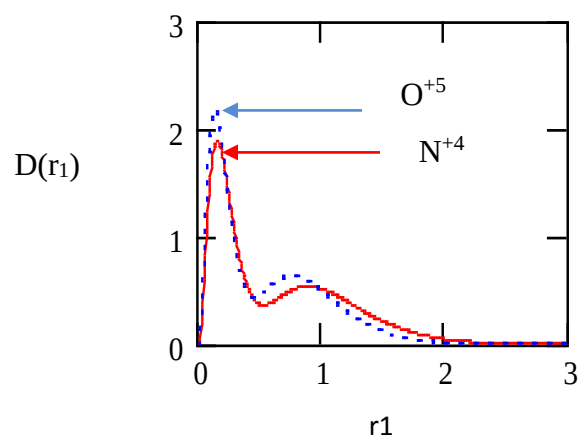
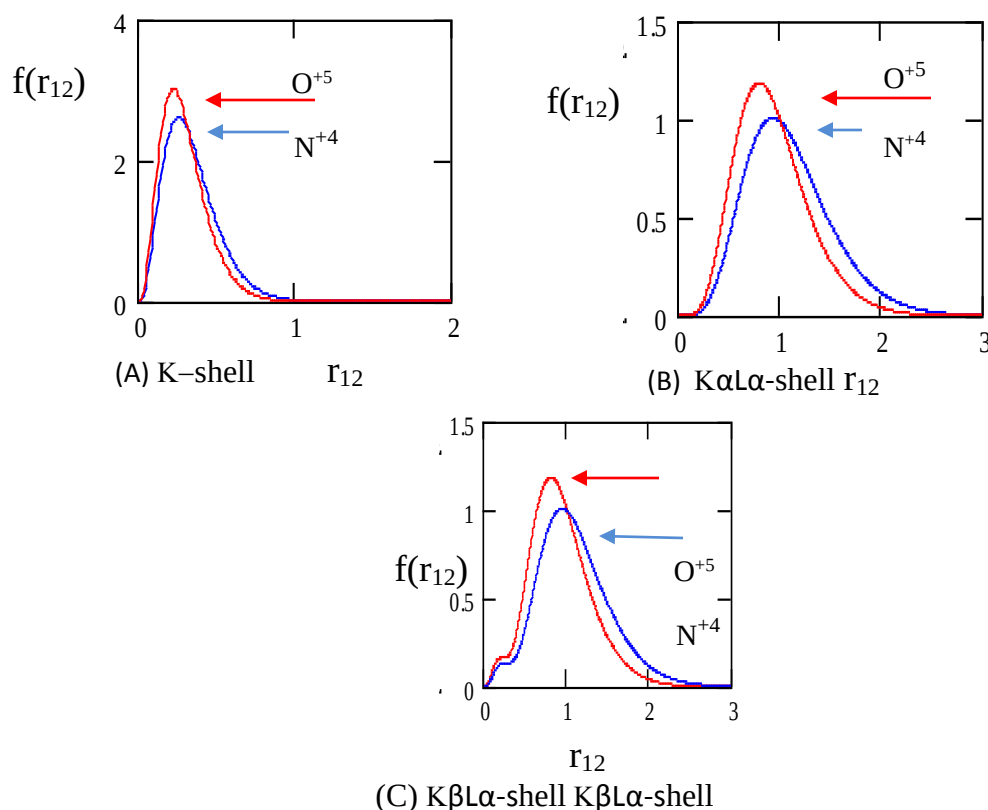


Fig.(1.b) the one- particle radial density function for $K\alpha L\alpha$ and $K\beta L\alpha$ -shells of N^{+4} and O^{+5} ions .



Fig(2) the inter-particle density distribution function of three electron systems for N^{+4} and O^{+5} ions
 (A) K-shell (B) $K\alpha L\alpha$ -shell (C) $K\beta L\alpha$ -shell

Table(3):The expectation values for all attraction, repulsion, kinetic and Hartree-Fock energies for K, $K\alpha L\alpha$, $K\beta L\alpha$ -shells and total systems of three electron systems.

Ion	shell	$-\langle V_{en} \rangle$	$\langle V_{ee} \rangle$	$-\langle V \rangle$	$\langle T \rangle$	$-\langle E_{HF} \rangle$
N^{+4}	K	46.7487	4.1455	42.6032	21.3016	21.3016
	$K\alpha L\alpha$	28.1679	1.0907	27.0772	13.5386	13.5386
	$K\beta L\alpha$	28.1679	1.1925	26.9753	13.4876	13.4876
	total	103.0843	6.4287	96.6557	48.3278	48.3278
O^{+5}	K	61.4227	4.7701	56.6526	28.3263	28.3263
	$K\alpha L\alpha$	37.1952	1.2804	35.9148	17.9574	17.9574
	$K\beta L\alpha$	37.1952	1.4044	35.7908	17.8954	17.8954
	total	135.8130	7.4548	128.358 2	64.1791	64.1791

Conclusion:

1-One-electron density function $D(r_1)$ increases as atomic number increases. For three shells and their locations are decreasing towards the nucleus which means increasing in probability of finding the electron when there is increasing in atomic number. Also inter particle density function $f(r_{12})$ increases when atomic number increases refer to important of nuclear charge on the electrons.

2-The results of K-shell is larger than those in the $K\alpha L\alpha$ and $K\beta L\alpha$ -shells for $D(r_1)$, and $f(r_{12})$ because K-shell is closer to the nucleus from others, so the Coulomb attraction force becomes larger.

3-Expectation value of one electron $\langle r_1^m \rangle$ and expectation value of two electrons when $m=-1, -2$ is increase as atomic number increases and when $m=1, 2$, these values decrease by increasing in atomic number.

4-Values of energies $\langle V_{en} \rangle$, $\langle V_{ee} \rangle$, $\langle V \rangle$, $\langle T \rangle$ and $\langle E_{HF} \rangle$ is increase when the atomic number increases which is interpreted as the influence of nuclear charge for all shells and for total system.

References

- [1] S. S. Reine, Ph.D, Thesis "Monte-Carlo Simulations of Atoms" University Of Oslo (2004).
- [2] D. P. Tew, W. Klopper, T. Helgaker, J. Comput Chem, V. 28(2007) 1307–1320.
- [3] D. G. Ellis, J. Physical Review A, V.53, No. 6 (1996) 3986- 3993.
- [4] Y. Kalugina, Ph.D.Sc., Thesis "Theoretical investigation of the potential energy, dipole moment and polarizability surfaces of the CH_4-N_2 and $C_2H_4-C_2H_4$ van der Waals complexes" Tomsk State University, Russia (2010).
- [5] A. Levitt, arXiv:1109.5473, V.1(2011).
- [6] F. Zimandl, Ph.D.Sc., Thesis "Conformational Study of a Flexibility of the Fluorescence Dye QSY21", University of South Bohemia(2010).
- [7] W. Uemura, arXiv:1102.4909, V.1.
- [8] S. Meyur and S. Debnath, J. Phys. Educ, V. 3, No. 2, (2009) 300 – 306.
- [9] M. Enstedt and M. Melgaard, J. Nonlinear Analysis, V. 69 (2008) 2125–2141
- [10] M. Laubenstein, International Journal of Quantum Information, V. 9 (2011) 145-154.
- [11] H. Friedrich "Theoretical Atomic Physics" third Edition (2006).
- [12] D. D. FITTS "Principles Of Quantum Mechanics as Applied to Chemistry and Chemical Physics" publisher : Cambridge University (2002)
- [13] N. J. Mauser And S. Trabelsi, arXiv:1002.1816, v.1 (2010).
- [14] C. Arguez, M. Melgaard, J. Nonlinear Analysis, V.75 (2012) 384–404.
- [15] I. Ema, J. M. Garcia and B. Miguel, J. Atomic Data and nuclear Data Tables, V. 72(1999)57-99.
- [16] B. Cakir, A. Ozmen, U. Atav And Yuksel, International Journal of Modern Physics C, V. 19, No. 4 (2008) 599-609

- [17] C. E. Hudson, C. A. Ramsbottom, P. H. Norrington, and M. P. Scott, *J. Astronomy & Astrophysics*, V. 494, (2009) 729–737
- [18] A. B. Gilbert, N. A. Besley, and P. W. Gill, *J. Phys. Chem. A*, V.112 (2008) 13164–13171.
- [19] I.I.Guseinov, Merturk and E .Sahin, *J. Phys*, V. 76, No. 1(2011) 109–117.
- [20] John E. Harriman, *J. Chemical physics*, V.54, No.3(1971) 902-908.
- [21] K. Yasuda, *J. Physical Review A*, V. 59, No. 6 (1999) 4133- 4149.
- [22] L.Greenman and D. A. Mazziotti, *J. Chemical Physics*, V. 128, No. 114109 (2008) 114109-1to 114109-7.
- [23] T. Koga and Y. Kawata, *J. Chemical Physics*, V. 117, No. 20(2002) 9133-9137 .
- [24] T. Koga and H. Matsuyama, *J. Chemical Physics*, V. 120, No. 17(2004) 7831- 7836.
- [25] N. Helbig, G. Theodorakopoulos, and N. N. Lathiotakis, *J. Chemical Physics*, V. 135, No. 054109 (2011) 054109-1 to 054109-9.
- [26] S. Goedecker and C. J. Umrigar, *J. Physical Review Letters*, V. 81, No.4(1998) 866-868 .
- [27] M. Fukuda and K. Fujisawa, *arXiv*: 1010.4095, V.2 (2011).
- [28] T. Koga and M. Sekiya, *J Math Chem*, V.48 (2010) 988–1000.
- [29] T. Koga and H. Matsuyama, *J. Theor Chem Acc*, V.118 (2007) 931–935 .
- [30] T. Koga and H. Matsuyama, *J. Theor Chem Acc*, V.115(2006) 59–64.
- [31] P. R. Dressel and F. W. King, *J. Chemical physics*, V. 100, No. 10 (1994) 7515– 7522.
- [32] Robert Benesch and Vedene H. Smith, *J. Chemical Physics*, V. 55, No. 2 (1971) 482- 488.
- [33] N.Moisseyev, J.Katriel and R.J.Boyd, *J. Theoretica Chimica Acta*, V. 45, (1977) 61 – 67.
- [34] A. Gupta and R. J. Boyd, *J. Chemical physics*, V. 68, No. 4 (1978) 1951 – 1957.
- [35] A.F. Riveros and A. R.Contreras, *J. Physics Letters A*, V. 372 (2008)6175-6182.
- [36] J. P. Lowe and K. A. Peterson “Quantum Chemistry” Third Edition, Elsevier Academic Press (2006).
- [37] S.Otranto, G.Gasaneo and C.R. Garibotti, *J. Nuclear Instruments And Methods In Physics Research B*, V. 217, (2004) 12-17 .
- [38] T. Oyamada, K. Hongo, Y. Kawazoe, and H. Yasuhara, *J. Chemical Physics*, V. 133, No. 164113 (2010) 164113-1 to 164113-19.
- [39] K.J.AL-Khafaji Ph.D. Thesis "A Study of Correlation Energy and Orbital Correction Function for two and three Electron-system" College of Science, Al-Mustansiriyah University (2005).
- [40] K. D. Sen and V. S. Reddy, *J. Chemical Physics*, V. 81, No. 5213 (1984) 5213-5214 .
- [41] E.Clement and C. Roetti, *J. Atomic Data and Nuclear Data Tables* V.14, No. 3-4 (1974) 177-478.