

Evaluation of the ground state correlation energy for two and three electron systems have (Z=15 – 20)

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Abstract: Correlation energies for all like ions of two electrons systems (P⁺¹³, S⁺¹⁴, Cl⁺¹⁵, Ar⁺¹⁶, K⁺¹⁷ and Ca⁺¹⁸) and three electrons systems (P⁺¹², S⁺¹³, Cl⁺¹⁴, Ar⁺¹⁵, K⁺¹⁶ and Ca⁺¹⁷) are obtained by taking difference between theoretical total energies of Hartree- Fock calculations and experimental total energies.

The atomic properties are calculated very important to describe the dynamics in atomic systems.

In this research used the division technique for the analysis the three electron system, also all the examining atomic properties were normalized and we used the atomic units in our calculations and the results is get by using Mathcad 14 program.

Keywords: correlation energy , Hartree- Fock, atomic units , atomic properties, Hamiltonian operator.

I. INTRODUCTION

The Hartree-Fock(HF) approximation ignores the correlation between electrons, but gives roughly 99% of the total electronic energy. Moreover, it is often accurate for the predication of atomic structure. Unfortunately, the part of the energy which the Hartree-Fock approximation ignores can have important chemical effects and this is particularly true when bonds are formed and/or broken. Consequently, realistic model chemistries require a satisfactory treatment of electronic correlation. The concept of electron correlation E_C was introduced by Wigner and defined as[1],

$$E_C = E - E_{HF} \tag{1}$$

Where E is the exact non-relativistic energy, i.e., the difference between the correlated and the Hartree-Fock energies E_{HF}

II. THEORY

The wave function $\Psi(r_1, r_2, r_3, \dots, r_n)$ of any system is a mathematical expression which describes the system properties as position, momentum, energy, etc. In the uncorrelated wave function approximation, each particle is assumed to move in only the average field of all the other particles of the system. This kind uses approximation that called Hartree-Fock approximation (HF). In the correlated wave function approximation one can take into account the correlation between all the particles of the system by using the configuration interaction approximation (CI). The wave function for the one-particle is defined as :

$$\Psi_{n \ell m_\ell m_s}(\vec{r}) = R_{n\ell}(r) Y_{\ell m_\ell}(\theta, \phi) \sigma(s) \tag{2}$$

the radial factor $R_{n\ell}(r)$ is related to the distance of electron from the nucleus and depends on the n (principal quantum number) and ℓ (angular momentum quantum number) while the angular factor (spherical harmonic) $Y_{\ell m_\ell}(\theta, \phi)$ supplies an angle dependence and depends on the ℓ and m_ℓ (magnetic quantum number) [2].

The Hartree-Fock (HF) atomic wave functions are independent particle-model approximations to non-relativistic Schrödinger equation for stationary states. The single determinant can be written as the ant symmetrized product of all occupied HF spin-orbital for atoms [3].

$$\Psi_{HF}(123\dots N) = A \Pi(123\dots N) \tag{3}$$

Where A is the ant symmetrized operator given by :

$$A = \frac{1}{\sqrt{N!}} \sum_P (-1)^P P \tag{4}$$

$(-1)^P$ Takes the values +1 and -1 for even and odd permutation, P is any permutation of the electron, and the factor $\frac{1}{\sqrt{N!}}$ introduced to ensure that the wavefunction is normalized. For our purpose the wavefunction can be written as

$$\Psi_{HF}(123\dots N) = \sum_{i < j} A_{ij}^{mn} (-1)^P A \Pi_{ij} \tag{5}$$

where the pair function A_{ij}^{mn} can be defined as:

$$A_{ij}^{mn} = \phi_i(m)\phi_j(n) - \phi_j(m)\phi_i(n) \tag{6}$$

And Π_{ij} represents the product of all occupied HF-spin orbital except $\phi_i(m)$ and $\phi_j(n)$. i and j represent spin orbital labels, also m and n refer to electron labels.

The product $\Pi(123\dots N)$ in equation (3) can be defined as:

$$\Pi(123\dots N) = \left| \phi_1(1)\phi_2(2)\phi_3(3)\dots\phi_N(N) \right| \tag{7}$$

Equation(5) can be expressed in terms of Slater determinant as follows:

$$\Psi_{HF}(123\dots N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(1)\phi_1(2) & \dots & \dots & \phi_1(N) \\ \phi_2(1)\phi_2(2) & \dots & \dots & \phi_2(N) \\ \dots & \dots & \dots & \dots \\ \phi_N(1)\phi_N(2) & \dots & \dots & \phi_N(N) \end{vmatrix} \tag{8}$$

For any atom or ion, the Hartree-fock spatial orbital may be written as:

$$\phi = \sum_{i=1}^j c_i \chi_i \tag{9}$$

Where c_i represents the constant coefficient yield from the SCF method And χ_i is the basis function as a standard normalized Slater-type orbital (STO's), which is given by:

$$\chi_{n\ell m_\ell}(r, \theta, \phi) = R_{n\ell}(r) Y_{\ell m_\ell}(\theta, \phi) \tag{10}$$

Many of the properties of an element depend on the energies of its electrons, that mean in each moment, we can specify the energy of the an electron precisely, but not its location at a given instant. So in quantum mechanics when we want determined the location we talk about the probability of finding an electron in specific region from the space at given instant[4].

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

defined as[5]

$$D(r_1) = \int_0^\infty D(r_1, r_2) dr_2 \tag{11}$$

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 He(¹S) in the ground state[6,7]

Pair distribution function can be written as [8].

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

The one-electron expectation value $\langle r_1^n \rangle$ is determined by the expression as [9]

$$\langle r_1^n \rangle = \int_0^\infty D(r_1) r_1^n dr_1 \tag{13}$$

the inter-electron expectation values $\langle r_{12}^n \rangle$ is given by the relation [8]

$$\langle r_{12}^n \rangle = \int_0^\infty f(r_{12}) r_{12}^n dr_{12} \tag{14}$$

The virial theorem is a necessary condition for any stationary state. From the theorem, we are led to[10]

$$\langle E \rangle = \langle T \rangle + \langle V \rangle \tag{15}$$

$$\langle E \rangle = -\langle T \rangle = \langle V \rangle / 2 \tag{16}$$

Expectation value of potential energy proportional to the expectation values of $\langle r_1^{-1} \rangle$ and $\langle r_{12}^{-1} \rangle$ respectively , where [11]

$$\langle V_{en} \rangle = -Z \cdot \langle r_1^{-1} \rangle \tag{17}$$

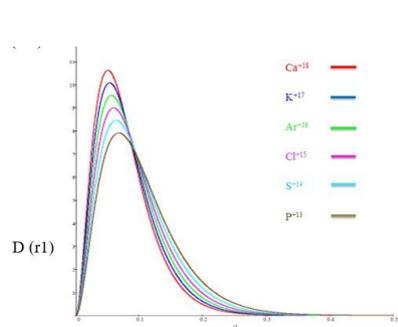
$$\langle V_{ee} \rangle = \langle r_{12}^{-1} \rangle \tag{18}$$

III. RESULTS AND DISCUSSION

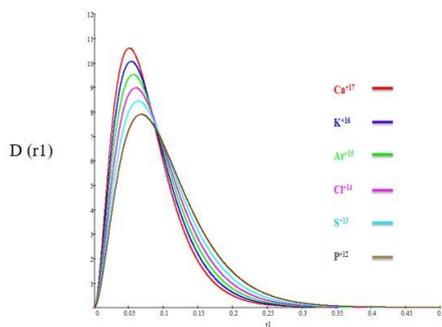
Figure1 represented the relation between one-particle radial density distribution function D (r₁) with the position (r₁) for two-electron system ,the figures 2,3 for k and KαLα≡ KβLα shells in three -electron system and figures (2,3) for three-electrons systems. From these figures observed that the maximum values of D(r₁) increases as Z increases , while the

locations of these peaks are contracted toward the nucleus where we note the maximum probability density distribution function $D(r_1)$ for Ca^{+18} is closer to the nucleus from $D(r_1)$ for P^{+13} . This difference occurs because the Ca^{+18} nucleus $Z=20$ exerts a much stronger attractive force on electrons than does the P^{+13} nucleus ($Z=15$), it was also observed from these figures when the distance equal to zero the probability of finding an electron equal to Zero { when $r=0$ $D(r_1) = 0$ }. This means that the electron is cannot be existed inside the nucleus and when the distance is far away the probability of finding an electron equal to Zero also { when $r = \infty$ $D(r_1) = 0$ }. That means not possible that the electron to be existed outside the atom.

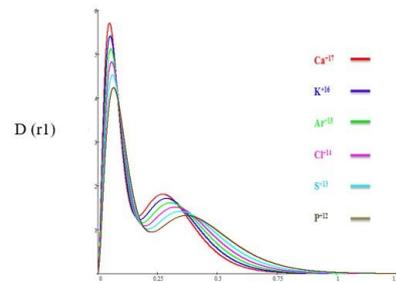
According to the figure (3), it is found there are two peaks for $\alpha\text{L}\alpha$ and $\beta\text{L}\alpha$ Shells. The first peak represented the probability of finding the electron in the α -shell, the second peak represented the probability of finding the electron in the L-shell and we can, also, found that the probability of finding an electron in the K-shell is larger than that in the L-shell because α -shell is the nearest to nucleus, so that attraction force between the nucleus and the electron is larger for K-shell than for L-shell According to coulomb law. In general we note the maximum probability density distribution function $D(r_1)$ in two-electron system Slightly less than three-electron system because the two system have just two electron in K-shell but the three system have two electron in K-shell and one electron in L-shell this electron reduces attraction nuclear force and thus increasing distance.



Fig(1):Relation between $D(r_1)$ with the position (r_1) for two- electron system

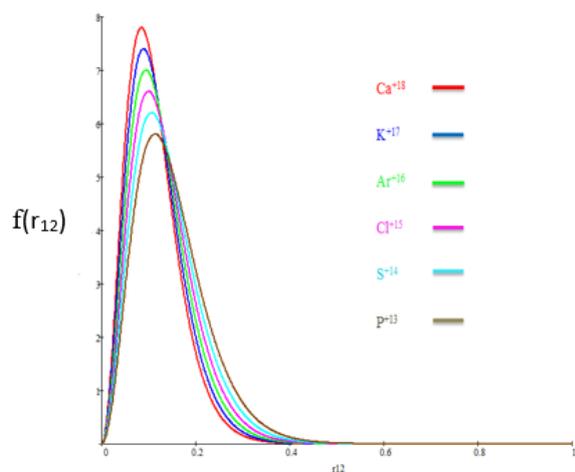


Fig(2): Relation between $D(r_1)$ with the position (r_1) for K -shell.(Three-electron system)

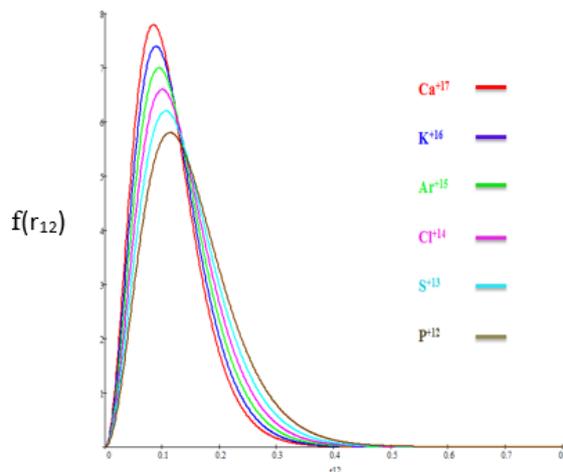


Fig(3): Relation between $D(r_1)$ with the position (r_1) for ($K\alpha, L\alpha \equiv K\beta, L\alpha$) shells.

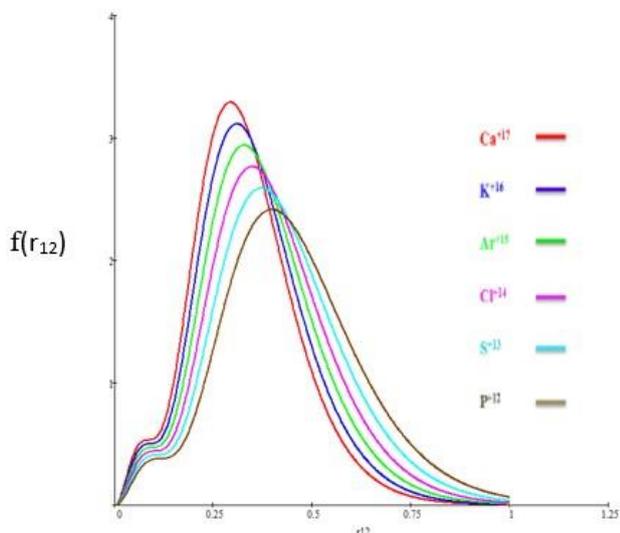
Figure 4 for two-electron system, figures 5,6 and 7 for three-electron system representing the inter-particle distribution function $f(r_{12})$, which describes the probability of locating two electrons separated by distance r_{12} from each other.



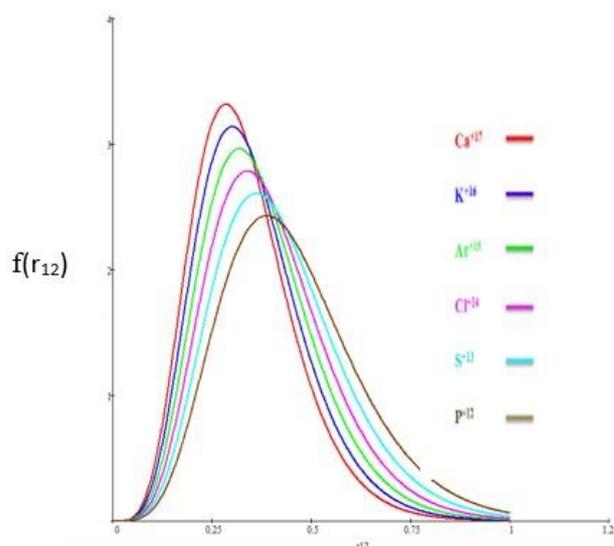
Fig(4): The relation between $f(r_{12})$ with corresponding position r_{12} for two- electron system system.



Fig(5): The relation between $f(r_{12})$ with corresponding position r_{12} for three- electron system system.



Fig(6): The relation between $f(r_{12})$ with corresponding position r_{12} $K\beta L\alpha$ - shell of three -electron system.



Fig(7): The relation between $f(r_{12})$ with corresponding position r_{12} $K\alpha L\alpha$ -shell of three electron system.

from fig(4) where z increases the maximum value of the inter particle distribution function increases $f(r_{12})_{P-ion} > f(r_{12})_{S-ion} > f(r_{12})_{Cl-ion} > f(r_{12})_{Ar-ion} > f(r_{12})_{K-ion} > f(r_{12})_{Ca-ion}$ for two-electron system also like three-electron system fig(5) , and observed that when $r_{12} = 0$ The probability of the inter particle distribution function $f(r_{12}) = 0$ this means that the electron not be closed on another electron and when the distance is far away ($r_{12} = \infty$) the probability of the inter particle distribution function $f(r_{12})$ equal to Zero also That means the diameter is not found out the atom. From figure (7) it can be noted that one peak in the $K\alpha L\alpha$ - shell and two peaks in the $K\beta L\alpha$ -shell because in the $K\alpha L\alpha$ shell the electron α in the K -shell associated with the electron α in the L- shell ,so the two electrons are parallel (has the same spin) and according to Pauli exclusion principle (no two electrons can occupy the same spin state) therefore; there is one probability of finding two electrons simultaneous in $K\alpha L\alpha$ -shell ,while in the $K\beta L\alpha$ shell has two peaks ,the first peak represent the probability of finding two electrons in small distance r_{12} and the second peak represented the probability of finding two electrons in the larger distance between them (r_{12}). Table (1) and table (2) shown The one-electron expectation value $\langle r_1^n \rangle$ and The inter-particle expectation values $\langle r_{12}^n \rangle$ for two and thre-electrons systems respectively

Table (1): Expectation values $\langle r_1^{-1} \rangle$, $\langle r_1^1 \rangle$, $\langle r_{12}^{-1} \rangle$ and $\langle r_{12}^1 \rangle$ for two-electron system

ion	Result and comparison	$\langle r_1^{-1} \rangle$	$\langle r_1^1 \rangle$	$\langle r_{12}^{-1} \rangle$	$\langle r_{12}^1 \rangle$
P^{+13}	Present work	14.68774	0.10257	9.15305	0.149670
	Ref[12]	14.68774	0.102572	9.15305	0.1497
S^{+14}	Present work	15.68773	0.09601	9.77804	0.14011
	Ref[12]	15.68772	0.096006	9.77804	0.14011
Cl^{+15}	Present work	16.68728	0.09023	10.40259	0.13167
	Ref[12]	16.68728	0.090229	10.40259	0.13167
Ar^{+16}	Present work	17.68736	0.08511	11.02769	0.12419
	Ref[12]	17.68736	0.08511	11.02769	0.12419
K^{+17}	Present work	18.68727	0.08054	11.65259	0.11752
	Ref[12]	18.68727	0.080539	11.65259	0.11752
Cu^{+18}	Present work	19.68759	0.07644	12.27797	0.11153

Table (2): Expectation values $\langle r_1^{-1} \rangle$, $\langle r_1^1 \rangle$, $\langle r_{12}^{-1} \rangle$ and $\langle r_{12}^1 \rangle$ for three-electron system

ion	shell	$\langle r_1^{-1} \rangle$	$\langle r_1^1 \rangle$	$\langle r_{12}^{-1} \rangle$	$\langle r_{12}^1 \rangle$
P ⁺¹²	k	14.67506	0.10270	9.14316	0.14989
	kβLα	9.02590	0.26975	2.87951	0.45070
	kαLα	9.02590	0.26975	2.60122	0.45349
	Average	10.90895	0.21406	4.87463	0.35136
S ⁺¹³	k	15.67503	0.09612	9.76823	0.14029
	kβLα	9.65112	0.25162	3.08985	0.42018
	kαLα	9.65112	0.25162	2.78953	0.42282
	Average	11.65909	0.19978	5.21587	0.32776
Cl ⁺¹⁴	k	16.67488	0.09033	10.39316	0.13183
	kβLα	10.27623	0.23577	3.30006	0.39353
	kαLα	10.27623	0.23577	2.97778	0.39602
	Average	12.40911	0.18729	5.557	0.30712
Ar ⁺¹⁵	k	17.67463	0.08520	11.01786	0.12434
	kβLα	10.90300	0.22181	3.51125	0.37007
	kαLα	10.90300	0.22181	3.16634	0.37244
	Average	13.16021	0.17627	5.89848	0.28895
K ⁺¹⁶	k	18.67449	0.08062	11.64287	0.11765
	kβLα	11.52636	0.20940	3.72042	0.34924
	kαLα	11.52636	0.20940	3.35414	0.35149
	Average	13.90907	0.16647	6.23914	0.27279
Ca ⁺¹⁷	k	19.67396	0.07651	12.26731	0.11165
	kβLα	12.15124	0.19831	3.93050	0.33064
	kαLα	12.15124	0.19831	3.54225	0.33279
	Average	14.65881	0.15771	6.58002	0.25836

Tables (1) and (2) we note that the one-particle expectation value $\langle r_1^n \rangle$ for K-shell increases when n take value -1, while when n take value +1 this lead to increases to the attraction force between the nucleus and the electrons where the $\langle r_1^{-1} \rangle$ related to the attraction energy expectation value $\langle V_{en} \rangle = -Z [N. \langle r_1^{-1} \rangle]$, N represents the number of electrons in the shell. Also from tables when Z increases the inter-particle expectation value $\langle r_{12}^n \rangle$ and $\langle r_1^n \rangle$ increases where $\langle r_{12}^{-1} \rangle$ represents repulsion energy between two-electrons, the values of $\langle r_{12}^n \rangle$ when $n=-1$ in the $K\alpha L\alpha$ – shell is smaller than those in $K\beta L\alpha$ shell because the two electrons in the $K\alpha L\alpha$ – shell are parallel this lead the distance between the two electrons decreased so the $\langle r_{12}^{-1} \rangle$ (which represent the repulsion energy between two electrons) is smaller in the $K\alpha L\alpha$ – shell, and when $n=1$ in the $K\alpha L\alpha$ – shell is greater than those in $K\beta L\alpha$ shell because the two electrons in the $K\alpha L\alpha$ – shell had the same spin so the distance must be large between them than the distance between the electrons had antiparallel spins according to Fermi effect. When comparison we find the expectation values $\langle r_1^{-1} \rangle$ and $\langle r_{12}^{-1} \rangle$ in three-electron system less than two-electron system because influence of third electron in L-shell for three-electron system with electron found in K-shell and with nucleus. Table(3) and table(4) shows the expectation value energies of two and three-electrons systems as electron-nucleus attraction expectation value $\langle V_{en} \rangle$, the electron-electron repulsion expectation value $\langle V_{ee} \rangle$ the potential energy expectation value $\langle V \rangle$ and the expectation values of Hartree-Fock energy $\langle E_{HF} \rangle$.

Table (3): The expectation values for all attraction, repulsion, kinetic and Hartree-Fock energies for two-electron system

ion	Result and comparison	$-\langle V_{en} \rangle$	$\langle V_{ee} \rangle$	$-\langle V \rangle$	$\langle T \rangle$	$-\langle E_{HF} \rangle$
P ⁺¹³	Present work	440.63220	9.15305	431.47915	215.73958	215.73958
	Ref[12]	440.63223	9.15305	431.47918	215.73959	215.73959
S ⁺¹⁴	Present work	502.00736	9.77804	492.22932	246.11466	246.11466
	Ref[12]	502.00729	9.77804	492.22926	246.114628	246.114628
Cl ⁺¹⁵	Present work	567.36752	10.40259	556.96493	278.48246	278.48246
	Ref[12]	567.36758	10.40259	556.965	278.482499	278.482499
Ar ⁺¹⁶	Present work	636.74496	11.02769	625.71727	312.85864	312.85864
	Ref[12]	636.7451	11.02769	625.71741	312.858707	312.858707
K ⁺¹⁷	Present work	710.11626	11.65259	698.46367	349.23183	349.23183
	Ref[12]	710.11633	11.65259	698.46375	349.231873	349.231873
Ca ⁺¹⁸	Present work	787.50360	12.27797	775.22563	387.61282	387.61282
	Ref[13]	775.22035	387.60930	387.61106

Table (4): The expectation values for all attraction, repulsion, kinetic and Hartree-Fock energies for three-electron system

Ion	shell	$-\langle V_{en} \rangle$	$\langle V_{ee} \rangle$	$-\langle V \rangle$	$\langle T \rangle$	$-\langle E_{HF} \rangle$
P^{+12}	K	220.12590	9.14316	210.98274	105.49137	105.49137
	$K\beta L\alpha$	135.38850	2.87951	132.50899	66.25449	66.25449
	$K\alpha\alpha$	135.38865	2.60122	132.78743	66.39371	66.39371
	total	490.90305	14.62389	476.27916	238.13957	238.13957
						238.14042 [13]
S^{+13}	K	250.80048	9.76823	241.03225	120.51613	120.51613
	$K\beta L\alpha$	154.41792	3.08985	151.32807	75.66403	75.66403
	$K\alpha\alpha$	154.41776	2.78953	151.62823	75.81411	75.81411
	total	559.63616	15.64761	543.98855	271.99427	271.99427
						271.99241 [13]
Cl^{+14}	K	283.47296	10.39316	273.07980	136.53990	136.53990
	$K\beta L\alpha$	174.69591	3.30006	171.39585	85.69792	85.69792
	$K\alpha\alpha$	174.69591	2.97778	171.71813	85.85907	85.85907
	total	632.86478	16.671	616.19378	308.09689	308.09689
						308.09443 [13]
Ar^{+15}	K	318.14334	11.01786	307.12548	153.56274	153.56274
	$K\beta L\alpha$	196.25400	3.51125	192.74275	96.37138	96.37138
	$K\alpha\alpha$	196.24356	3.16634	193.07722	96.53861	96.53861
	total	710.64090	17.69545	692.94545	346.47273	346.47273
						346.44647 [13]

From the tables (3) and (4) we noted that increasing all energies as nuclear charge increase. We note the attraction energy expectation values $\langle V_{en} \rangle$ are larger than the repulsion energy expectation value $\langle V_{ee} \rangle$ because the distances between the electrons and the nucleus are smaller than the distances between the electrons, and it can be observed from table(4) the expectation value of repulsion energy in the $K\alpha\alpha$ is smaller than that in the $K\beta L\alpha$ because the distance between two electrons in the $K\alpha\alpha$ is larger than that in the $K\beta L\alpha$.

Also it noted that energies largest in three-electron than two-electron system because it have three term of attraction force between nucleus and electron, also has three repulsion terms resulted from the interaction between the electrons while two-electron system has two term of attraction force and the repulsion term.

Tables (5) and (6) represented Correlation Energy E_{corr} for two-electron system and three electron system respectively

Table (5): the correlation energy for two-electron

ion	$-E_o$	E_{HF}	E_{corr}
P^{+13}	216.34325	215.73958	0.60367
S^{+14}	246.89231	246.11466	0.77765
Cl^{+15}	279.47886	278.48246	0.99640
Ar^{+16}	314.10657	312.85864	1.24793
K^{+17}	350.78647	349.23183	1.55464
Ca^{+18}	389.51488	387.61282	1.90206

Table (6): the correlation energy for three-electron

ion	$-E_o$	E_{HF}	E_{corr}
P^{+12}	238.82947	238.13957	0.68990
S^{+13}	272.88055	271.99427	0.88628
Cl^{+14}	309.22491	308.09689	1.12802
Ar^{+15}	347.84270	346.47273	1.36997
K^{+16}	388.76515	387.04969	1.71546
Ca^{+17}	432.06541	429.89426	2.17115

the correlation energy is the difference between the exact non-relativistic energy (E_o) and the Hartree-Fock (HF) energy (E_{HF}) of a system $E_{corr} = E_o - E_{HF}$ and we noted from above tables that correlation energy depended on nucleus charge so it increases when nucleus charge increases. Also note that the correlation energy largest in three-electron system than two electron system because the exact energy bigger of three-electron system than two-electron system.

IV. CONCLUSION

1. When the atomic number Z increases, the one-particle radial density distribution function $D(r_1)$ and the inter-particle distribution function $f(r_{12})$ are increased for two and three electrons systems.
2. For both one-particle expectation $\langle r_1^n \rangle$, and inter-particle expectation $\langle r_{12}^n \rangle$ increase when Z increase for two and three electrons systems.
3. All the expectation values of the energies $\langle V_{en} \rangle$, $\langle V_{ee} \rangle$, $\langle V \rangle$, $\langle T \rangle$ and $\langle E_{HF} \rangle$ increase when the atomic number increases for two and three electrons systems.
4. It can be observed that flat region at small r_{12} of inter particle density function for $K\alpha L\alpha$ -shell due to Fermi effect which means there is no probability to find two electrons in the same spin together in small distance between them
5. The correlation energy increases with increases in atomic number for all studied systems.

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Disclaimer: None

Conflict of interest: There are no conflicts of interest to declare.

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