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### Calculation of the Energy of Subshells for Five\_Electron Systems

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#### Abstract

This study aims to calculate the important atomic properties such as Two Particle Density  $\Gamma_{HF}(r_1, r_2)$ , the electron-electron radial density distribution  $D(r_1, r_2)$ , One-electron radial density distribution  $D(r_1)$ , the expectation values  $\langle r_{12}^n \rangle, \langle r_1^n \rangle$ , the standard deviation  $\Delta r_{12}, \Delta r_1$ , the inter-electronic distribution function  $f(r_{12})$  and the energy expectation value  $\langle E_{HF} \rangle, \langle V_T \rangle, \langle V_{en} \rangle, \langle V_{ee} \rangle$  and  $\langle T \rangle$  the

1s, 2s and 2p-shells for the five\_electron system are examined in position space within the ground state in the (Ne<sup>+5</sup>, Na<sup>+6</sup>, Mg<sup>+7</sup>, Al<sup>+8</sup>, Si<sup>+9</sup> and P<sup>+10</sup> ions) by using Hartree-Fock wave function. These parameters are very important in studying of physical and chemical properties of the atoms, and for this purpose a computer program was designed in MATHCAD14 to calculate these parameters for ions.

**Keywords:** Hartree-Fock, Atomic Properties, Hamiltonian Operator, Hartree-Fock Energies, Five Electron System

#### Introduction

The Hartree-Fock Self-Consistent Field approximation (HF-SCF), which is represented by the wave function, is a decent approximation to many-electron systems. The goal of the HF-SCF approximation is to approximate the complex many-electron problem as a simple one-electron problem with an average approach to handling electron-electron repulsion [1]. The approximation is based on two premises. First, according to the central field approximation, each electron flows independently in the potential field of the nucleus plus N-1 additional electrons [2]. When entering the calculation, the second must have an initial wave function that is compatible with the final one. The Pauli exclusion principle is followed by the wave functions  $\Psi(x_i)$  where  $x_i$  spin orbitals include four quantum numbers ( $n, l, ml, ms$ ), making the wave function antisymmetric when two electrons swap places.

#### Theory:

Wave functions must be expressed as the John C. Slater determinant to meet the antisymmetric principle [3].

$$\Psi_{HF} = \begin{vmatrix} \Phi_1(x_1) & \Phi_1(x_2) & \dots & \Phi_1(x_N) \\ \Phi_2(x_1) & \Phi_2(x_2) & \dots & \Phi_2(x_N) \\ \vdots & \vdots & \dots & \vdots \\ \Phi_N(x_1) & \Phi_N(x_2) & \dots & \Phi_N(x_N) \end{vmatrix} \quad (1)$$

The Slater-type orbitals (STO's), which were developed by Slater, are such a base set of functions and are written [4].

$$\chi_{nlm}(\vec{r}, \zeta) = R_{nl}(r, \zeta) Y_{lm}(\theta, \phi) \quad (2)$$

Where  $R_{nl}(r, \zeta)$  showed up for the radial component of the wave function, and its value is provided in [5].

$$R_{nl}(r, \zeta) = (2\zeta)^{n+\frac{1}{2}} [(2n)!]^{-\frac{1}{2}} r^{n-1} e^{-\zeta r} \quad (3)$$

Where  $n$  is the principle quantum number,  $r$  is the distance between the atomic nucleus and the electron,  $Y_{l,m}$  is the spherical harmonic, and  $(\zeta)$  is the orbital exponent.

A linear combination of Slater orbitals from the function known as basis functions denoted as can be used to explain the Hartree-Fock spin orbitals<sup>[6]</sup>.

$$\Psi(\vec{r}) = \sum_j C_j x_{ij}(\vec{r}) \quad (4)$$

Where  $C_i$  is a parameter of the theory (the expansion coefficients), and  $\vec{r} = (r, \theta, \phi)$ , the basic functions  $x_{ij}(\vec{r})$  are a Slater-type orbital with quantum numbers.

### Atomic Properties:

#### a. Two-Particle Density function $\Gamma_{HF}(X_m, X_n)$

For any atomic system with N electrons, the density function of the two particles  $\Gamma_{HF}(X_m, X_n)$  may be expressed as follows<sup>[7]</sup>:

$$\Gamma_{HF}(X_m, X_n) = \binom{N}{2} \int \Psi^*(X_m, X_n, X_p \dots X_N) \Psi(X_m, X_n, X_p \dots X_N) dX_p \dots dX_N \quad (5)$$

Where  $dX_p \dots dX_N$  refers to the integral density of all electrons with the exception of m, n, and  $x_i$  represents the sum of the space vector and electron spin of i.

Assuming that  $\Gamma_{HF}(X_m, X_n)$  is a function of the particles m, n, and that  $\binom{N}{2}$  represents the number of electronic couples, we may calculate the number of twins in the system as follows:

$$\int \Gamma_{HF}(X_m, X_n) dx_m dx_n = \binom{N}{2} = \frac{N!}{[2!(N-2)!]} \quad (6)$$

#### b. The Two-Particle Radial Density Distribution $D(r_1, r_2)$ :

The radial density of an electron A distance between  $r_1$  and  $r_1+dr_1$  from the coordinate origin is represented by the probability density function  $D(r_1)$  as follows<sup>[8]</sup>:

$$D(r_1, r_2) = \iint \Gamma(r_1, r_2) r_1^2 r_2^2 d\Omega_1 d\Omega_2 \quad (7)$$

Where  $d\Omega_k = \sin \theta_k \cdot d\theta_k \cdot d\phi_k$ ,  $K=1$  or  $2$  and that  $D(r_1, r_2)$  must be Normalization.

$$\iint_0^\infty D(r_1, r_2) dr_1 dr_2 = 1 \quad (8)$$

Where  $D(r_1, r_2)$  is the probability density of concurrently discovering electrons 1 at  $r_1$  and 2 at  $r_2$  from the nucleus<sup>[9]</sup>.

#### c. One-particle radial density distribution function $D(r_1)$ :

For the study of electrons in an atom or ion, the one-particle radial density distribution function  $D(r_1)$  is important since it represents the possibility of having electrons in each electron shell, which is known as the following<sup>[10]</sup>.

$$D(r_1) = \int_0^\infty D(r_1, r_2) dr_2 \quad (9)$$

#### d. One-Particle Expectation Value $\langle r_1^n \rangle$ :

The following equation may be used to describe the high probability of an electron's presence at a certain location in relation to the nucleus and its density of radial probability<sup>[11, 12]</sup>.

$$\langle r_1^n \rangle = \int_0^\infty D(r_1) r_1^n dr_1 \quad (10)$$

#### e. Standard Deviation $\Delta r_1$ :

The term "Standard deviation" refers to how much the electron deviates from its initial location from the expected value of its existence, and it is described by the following formula<sup>[13]</sup>.

$$\Delta r_1 = \sqrt{\langle r_1^2 \rangle - \langle r_1 \rangle^2} \tag{11}$$

**f. The Electron-Electron Distribution Function f (r<sub>12</sub>):**

Coulson and Neilson's initial investigation into the role of interstitial distribution focused on the interaction between electrons and helium in its ground state. They came up with the following formula<sup>[14]</sup>.

$$f_{ij}(r_{12}) = \int \Gamma_{ij}(r_1, r_2) dr_1 dr_2 \tag{12}$$

As the (i, j) represents Orbital spin.

**g. Inter-Electron Expectation Values  $\langle r_{12}^n \rangle$ :**

The following equation represents the expected value of the separation between two electrons<sup>[15]</sup>:

$$\langle r_{12}^n \rangle = \int_0^\infty f(r_{12}) r_{12}^n dr_{12} \tag{13}$$

**h. Standard Deviation  $\Delta r_{12}$ :**

Between the two electrons, the electronic distance standard deviation is described as<sup>[16]</sup>.

$$\Delta r_{12} = \sqrt{\langle r_{12}^2 \rangle - \langle r_{12} \rangle^2} \tag{14}$$

**i. Energy Expectation Value  $\langle E \rangle$ :**

A desired system for any stable state is the virus theorem. The viral theorem leads one to<sup>[17]</sup>:

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

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

Potential energy's expected value is proportional to those of  $\langle r_1^{-1} \rangle$  and  $\langle r_{12}^{-1} \rangle$ , respectively, where<sup>[18]</sup>

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

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

**Results and Discussion**

Table (1) displays the results of the maximum values one-particle radial density distribution function D(r<sub>1</sub>) and the corresponding position values (r<sub>1</sub>) for five\_electronic systems. Figures (1) for 1s shell, (2) for 2s and (3) for 2p shell show the relationship between the one-particle radial density distribution function D (r<sub>1</sub>) and the position (r<sub>1</sub>) for five\_electronic systems.

**Table 1:** The maximum value of the radial density distribution function of a one particle Dmax(r<sub>1</sub>) with the positions corresponding to r<sub>1</sub> for five electronic systems

ions	Atomic Number(Z)	1s shell		2s shell			2p shell	
		r <sub>1</sub>	D <sub>max</sub> (r <sub>1</sub> )	peak	r <sub>1</sub>	D <sub>max</sub> (r <sub>1</sub> )	r <sub>1</sub>	D <sub>max</sub> (r <sub>1</sub> )
Ne <sup>+5</sup>	10	0.1028	5.1737	Peak1	0.0801	0.52503	0.5158	1.4370
				Peak2	0.6170	1.5080		
Na <sup>+6</sup>	11	0.0932	5.7137	Peak1	0.0727	0.37586	0.4578	1.6350
				Peak2	0.5514	1.7010		
Mg <sup>+7</sup>	12	0.0853	6.2537	Peak1	0.0664	0.42692	0.4089	1.8326
				Peak2	0.4964	1.8935		
Al <sup>+8</sup>	13	0.0786	6.7943	Peak1	0.0612	0.4552	0.3708	2.0297
				Peak2	0.47816	2.0861		
Si <sup>+9</sup>	14	0.0729	7.3347	Peak1	0.0566	0.52728	0.3390	2.2270
				Peak2	0.4199	2.2536		
P <sup>+10</sup>	15	0.0679	7.8753	Peak1	0.0527	0.58096	0.3114	2.4237
				Peak2	0.3877	2.4705		

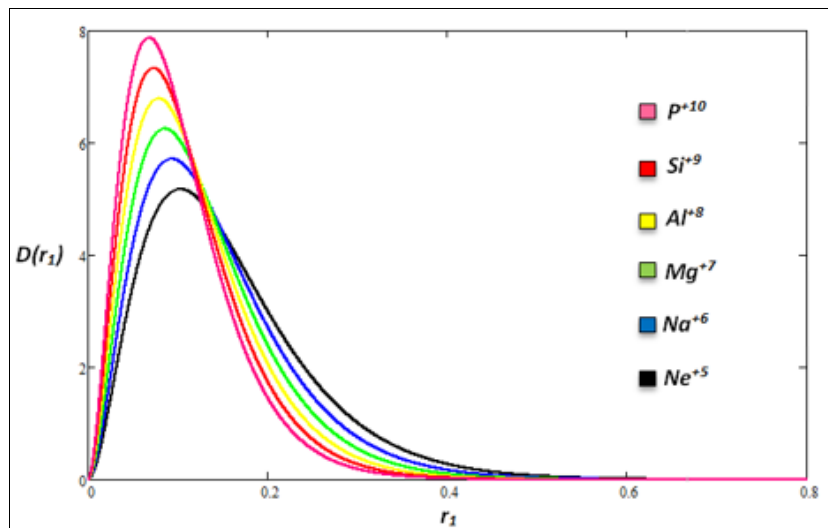


Fig 1: Relationship between one\_particle radial density distribution function and location  $r_1$  for 1s shell in a five\_electron system

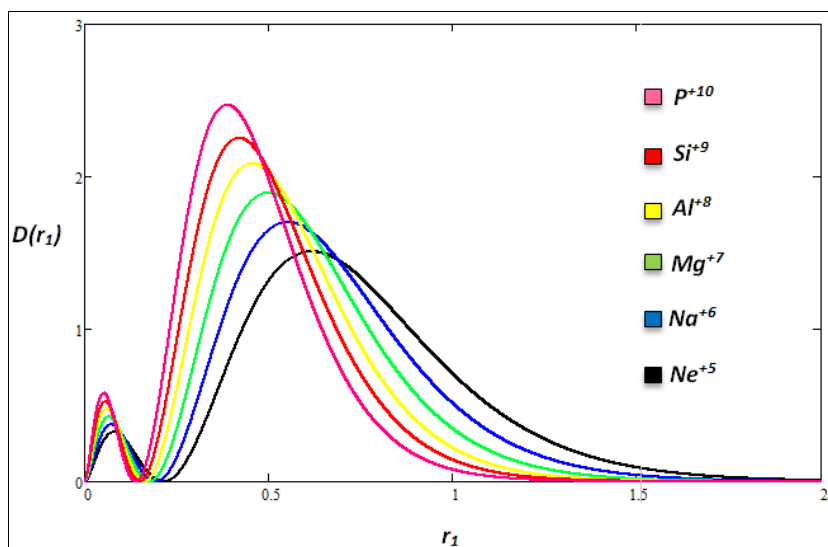


Fig 2: Relationship between one\_particle radial density distribution function and location  $r_1$  for 2s shell in a five\_electron system

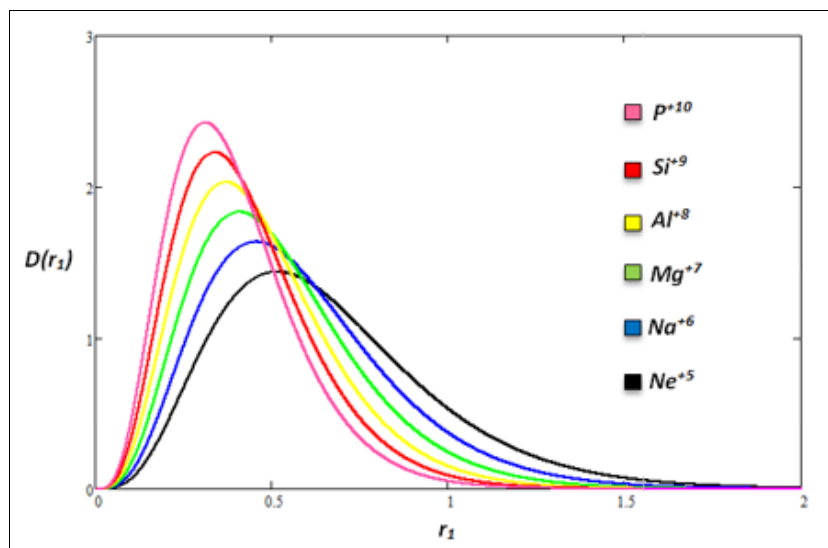


Fig 3: Relationship between one\_particle radial density distribution function and location  $r_1$  for 2p\_shell in a five\_electron system

The maximum values of radial density of a one particle  $D(r_1)$ , as shown in Table (1) for five\_electronic systems, increases with increasing atomic number  $Z$ . This value increase occurs for all shells (1s), (2s) and (2p). because an increase in atomic number leads to increases in the attraction force between the nucleus and the electrons.

$$D(r_1)_{P^{+10}} > D(r_1)_{Si^{+9}} > D(r_1)_{Al^{+8}} > D(r_1)_{Mg^{+7}} > D(r_1)_{Na^{+6}} > D(r_1)_{Ne^{+5}}$$

Whereas the positions of maximum ( $r_1$ ) values decrease, it is also important to note that from all these figures, the probability of finding an electron equals zero when the distance equals zero. This means that the electron cannot exist inside the nucleus, whereas when the distance is far away, the probability of finding an electron equal zero, which means that the electron cannot exist outside the atom.

Figures (1) and (3) for 1s and 2p shells, respectively, show that for each of the two examined systems, there is one peak that refers to the probability of finding the electron in the 1s shell or 2p shell.

Figure (2) show that for each of the examined system, the first peak represents an electron that can penetrate the 1s\_shell and settle for a short period of time, known as a penetration phenomenon, and the second peak represents the probability of finding the electron in the 2s\_shell.

Furthermore, as the distance between the nucleus and the electron reduces because of an increase in the atomic number, the force of attraction causes the nucleus' location to decrease. Because the 1s shell is closer to the nucleus than the 2s shell, it has a higher probability of containing an electron.

The results of the one-particle expectation values  $\langle r_1^n \rangle$  and standard deviation  $\Delta r_1$  for 1s, 2s and 2p shell and 2p shell for five electronic systems, are shown in tables (2), (3) and (4) for the ground state.

**Table 2:** Expectation values  $\langle r_1^n \rangle$  where  $-2 \leq n \leq 2$  and standard deviation for 1s shell for five electron system

ions	$\langle r_1^{-2} \rangle$	$\langle r_1^{-1} \rangle$	$\langle r_1^{+1} \rangle$	$\langle r_1^{+2} \rangle$	$\Delta r_1$
$Ne^{+5}$	188.31600	9.65500	0.15700	0.03300	0.09167
$Na^{+6}$	229.06405	10.65343	0.14185	0.02700	0.08292
$Mg^{+7}$	273.80320	11.65167	0.12962	0.02253	0.07570
$Al^{+8}$	322.55078	12.65056	0.11933	0.01909	0.06963
$Si^{+9}$	375.29775	13.64934	0.11054	0.01637	0.06446
$P^{+10}$	432.04838	14.64846	0.10297	0.01420	0.06000

**Table 3:** Expectation values  $\langle r_1^n \rangle$  where  $-2 \leq n \leq 2$  and standard deviation for 2s shell for five electron systems

ions	$\langle r_1^{-2} \rangle$	$\langle r_1^{-1} \rangle$	$\langle r_1^{+1} \rangle$	$\langle r_1^{+2} \rangle$	$\Delta r_1$
$Ne^{+5}$	15.61278	1.96290	0.73820	0.63955	0.30759
$Na^{+6}$	19.84721	2.21333	0.65684	0.50589	0.27284
$Mg^{+7}$	24.58145	2.46371	0.59170	0.41020	0.24514
$Al^{+8}$	29.81799	2.71407	0.53837	0.33940	0.22262
$Si^{+9}$	35.25716	2.95055	0.49689	0.28941	0.20619
$P^{+10}$	41.79090	3.21463	0.45619	0.24351	0.18813

**Table 4:** Expectation values  $\langle r_1^n \rangle$  where  $-2 \leq n \leq 2$  and standard deviation for 2p shell for five electron systems

ions	$\langle r_1^{-2} \rangle$	$\langle r_1^{-1} \rangle$	$\langle r_1^{+1} \rangle$	$\langle r_1^{+2} \rangle$	$\Delta r_1$
$Ne^{+5}$	5.05548	1.92336	0.66201	0.53351	0.30864
$Na^{+6}$	6.46069	2.17747	0.58347	0.41369	0.27065
$Mg^{+7}$	8.03237	2.43070	0.52179	0.33040	0.24112
$Al^{+8}$	9.77112	2.68338	0.47200	0.27006	0.21744
$Si^{+9}$	11.68261	2.93645	0.43081	0.22476	0.19790
$P^{+10}$	13.74794	3.18735	0.39656	0.19036	0.18194

Tables (2), (3) and (4) for the five electron system in the ground state, show that the one-particle expectation value  $\langle r_1^n \rangle$  increases when  $n$  takes negative values (-2,-1), where  $n = -2$  is used in the calculation correlation factor and  $n = -1$  the  $\langle r_1^{-1} \rangle$  which represents the attraction energy expectation value  $\langle V_{en} \rangle = -Z[\langle r_1^{-1} \rangle]$ , increases where the atomic number  $Z$  increases for each 1s, 2s and 2p\_shells, this is due to an increase in the attraction energy between the nucleus and electron.

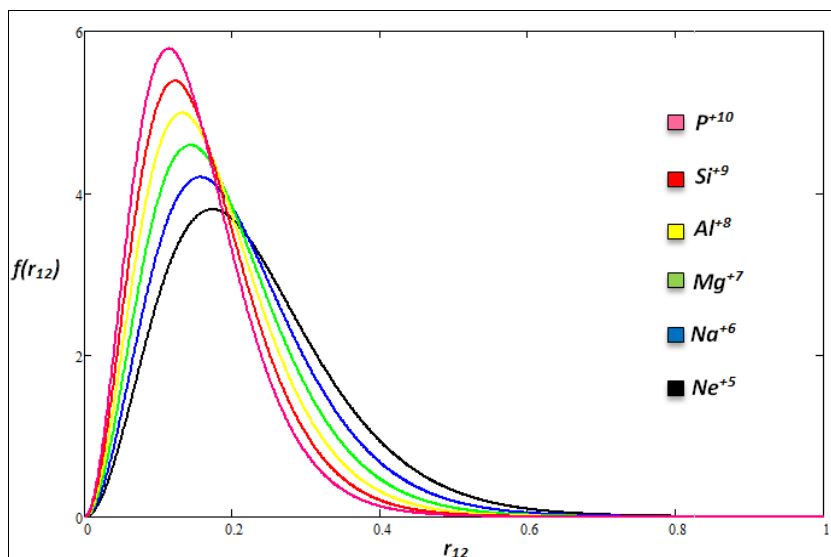
Also from all tables, the maximum value of  $\langle r_1^{-1} \rangle$ , is in the 1s\_shell and the lowest value of  $\langle r_1^{-1} \rangle$ , in the 2p shell for all ions.  $n$  takes positive values (+1,+2), when  $n = +2$  it is used in the standard deviation calculation, when  $n = +1$ ,  $\langle r_1^{+1} \rangle$  indicates the distance between the nucleus and electron. For positive numbers (+1, +2), the one-expectation value  $\langle r_1^n \rangle$  decreases as the atomic number ( $Z$ ) increases. When  $n$  equals zero, the one-particle expectation value  $\langle r_1^n \rangle$  equals unity for all examined systems, and this constitutes the normalization condition since the one-particle radial density distribution function  $D(r_1)$  is normalized  $[\int_0^\infty D(r_1)r_1^n dr_1 = 1]$ .

The lowest value of  $\langle r_1^{+1} \rangle$  from all tables is in the 1s shell for all ions, whereas the highest value of  $\langle r_1^{+1} \rangle$  is in the 2p shell for all ions.

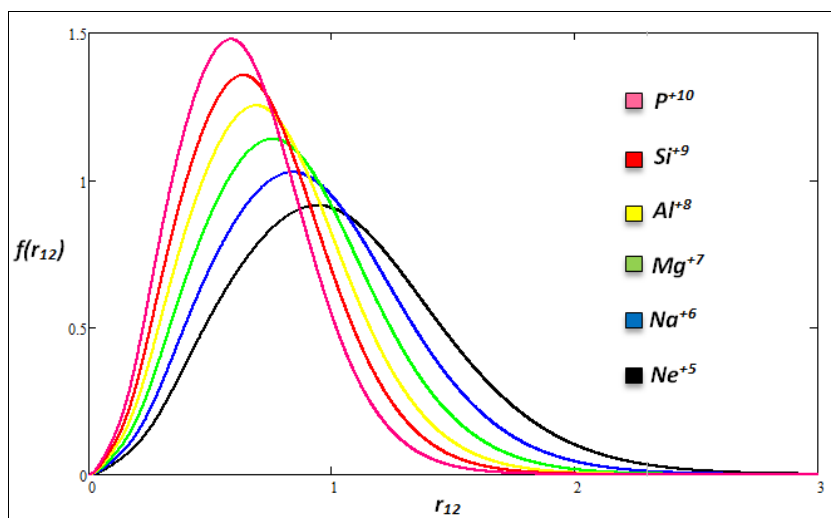
Table (5), which present the greatest values of  $f(r_{12})$  and their related locations, give documentation of the findings. Figures (4) for 1s\_shells and (5) for 2s shells for the five electronic systems, demonstrate the relationship between the inter-electron distribution function  $f(r_{12})$  and the distance between electrons  $r_{12}$ .

**Table 5:** Maximum  $f(r_{12})$  Values with Corresponding Values of  $r_{12}$  in 1s and 2s shells for five\_electron System Under Study in a.u

ions	Atomic number(z)	1s shell		2s shell	
		$r_{12}$	$f_{max}$	$r_{12}$	$f_{max}$
$Ne^{+5}$	10	0.173	3.7979	0.940	0.91331
$Na^{+6}$	11	0.157	4.1949	0.839	1.02650
$Mg^{+7}$	12	0.144	4.5920	0.757	1.13960
$Al^{+8}$	13	0.132	4.9897	0.690	1.25250
$Si^{+9}$	14	0.122	5.3870	0.636	1.35560
$P^{+10}$	15	0.114	5.7849	0.585	1.47780



**Fig 4:** The Inter particle Distribution Function and  $r_{12}$  for 1s\_shell for five electron system Relationship



**Fig 5:** The Inter particle Distribution Function and  $r_{12}$  for 2s shell for five electron system Relationship

The maximum value in the inter particle distribution function  $f(r_{12})$  grows with increasing atomic number ( $Z$ ) as the distance between electrons  $r_{12}$  decreases in Table (5) for five\_electron system for 1s and 2s\_shells.

The maximum value of  $f(r_{12})$  in the 1s\_shell and the minimum value of  $f(r_{12})$  in the 2s\_shell for each state because the nuclear attraction of the 1s\_shell is greater than the other shells, resulting in a decrease in the distance between the electrons  $r_{12}$ , which increases  $f(r_{12})$  in the 1s\_shell relative to the other shells. It was also observed from the figures (4) and (5) for five\_electron systems for 1s and 2s shells that when  $r_{12} = 0$ , the probability of distribution between particles  $f(r_{12}) = 0$ , which means that there is no distance between electron and itself, and when the distance is far, the probability of the inter\_particle distribution function  $f(r_{12}) = 0$ .

The findings of the inter-electron expectation values  $\langle r_{12}^n \rangle$  and standard deviation  $\Delta r_{12}$ , when  $n = -1$ , are shown in Tables (6) and (7) The repulsion energy expectation value between two electrons is represented by the inter-particle expectation value  $\langle r_{12}^{-1} \rangle$ , or  $\langle V_{ee} \rangle = \langle r_{12}^{-1} \rangle$ .

**Table 6:** Expectation values  $\langle r_{12}^n \rangle$  where  $-2 \leq n \leq 2$  and standard deviation for 1s shell for five electron systems in a.u.

ions	$\langle r_{12}^{-2} \rangle$	$\langle r_{12}^{-1} \rangle$	$\langle r_{12}^{+1} \rangle$	$\langle r_{12}^{+2} \rangle$	$\Delta r_{12}$
Ne <sup>+5</sup>	61.78916	6.00261	0.22875	0.06587	0.11637
Na <sup>+6</sup>	75.26252	6.62617	0.20714	0.05400	0.10530
Mg <sup>+7</sup>	90.06626	7.24982	0.18926	0.04506	0.06914
Al <sup>+8</sup>	106.21012	7.87410	0.17422	0.03818	0.08845
Si <sup>+9</sup>	123.68128	8.49806	0.16138	0.03275	0.08189
P <sup>+10</sup>	142.48889	9.12255	0.15031	0.02841	0.07623

**Table 7:** Expectation values  $\langle r_{12}^n \rangle$  where  $-2 \leq n \leq 2$  and standard deviation for 2s shell for five electron systems a.u.

ions	$\langle r_{12}^{-2} \rangle$	$\langle r_{12}^{-1} \rangle$	$\langle r_{12}^{+1} \rangle$	$\langle r_{12}^{+2} \rangle$	$\Delta r_{12}$
Ne <sup>+5</sup>	2.46658	1.22426	1.04173	1.27910	0.44033
Na <sup>+6</sup>	3.11997	1.37554	0.92680	1.01177	0.39090
Mg <sup>+7</sup>	3.84970	1.52673	0.83481	0.82040	0.35143
Al <sup>+8</sup>	4.65565	1.67776	0.75952	0.67880	0.31927
Si <sup>+9</sup>	5.47609	1.81801	0.70124	0.57882	0.29510
P <sup>+10</sup>	6.49621	1.97951	0.64353	0.48701	0.26995

Notice from Tables (6) and (7) that for all shells when values  $n = -2, -1$ , the inter-electron expectation value  $\langle r_{12}^n \rangle$  increases when  $Z$  increases. when  $n = +1, +2$  inter-electron expectation value  $\langle r_{12}^n \rangle$  decreases when  $Z$  increases, as seen in Tables for each shell, where  $\langle r_{12}^n \rangle$  represents the  $\langle V_{ee} \rangle$  values for electron-electron repulsion. In other words, when the nucleus's attraction force increases, the space between electrons gets smaller. The repulsive force in the 1s shell is greater than those in the other shells, and because the distance between two electrons is less in the 1s shell, the value of  $\langle r_{12}^{-1} \rangle$  in all Tables for all systems is highest in the 1s shell, while it is lowest in the 2s shell.

Where  $\langle r_{12}^{+1} \rangle$  denotes the separation between two electrons, When  $Z$  increases, the inter-particle expectation value  $\langle r_{12}^{+1} \rangle$  decreases for the five-electron system because an increase in the attraction nuclear force causes the distance between electrons to decrease. Also, notice that the value  $\langle r_{12}^{+1} \rangle$  is highest in the 2s shell and lowest in the 1s shell because the repulsion between two electrons in the 2s shell is stronger than that in the 1s shell.

Because decreasing the distance between electrons makes the deviation on the expectation value small, it can be seen from Table that the standard deviation  $\Delta r_{12}$  decreases as ( $Z$ ) increases, and it is important to note that for each shell of the five electronic systems,  $\Delta r_{12}$  is largest in the 2s shell and smallest in the 1s shell.

The results of the calculations of the expected values for the energies of the five-electron system are organized in Table (8).

**Table 8:** Expectation Values for All Attraction, Repulsion Potential, Kinetic and Total Energy for 1s, 2s and 2p shells for five electron system in a.u.

ions	shells	$\langle V_{en} \rangle$	$\langle V_{ee} \rangle$	$\langle V_T \rangle$	$\langle T \rangle$	$\langle E_T \rangle$
Ne <sup>+5</sup>	1s	193.08000	6.00199	187.07801	93.53900	93.53900
	2s	39.25520	1.22418	38.03102	19.01551	19.01551
	2p	19.23360	—	19.23360	9.61680	9.61680
Na <sup>+6</sup>	1s	234.37546	6.62617	227.74929	113.87465	113.87465
	2s	48.69326	1.37554	47.31772	23.65886	23.65886
	2p	23.95217	—	23.95217	11.97608	11.97608
Mg <sup>+7</sup>	1s	279.64008	7.24982	272.39026	136.19513	136.19513
	2s	59.12904	1.52673	57.60231	28.80115	28.80115
	2p	29.16840	—	29.16840	14.58420	14.58420
Al <sup>+8</sup>	1s	328.91456	7.87410	321.04046	160.52023	160.52023
	2s	70.56582	1.67776	68.88806	34.44403	34.44403
	2p	34.88394	—	34.88394	17.44197	17.44197
Si <sup>+9</sup>	1s	382.18152	8.49806	373.68346	186.84173	186.84173
	2s	82.61540	1.81801	80.79739	40.39869	40.39869
	2p	41.11030	—	41.11030	20.55515	20.55515
P <sup>+10</sup>	1s	439.45380	9.12255	430.33125	215.16563	215.16563
	2s	95.42880	1.97951	93.44929	46.72464	46.72464
	2p	47.81025	—	47.81025	23.90512	23.90512

When the atomic number ( $Z$ ) increases, it is shown in Tables (8):

For each shell, the energy of the  $\langle V_{en} \rangle$  attraction potential between the electron and the nucleus increases and the potential energy electron repulsion  $\langle V_{ee} \rangle$  is increased by the repulsive energy,

The total potential energy  $\langle V_T \rangle$  will increase in the shell when it reaches a value that is equal to the sum of the attractive potential energy of the electron core  $\langle V_{en} \rangle$  and the potential energy of electron repulsion  $\langle V_{ee} \rangle$ .

When the attraction potential between the electron and the nucleus increases, which decreases the distance between electrons and hence preserves the stability of the atomic system, is predicted to increase the velocity of the electron rotation in the orbital, leading to an increase in the expected value of the kinetic energy  $\langle T \rangle$ .

When the system's total energy (also known as the Hartree-Fock energy, or  $\langle E_{HF} \rangle$ ) increases together with the potential and kinetic energies, it does so as well (HF energy).

### Conclusions

1. It is obvious that as the atomic number  $Z$  increases, the maximum values of the radial density of a particle  $D(r_1)$  increase for the five-electron system, with distances  $(r_1)$  decreasing as the atomic number increases and for all shells.
2. When the value of  $(n)$  is negative and for all of the shells, the maximum values of the one-particle expectation values  $\langle r_1^n \rangle$  increase as the atomic number  $Z$  increases, while  $(n)$  is the positive value of  $\langle r_1^n \rangle$  decreases as the atomic number  $Z$  increases and for all the shells in the system. Additionally, it should be noticed that when  $Z$  increases, the value of standard deviation  $\Delta r_1$  reduces.
3. The maximum value of inter-particle distribution function  $f(r_{12})$  increases with the atomic number  $Z$ .
4. With increasing atomic number  $Z$ , the maximum value of the inter-particle expectation values for the two-electron system  $\langle r_{12}^n \rangle$  increases when  $(n)$  takes negative values, and decreases when  $(n)$  takes positive values. Additionally, the actual results showed that the standard deviation is  $\Delta r_{12}$  decreases by increasing the system's total number of atomic  $Z$  shells.
5. The expectation value of the potential energy  $\langle V_T \rangle$ ,  $\langle V_{en} \rangle$  and  $\langle V_{ee} \rangle$  will increase with an increase in the atomic number  $Z$ .
6. By increasing the atomic number  $Z$  in all of the system's shells, the expectation values of Kinetic energy  $\langle T \rangle$  and the total energy (Hartree-Fock energy,  $\langle E_{HF} \rangle$ ) increase.

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