



Energies of K-Shell for Chemical Elements From (Ne to Si) By Hartree-Fock Method

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ABSTRACT:

The energies of the K-shell, as well as the atomic characteristics of the (Ne, Na, Mg, Al, and Si) atoms were computed using the algebraic approximation of the Hartree-Fock method (HF) and compared to some experimental results from extensive studies. The calculated atomic energies for atomic number ($10 \leq Z \leq 14$) were assessed. The study demonstrated that the estimates used to calculate the atomic properties using this method were accurate. The function $f(r_{12})$ for the inter-particle distribution is one of the atomic characteristics. According to this approximation, the two techniques should yield values for the one-particle radial density distribution function $D(r)$, ($\langle r_1^n \rangle$, $\langle r_{12}^n \rangle$), where n is an integer number from -2 to 2, and the standard deviation Δr_1 and Δr_{12} . The properties of the energies expectation values are repulsion potential energy $\langle V_{ee} \rangle$, attractive potential energy $\langle V_{en} \rangle$, total potential energy $\langle V \rangle$, kinetic energy $\langle T \rangle$ and total energy $\langle E \rangle$. In conclusion increasing the atomic number leads to an increase in all values studied energies. Finally, the equations were programmed in Mathematics 2015 and all calculations were calculated in atomic units.

1. Introduction

Planetary motion, additionally to the behavior of electrons and subatomic particles, according to quantum mechanics. As a result, In quantum mechanics, there is classical mechanics as a subset. Even though they have the beginning condition, In the quantum theory, events are not deterministic but rather depend on probability, with one significant exception. Quantum theory is the theory of probability since it is a statistical theory, even for a single particle. The choices are not limited to the nature of the state that serves as the representation of the method or the number of states that need to be normalized in the system [1].

Schrodinger introduced wave mechanics into the collection of ideas, equations, interpretations, and theories that were common in order to explain the growing body of observations of the wave equation that it obeys. The basis for our current understanding of quantum phenomena and the mathematical techniques

we use to test them is Schrodinger's wave mechanics. The Schrodinger equation with time independence [2].

$$\hat{H}\psi = E\psi \quad (1)$$

Where ψ denotes the wave function and controls how the electron behaves. The Schrödinger equation was discovered to be an Eigen value equation when stated as in equation (1), hence the equation becomes [3].

{(operator). (function) = constant factor × same function}

The eigenvalue of the operator H is designated as E . The Hamiltonian operator, which is defined for a single electron of an atom with a charge of Ze , is the component H in equation (1), where the Eigen function is the wave function corresponding to the energy [4].

$$H = -\frac{\hbar^2}{2m} \nabla^2 - \frac{Ze^2}{r} \quad (2)$$

Where $\hbar = \frac{h}{2\pi}$, h : is Planck's constant, m_e : is the mass of an electron and ∇^2 : Laplacian operator, which can be written in spherical coordinate (r, θ, ϕ) as follows [5].



$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \left(\frac{\partial^2}{\partial \phi^2} \right)$$

3

The Hamiltonian for an atom with N electrons is given by [6]:

$$\hat{H} = -\frac{\hbar^2}{2m_e} \sum_{i=1}^N \nabla_i^2 + \sum_{i=1}^N \frac{Ze^2}{r_i} + \sum_{i=1}^N \sum_{j>i}^N \frac{e^2}{r_{ij}}$$

4

As a result, the kinetic energy operator is the first component for N-electrons, while potential energy is the second term for the attraction of the electrons to the charge nucleus. The final item is the potential energy of the electron, and Ze , r_i is the separation between the nucleus and the electron [7]. At an infinite distance from the nucleus' center, this term equals 0. The constraint $j > i$ prevents counting the same inter electronic repulsion twice and avoids expressions like $\frac{e^2}{r_i}$. An electron's potential energy in an atom is a negative amount since it is lower than when the nucleus and electron are separated by an infinite distance [8]. Because of the inter-electronic repulsion factors $\frac{e^2}{r_{ij}}$, the Schrödinger equation for the atom cannot be separated [9]. The atomic Hartree-Fock equations have numerical computational methods developed by Froese Fischer [10]. a solitary substance The Green's function approach and related many body approaches have been used frequently to determine the ionization and electron attachment spectra of atoms and molecules. Recent review papers provide thorough descriptions of the various techniques created in this topic as well as an overview of applications [11].

For the ground states of all the neutral atoms from He to Xe, singly charged cations from Li^+ to Cs^+ , and stable singly charged anions from H^- to I^- , improved Roothaan-Hartree-Fock wave functions are presented [12]. Mg is one of the two-electron atomic systems explored in this paper, along with the ions Al^{+1} , Si^{+2} , P^{+3} and S^{+4} . Hartree-Fock approximation is used to calculate the atomic parameters, such as the one electron radial density function $D(r_1)$ [13]. The study of the atomic system with two electrons covered the wave functions of the neutral atoms O, F, and Ne [14]. The treatments were used on diatomic molecules like Li_2 , N_2 , F_2 , and Se_2 as well as the atoms in group 15 of the periodic table, which include ^{7}N , ^{15}P , ^{33}As , ^{51}Sb , ^{83}Bi , and ^{115}U up. Three fundamental techniques—basis-set, Hamiltonian, and method type—were dependent on the treatments [15].

Another investigation of intraocular densities, Coulomb holes, and high-accuracy correlation energies for the lithium cation, helium, hydride ion, and system with the crucial nuclear charge, ZC, for binding two electrons. A Laguerre-based wave function is used to calculate both the completely correlated (FC) and Hartree-Fock (HF) wave functions [16]. Consequently, the goal of our research was to examine the energy of atoms in this orbit that have two electrons.

2. Calculations

Many important atomic properties of studied ions are discussed below:

2.1 Radial density distribution function $D(r_1)$ for one particle

Using the electron radial density distribution function as in equation (5), the researchers calculated the likelihood of finding an electron in a spherical shell at a radius of r_1 from the nucleus [17]

$$D(r_1) = R_{1s}^2(r_1)R_{1s}^2(r_2) \quad 5$$

2.2 Inter-particle Distribution Function [18]:

The pair distribution function from the following equation was evaluated (6)

$$f(r_{12})_{(2s)} = 0.5r_{12} \left[\int_{r_1}^{\infty} \int_{r_1-r_{12}}^{r_1+r_{12}} R_{2s}^2(r_1)R_{2s}^2(r_2)r_2 dr_2 dr_1 + \int_{r_1}^{r_{12}} \int_{r_{12}-r_1}^{r_{12}+r_1} R_{2s}^2(r_1)R_{2s}^2(r_2)r_2 dr_2 dr_1 \right] \quad 6$$

Is the coulomb repulsion of two electrons in a k-shell with opposite spins, which was used to determine the relationship between $f(r_{12})$ and inter-electronic distance r_{12} .

2.3 One-particle expectation value $\langle r_1^m \rangle$

We calculated the one-particle expectation value by using equations (7) [19]:

$$\langle r_1^m \rangle = \int_0^{\infty} D(r) r_1^m dr_1 \quad 7$$

For m, an integer number that takes the values, successively for various values $-2 \geq m \geq 2$, the results of the radial expectation values of $\langle r_1^m \rangle$ and standard deviation.

2.4 Inter-particle Expectation Value $\langle r_{12}^m \rangle$

Using the equation (8) below, we assessed the inter-particle expectation value $\langle r_{12}^m \rangle$ [20]:



$$\langle r_{12}^m \rangle = \int_0^\infty f(r_{12}) r_{12}^m dr_{12} \quad 8$$

which show the relationship between $\langle r_{12}^m \rangle$ with (m).

2.5 The expectation value for energy $\langle E \rangle$

The total energy and the potential energy were calculate by using equations (9 and 10)[21]:

$$\langle E \rangle = \frac{1}{2} \langle V \rangle \quad 9$$

$$\langle V \rangle = Z \left\langle \frac{1}{r_1} \right\rangle + \left\langle \frac{1}{r_{12}} \right\rangle \quad 10$$

3. Results and Discussions

Through the use of the above equations, the results were tabulated and plotted using the Mathematics 15 program:

Table 1. Lists the values of the positions for the analyzed atoms that correspond to the distribution function.

Atomic properties	Atoms				
	Ne	Na	Mg	Al	Si
r_1	0.102 0	0.093 0	0.086 0	0.079 0	0.073 0
$D_{max}(r_1)$	5.142 3	5.672 5	6.207 2	6.742 3	7.276 6
r_{12}	0.174 0	0.157 0	0.144 0	0.133 0	0.123 0
$f_{max}(r_{12})$	3.770 9	4.155 8	4.547 7	4.939 6	5.337 0

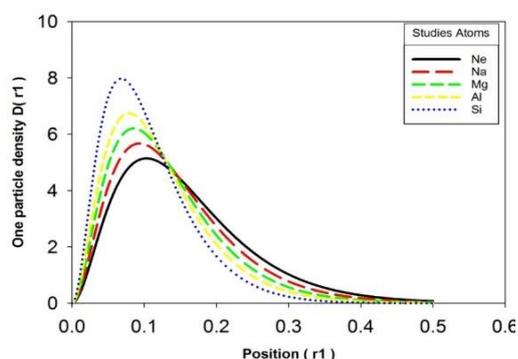


Figure 1. shows the connection between the examined atoms' distance r_1 and the radial distribution function $D(r_1)$.

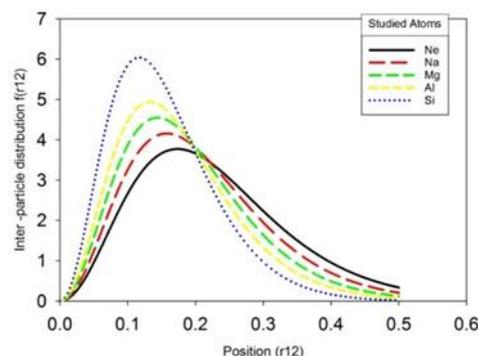


Figure 2. Shows the connection between the examined atoms' distance (r_{12}) and the inter-particle distribution function ($f(r_{12})$).

From Table 1 and Figures 1 and 2, we obtained several results, due to the maximum values for $D(r_1)$ rise as r_1 gets higher, detecting an electron becomes more likely as the gap between the nucleus and the electron narrows. Additionally, we observe that these peaks are concentrated closer to the nucleus, which is also where we observe the maximum probability density distribution function for the systems under study. When $D(r_1) = 0$ is attributed to $r = 0$ when the distance from the system equals zero, the chance of finding an electron is zero, indicating that the electron was not found in the nucleus. In contrast, when $r = \infty$, $D(r_1) = 0$, is attributed to $r = \infty$, the chance of discovering an electron is zero, indicating that the electron is not discovered in the atom.

Additionally, Table 1 demonstrates how, for the systems under study, the relationship between inter-distance r_{12} and maximum values of the inter-particle distribution function $f(r_{12})$ led us to notice that, as Z increases, the maximum value $f(r_{12})$ increases and, conversely, the inter-particle distance decreases due to an increase in atomic number, which increases the nucleus-electron attraction force and reduces the distance between electrons.

The distance r_{12} between two electrons decreases as atomic number increases, contrary to the trend seen in figure 3 where the inter-particle distribution function increases as each shell shrinks near the nucleus $r_{12} = 0$, $f(r_{12}) = 0$ and When $r_{12} = \infty$, $f(r_{12}) = 0$ because the coulomb interaction is ignored when there is a significant distance between two electrons. The relationship between (r_1) and $D_{max}(r_1)$ was likewise depicted, and it was a direct linear relationship. The relationship between (r_{12}) and $f(r_{12})$ similarly exhibited same pattern.



Table 2. Lists the one-particle expectation values for various (m) values.

Atoms	$\langle r_1^{-2} \rangle$	$\langle r_1^{-1} \rangle$	$\langle r_1^1 \rangle$	$\langle r_1^2 \rangle$
Ne	187.289550	9.618780	0.157710	0.033510
[22]	187.197184	9.618054	0.157631	0.033470
Na	227.538390	10.60336	0.143030	0.027580
[22]	227.533835	10.607384	0.142858	0.027481
Mg	271.975590	11.596050	0.130740	0.023030
[22]	271.847138	11.597954	0.130594	0.022956
Al	320.300750	12.586440	0.120410	0.019540
[22]	320.129366	12.589248	0.120258	0.019459
Si	372.63133	13.57914	0.11156	0.016770
[22]	372.382224	13.581150	0.111431	0.016701

All examined systems are shown in Table 2, and we discovered that the one-particle expected value $\langle r_1^m \rangle$ increases as the atomic number rises and decreases as m becomes negative (-2, -1) where the $\langle r_1^{-1} \rangle$ is related to the attraction energy expectation value $\langle V_{en} \rangle = -Z[N \langle r_1^{-1} \rangle]$, N denotes the number of electrons in the shell, and $\langle r_1^{-2} \rangle$ demonstrates how the distribution of density is dispersed near the nucleus. Additionally, we saw that the one-expectation value grows as Z increases $\langle r_1^m \rangle$ begins decreasing for (m) positive values (+1, +2), where $\langle r_1^1 \rangle$ represents the distance between electron and nucleus.

Table 3. Represents of expectation values $\langle r_{12}^m \rangle$ when $-2 \leq m \leq 2$.

Atom	$\langle r_{12}^{-2} \rangle$	$\langle r_{12}^{-1} \rangle$	$\langle r_{12}^1 \rangle$	$\langle r_{12}^2 \rangle$
Ne	61.24045 7	5.97170 3	0.23051 2	0.06703 8
Na	74.43582 5	6.58265 7	0.20903 8	0.05515 2
Mg	89.05579	7.2010	0.19105	0.04606 0
Al	104.9453 2	7.81785	0.17596	0.03909 0
Si	122.1830 6	8.43654	0.16301	0.03354 0

From analyzing the inter-particle expectation value $\langle r_{12}^m \rangle$ displayed in Table 3, we noted that the inter-particle expectation value $\langle r_{12}^m \rangle$ increases when Z increases and when (m) takes values -2, -1, where

$\langle r_{12}^{-1} \rangle$ represents repulsion energy between two-electrons. But when (m) takes positive values +1, +2, the inter-particle expectation value decreases with Z increasing.

The expected values for the investigations of the atomic attraction, repulsion, kinetic, and Hartree-Fock energies are all provided in Table 4 for the aforementioned equations.

Table 4. Expected values of (Attractive potential, Repulsive potential energies, kinetic energy and total energy (Hartree-Fock energy) and global comparison.

ATOMS	$-\langle V_{en} \rangle$	$\langle V_{ee} \rangle$	$-\langle V \rangle$	$\langle T \rangle$	$-\langle E_{HF} \rangle$
Ne	192.3 76	5.971 70	186.40 400	93.201 94	93.201 94
[14]	192.3 512	5.970 08	186.38 112	93.19 056	93.190 56
Na	233.27 392	6.582 657	226.69 1	113.34 60	113.34 60
Mg	278.30 5	7.201	271.10 4	135.55 21	135.55 21
Al	327.24 7	7.817 85	319.43	159.71 479	159.71 479
Si	380.2 16	8.436 54	371.77 9	185.88 969	185.88 969

The results of the anticipated values for the two-electron repulsion potential energy $\langle V_{ee} \rangle$ and the nucleus-electron attraction potential energy $\langle V_{en} \rangle$ are shown in Table 4.

The total energy or Hartree-Fock energy expectation values are in line with previously reported findings. Both $\langle V_{en} \rangle$ and $\langle V_{ee} \rangle$ for atoms increase as atomic number increases. All shells start to constrict toward the nucleus because of the stronger attraction between the proton and electrons when the distance between the nucleus-electron and electron-electron reduces.

Both the attraction potential energy and the repulsion potential energy rise as a result. The total potential energy expectation values $\langle V \rangle$ increase in each system because the increase of $\langle V_{en} \rangle$ is higher than that of $\langle V_{ee} \rangle$. In order to keep the atom's entity intact, it has also been found that when Z increases, the energy of attraction increases more than the energy of repulsion.

Moreover, the expectation energy for kinetic energy $\langle T \rangle$ increases when Z increases. The total energy or Hartree-



Fock energy becomes larger when Z increases, which also indicates the $\langle E_{HF} \rangle$ as a function of Z .

In order to sustain the entity of the atom, we observed that the energy of attraction increases more rapidly than the energy of repulsion does as Z increases. The energy of kinetic energy $\langle T \rangle$ increases as Z increases. Likewise, as Z increases, the total energy or Hartree-Fock energy $\langle E_{HF} \rangle$ similarly increases, indicating the function of Z .

Conclusions

According to the results of the current study, the maximum values for the inter-particle distribution function $f(r_{12})$ and the one-particle radial density distribution function $D(r_1)$ increase as Z increases, but their positions decrease as Z increases for some atomic properties for some atoms (Ne, Na, Mg, Al, and Si).

For one-particle expectations for both $\langle r_1^m \rangle$, and the expectation of two particles $\langle r_{12}^m \rangle$ increase when Z increases and when ($m = -2, -1$) and both decrease for ($m = +2, +1$) when $m = \text{zero}$ $\langle r_1^0 \rangle$. This value represents the normalization condition. The expectation values of all the energies must also be specified $\langle V_{en} \rangle$, $\langle V_{ee} \rangle$, $\langle V \rangle$, $\langle T \rangle$ and $\langle E_{HF} \rangle$ a rise as the atomic number rises.

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