

Energies of K-shell for some atoms electrons

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Using the equation approximation of the Hartree-Fock (HF) method, the K-shell energies and atomic properties of the (Neon(Ne), sodium(Na), Magnesium(Mg), Aluminium (Al), and Silicon(Si)) atoms were calculated and compared with available experimental data from comprehensive studies. For atomic numbers in the range $10 \leq Z \leq 14$, the computed atomic energies were thoroughly evaluated. The findings confirmed the reliability and accuracy of the approximations employed in determining these atomic characteristics. The single-particle radial density distribution function $D(r_1)$ and the interparticle distribution function $f(r_{12})$ were among the atomic properties analysed and the associated statistical moments, where n is between -2 and 2, $\langle r_1^n \rangle$ and $\langle r_{12}^n \rangle$. Additionally, several key energy expectation values were computed, including the)electron-electron repulsion potential $\langle V_{ee} \rangle$, the nucleus-electron attraction potential $\langle V_{en} \rangle$, the total potential $\langle V \rangle$, the kinetic $\langle T \rangle$, and the total (Hartree-Fock) $\langle E \rangle$ energies. In conclusion, all values of the examined energies rise as the atomic number increases. Ultimately, all computations were performed in atomic units, and the equations were programmed in Mathematics 2015.

1. Introduction

Electrons and other particles, including the nucleus, its contents, and elementary particles, move according to quantum mechanics, just as planets move according to classical mechanics. Unlike classical systems, however, quantum events are not strictly deterministic, even when initial conditions are known, they are influenced by probabilities, with one notable exception. Quantum mechanics is inherently a statistical framework, treating even individual particles probabilistically. Neither the type of state used to define the system nor the number of states that must be normalized inside it restrict the range of possibilities [1].

To account for the growing number of observations aligning with the wave equation, Wave mechanics was first brought by Schrödinger into the context of preexisting theories, equations, and interpretations. His formulation laid the groundwork for modern understanding of quantum behaviour and established the mathematical tools—particularly the time-independent Schrödinger equation—that are still used today to analyse quantum systems [2].

$$H\psi = E\psi \quad 1$$

The wave function, denoted by ψ , describes the behaviour of the electron. When formulated as Equation (1), the Schrödinger equation takes the form of an eigenvalue equation, which can then be expressed as:[3].

In this case, E stands for the Hamiltonian, or eigenvalue, of the operator H . For an atom with a nuclear charge of (Ze) , the Energy operator is represented by the letter H in Equation (1). The system's state is represented by the corresponding wave function, or eigenfunction, which is linked to a particular energy value[4].

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

The Laplacian operator ∇^2 can be expressed as follows in spherical coordinates (r, θ, ϕ) [5].

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin \theta} \left(\frac{\partial^2}{\partial \phi^2} \right) \quad 3$$

For an atom with N electrons, the Hamiltonian is provided by [6]:

$$\hat{H} = -\frac{\hbar^2}{2m_e} \sum_{i=1}^N \nabla_i^2 + \sum_{i=1}^N \frac{Ze^2}{r_i} + \sum_{i=1}^N \sum_{j>i}^N \frac{e^2}{r_{ij}} \quad 4$$

The kinetic energy operator of the electrons in a system with N electrons is represented by the first term. The second term accounts for the potential energy arising from the electrostatic attraction between the electrons and the positively charged nucleus. The potential energy of each electron depends on its distance from the nucleus, denoted by the variable r_i represents the distance between an electron and the nucleus, which carries a charge of Ze [7]. At an unbounded distance from the nucleus, the potential energy term approaches zero. The condition $j > i$ is applied to avoid double-counting electron–electron repulsion and to prevent expressions such as e^2/r_i from being erroneously included. Since the potential energy of an electron bound within an atom is lower than that of a free electron infinitely distant from the nucleus, it is inherently negative [8]. Due to inter-electronic repulsion terms like e^2/r_{ij} , the Schrödinger equation for multi-electron atoms cannot be separated into simpler, independent components [9].

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To address this complexity, Froese Fischer developed numerical methods for solving the atomic Hartree-Fock equations [10]. Atomic and molecular ionization potentials and electron attachment spectra are commonly calculated using methods like the one-particle Green's function and other many-body procedures. Recent review articles offer comprehensive overviews of these methodologies along with their applications [11].

For all neutral atoms from helium (He) to xenon (Xe), Additionally, upgraded (Roothaan-Hartree-Fock) wave functions have been created for singly charged cations (Li^+ to Cs^+) and stable singly charged anions (H^- to I^-) [12]. Additionally, ions such as Al^+ , Si^{2-} , P^{3+} , and S^{4+} , along with the magnesium atom, have been analysed as part of two-electron atomic systems. Within these studies, atomic characteristics like the radial density function of one electron $D(r_1)$ were calculated using the Hartree-Fock approximation [13]. Another study employed the fragmentation technique to estimate total atomic energies [14].

The wave functions of (oxygen (O), fluorine (F), and neon (Ne)) neutral atoms were explored in the context of two-electron systems [15]. The treatments were given to diatomic compounds like Li_2 , N_2 , F_2 , and Se_2 , in addition to the atoms in the periodic table's group 15, which comprises 7N, 15P, 33As, 51Sb, 83Bi, and 115Uup. The treatments employed three basic techniques: method type, Hamiltonian, and basis-set. [16].

High-precision studies have also examined correlation energies, intra-electronic density distributions, and Coulomb holes for systems such as the lithium cation, helium, the hydride ion, and others involving the critical nuclear charge Z_e required to bind two electrons. These analyses involved calculations using both fully correlated (FC) and Hartree-Fock (HF) wave functions, based on Laguerre-type orbitals [17].

Additionally, research in atomic physics has thoroughly investigated the properties of ten-electron systems—such as neon (Ne), sodium ion (Na^+), magnesium ion (Mg^{2+}), and aluminum ion (Al^{3+})—which are of substantial interest due to their relevance to industrial, nuclear, and other scientific applications [18]. Our study focuses on the atomic dynamics of two-electron systems, including magnesium and ions such as Al^+ , Si^{2+} , P^{3+} , and S^{4+} . Using the Hartree-Fock method, atomic properties like the one-electron radial density function $D(r_1)$ and its expected value were determined. Thus, this work aims to investigate the energy levels of two-electron atomic systems in their respective orbitals.

Calculations

The following discusses several significant atomic characteristics of the ions under study:

a) One particle radial density distribution function $D(r_1)$

The researchers determined the probability of discovering an electron in a spherical shell at a radius of r_1 from the nucleus using the electron radial density distribution function as in equation (5).

The researchers determined the likelihood that an electron would be found inside a spherical shell with a radius of r_1 from the nucleus using the electron radial density distribution function, which is displayed in Equation (5). This analysis provides insights into the probability of an electron being located at a specific distance from the nucleus in the three-dimensional space of the atom [19].

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

b) Inter-particle Distribution Function [20].

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

$$f(r_{12})_{(2s)} = 0.5r_{12} \left[\int_{r_{12}}^{\infty} r_1 \int_{r_1-r_{12}}^{r_1+r_{12}} R_{2s}^2(r_1)R_{2s}^2(r_2)r_2dr_2dr_1 + \int_{r_{12}}^{r_{12}+r_1} r_1 \int_0^{r_{12}-r_1} R_{2s}^2(r_1)R_{2s}^2(r_2)r_2dr_2dr_1 \right] \quad 6$$

The link between and inter-electronic distance r_{12} was ascertained using the coulomb repulsion of two electrons in a k -shell with opposing spins.

c) One –particle expectation value $\langle r_1^m \rangle$

Equations (7) were used to determine the one-particle expectation value [21]:

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

The results of the radial expectation values of $\langle r_1^m \rangle$ and standard deviation are found for m , an integer number that takes values for various values one after the other. $-2 \geq m \geq 2$.

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

We evaluated the inter-particle expectation value using the following equation (8). $\langle r_{12}^m \rangle$ [22]:

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

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

e) The expectation value for energy $\langle E \rangle$

As stated in Equation (9), the kinetic energy (E) and potential energy (V) are added together to determine the system's total energy (E). Equation (10) [23]:

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

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

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2. Results and Discussions:

The mathematics 15 program was used to tabulate and plot the results using the equations:

Table 1. The values of the places that correspond to the distribution function for the atoms under study

Atomic properties	Atoms				
	Ne	Na	Mg	Al	Si
r_1	0.102	0.093	0.086	0.079	0.073
$D_{\max}(r_1)$	5.142	5.673	6.207	6.742	7.277
r_{12}	0.174	0.157	0.144	0.133	0.123
$F_{\max}(r_{12})$	3.771	4.156	4.548	4.94	5.337

The increase in the maximum values of the radial density function $D(r_1)$ indicates that the likelihood of finding the electron increases as the distance between it and the nucleus decreases. with increasing r_1 . These peaks tend to be concentrated closer to the nucleus, which corresponds to the region where the maximum probability density for the system is found. When $D(r_1) = 0$ at $r = 0$, it indicates that the probability of finding the electron at the nucleus is zero—suggesting that the electron is not located within the nucleus. Similarly, when $r \rightarrow \infty$ and $D(r_1) = 0$, it implies that the electron is not found infinitely far from the nucleus, reaffirming that the electron remains bound within the atomic system.

Table 1 illustrates the relationship between the inter-electronic distance (r_{12}) and the peak values of the inter-particle distribution function. As the atomic number Z increases, the maximum of this function also increases, while the average inter-electronic distance decreases. This behaviour is attributed to the stronger electrostatic attraction between the nucleus and electrons as Z rises, which consequently pulls electrons closer together.

Additionally, a direct linear relationship was observed between r_1 and $D_{1\text{ax}}(r_1)$, as well as between r_{12} and $f(r_{12})$. These correlations highlight the structural and probabilistic behaviours of two-electron atomic systems as influenced by increasing nuclear charge.

Table 2. The relationship for the expected values of a single particle for a range of values of m .

Atoms	$\langle r_1^{-2} \rangle$	$\langle r_1^{-1} \rangle$	$\langle r_1^1 \rangle$	$\langle r_1^2 \rangle$
Ne	187.29	9.619	0.16	0.035
[18]	187.2	9.1681	0.158	0.035
[24]	187.2	9.618	0.158	0.034
Na	227.5	10.60	0.145	0.029
[24]	227.5	10.61	0.14	0.027
Mg	271.97	11.6	0.131	0.023
[24]	271.85	11.598	0.131	0.024
Al	320.31	12.586	0.121	0.0197
[24]	320.13	12.589	0.121	0.0195
Si	372.63	13.59	0.112	0.018
[24]	372.38	13.58	0.112	0.0167

Table 2 presents all the atomic systems examined in this study. The results show that the one-particle expectation value $\langle r_1^m \rangle$ increases with rising atomic number, while it decreases as the exponent m becomes more negative (e.g., -2, -1).

This behaviour reflects how the electron density is distributed near the nucleus and is closely related to the expectation value of the electron–nucleus attraction energy, given by $\langle V_{en} \rangle = -Z\langle N \rangle$, where Z is the nuclear charge and N is the number of electrons in the shell. Additionally, for positive values of m (e.g., +1, +2), which correspond to increasing distances between the electron and the nucleus, we observed that the one-particle expectation value $\langle r_1^m \rangle$ initially increases with atomic number Z , but eventually begins to decrease. This trend reflects the stronger nuclear attraction that pulls electrons closer as Z increases, leading to more compact electron distributions.

Table 3. calculations of expectation values $\langle r_1^m \rangle$ for the range of exponents $-2 \leq m \leq 2$.

Atoms	$\langle r_{12}^{-2} \rangle$	$\langle r_{12}^{-1} \rangle$	$\langle r_{12}^1 \rangle$	$\langle r_{12}^2 \rangle$
Ne	61.244	5.973	0.232	0.067
[18]	61.26	5.973	0.23	0.067
Na	74.436	6.584	0.209	0.056
Mg	89.056	7.201	0.193	0.0462
Al	104.95	7.819	0.176	0.0392
Si	122.184	8.437	0.163	0.0336

After looking at the inter-particle expectation values in Table 3, we discovered that the inter-particle expectation value increases with Z , or the repulsion energy between two electrons, when m takes negative values (-2, -1). On the other hand, the inter-particle expectation value falls as Z rises for positive values of m (+1, +2).

Table 4. calculated expectation values based on the previously described formulae for kinetic energy, total (Hartree-Fock) energy, electron-electron repulsion, and atomic attraction.

ATOMS	$-\langle V_{en} \rangle$	$\langle V_{ee} \rangle$	$-\langle V \rangle$	$\langle T \rangle$	$-\langle E_{HF} \rangle$
Ne	192.39	5.99	186.4	93.20	93.20
[18]	192.3625	5.9718	186.3906	93.19	93.1953
[15]	192.4	5.971	186.5	93.19	93.192
Na	233.28	6.583	226.7	113.4	113.35
Mg	278.31	7.201	271.1	135.6	135.56
Al	327.25	7.819	319.43	159.7	159.716
Si	380.22	8.437	371.78	185.9	185.89

One may say that Table 4 displays the expected values for the repulsive energy between two electrons and the nucleus-electron attraction energy. Furthermore, the overall energy, represented by the expected Hartree-Fock values, is consistent with previously published results. With the behaviour of increasing atomic number (Z), both the attractive and repulsive potential energies rise. This trend is attributed to the increasing proton-electron attraction, which causes electron shells to contract closer to the nucleus, thereby reducing the average distances between both nucleus-electron and electron-electron pairs.

Notably, the increase in attraction energy with Z is greater than that of repulsion energy, resulting in an overall rise in the total potential energy expectation values across the examined systems. This stronger attraction also contributes to the structural stability of the atom. Additionally, the kinetic energy expectation value increases with Z , which in turn leads to a corresponding increase in the total (Hartree-Fock) energy as the atomic number grows.

3. Conclusions

The findings of this study reveal that for elements such as Ne, Na, Mg, Al, and Si, the maximum values as atomic number (Z) rises, the peak positions of the one-particle radial density distribution function $D(r_1)$ and the inter-particle distribution function shift closer to the nucleus. For the one-particle expectation values $\langle r_1 m \rangle$, those corresponding to $m = -2$ and $m = -1$ increase with Z , whereas values for $m = +1$ and $m = +2$ decrease. At $m = 0$, the normalization condition holds. Furthermore, all computed energy expectation values—including nucleus-electron attraction, electron-electron repulsion,

kinetic energy, and total Hartree-Fock energy—demonstrated an overall increase with rising atomic number, reflecting enhanced binding and atomic stability.

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