

The isotropic Compton profile in C-like ions: individual shells analysis

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ABSTRACT

The Compton profiles of intra- and inter-shell interactions in the carbon atom were calculated and analyzed using the Roothaan-Hartree-Fock method. To examine the effect of increasing nuclear charge, the study was extended to include selected carbon-like ions: N^+ , O^{2+} , and F^{3+} . All calculations were performed for the ground state and reported in atomic units. A progressive narrowing of the orbitals with increasing nuclear charge appears to reduce the height of the central peak and extend the momentum distribution toward higher momentum values. The crossover points between the profiles were also identified, revealing regions in which the momentum density expands in response to ionization. The Compton profile of intra-shell interactions appears to contain two main regions: one near $q = 0$ and another at intermediate q values. For inter-shell interactions, more than one region was observed, reflecting the contribution of exchange processes. Overall, the findings are in good agreement with the published literature.

Keywords: *Compton profile, Momentum space, Roothaan-Hartree-Fock method*

1 INTRODUCTION

Compton scattering is an inelastic interaction between an incident photon and a bound electron. It was first reported by A. H. Compton in 1923 [1]. This phenomenon provided strong evidence for the quantum nature of X-rays and remains a fundamental concept in the study of light-matter interactions [2]. Compton scattering provides important information about electronic structure, electron correlation, and momentum distributions. Owing to its broad applications, it is widely used in atomic, molecular, condensed-matter, and nuclear physics [3,4].

Several theoretical approaches have been developed to describe Compton scattering. One of the earliest and simplest models is the free-electron approximation (FEA), which was introduced through the Klein-Nishina formulation in 1929 [5]. In this approximation, electrons are treated as free particles, and atomic binding and many-body effects are neglected. Although this model

is widely used because of its analytical simplicity, it does not fully describe the complexity of real atomic systems. To address the limitations of the free-electron model, the impulse approximation (IA) was developed [6]. The IA considers the momentum distribution of bound electrons and expresses the Compton scattering cross section in terms of the Compton profile, $J(p_z)$ [7,8]. Compared with the FEA, the IA provides better agreement with experimental data while maintaining computational practicality [9].

During the past several decades, many theoretical and experimental studies have investigated the Compton profiles of atomic systems. One of the earliest major contributions was by Biggs et al. (1975), who tabulated Compton profiles for a wide range of atomic systems using the IA and accurate Hartree-Fock (HF) wavefunctions for the main shells. These tabulated profiles formed a basis for later theoretical and experimental studies in momentum-space atomic physics [10]. Subsequently,

Brown et al. (1977) calculated the Compton profiles of first-row elements from H to Ne using HF wavefunctions. They found systematic changes in profile shape with increasing atomic number, which were consistent with experimental results, particularly in the low-momentum region where electron-correlation effects are most important [11].

Gadre et al. (1983) calculated the Compton profiles of light atoms using HF wavefunctions and reported good agreement with experimental data. Their study also demonstrated the relationship between the radial distribution of atomic orbitals and the corresponding Compton profile, thereby contributing to the theoretical understanding of the electronic structure of light atoms [12]. Esquivel et al. (1992) used a nonrelativistic HF framework to compute radial and Compton profiles for light atoms, including Li, Be, and B. Their work emphasized the importance of valence orbitals in determining the momentum distribution and examined the relationship between real-space electron density and momentum-space density [13].

Talukdar et al. (2003) studied the effect of electron correlation on the momentum characteristics, moments, and Compton profile of the helium atom. Their simplified analytical method estimated correlation effects using the Hartree–Fock–Roothaan wavefunction. The findings showed good agreement with more advanced theoretical models, indicating that the method provides a practical and convenient approach for evaluating such properties [14]. Al-Sharif et al. (2005) measured the Compton profile of phosphorus using high-energy X-ray scattering and compared the results with HF and density functional theory (DFT) calculations. Their results were similar to DFT predictions in the low-momentum region, whereas differences at higher momentum values reflected correlation effects. The study also showed that second-derivative analysis can help resolve core and valence contributions to the momentum distribution [15].

Khera et al. (2007) used Compton profile analysis to investigate the electronic structure of hafnium. Their experimental findings were compared with theoretical results obtained using DFT and relativistic corrections. The agreement between theory and experiment in several regions confirmed the usefulness of Compton scattering as a tool for studying heavy elements [16]. Alzubadi et al. (2010) studied isotopic Compton profiles of light atoms, including He, Li, Be, and B, using optimized Roothaan–Hartree–Fock (RHF) orbitals. Their theoretical results, particularly for helium, were in good

agreement with experimental data and highlighted the importance of electron–electron interactions at higher momentum values [17].

Ozdogan et al. (2016) derived analytical expressions for momentum density and Compton profiles based on the Hartree-Fock-Roothaan method for atoms with atomic numbers $2 \leq Z \leq 10$. They found that all Compton profiles converge at high momentum transfer values, $q > 3$ a.u., because the inner-shell contributions become similar. However, differences are evident at lower momentum values, $q < 2$ a.u., owing to differences in the treatment of interactions and correlation effects, although valence-electron contributions in this range are relatively small [18]. Mukherjee et al. (2020) examined the effects of confinement on the Compton profiles of hydrogen-like atoms and Onicescu energy using Shannon entropy. They reported that increasing pressure increases momentum uncertainty, whereas decreasing nuclear charge reduces the profile width [19].

Al-Jibbouri (2021) studied radial density and Compton profiles of atomic states with $2 \leq Z \leq 10$ using the configuration interaction (CI) method with a Coulomb-Sturmian basis set. The study emphasized the role of electron correlation in determining momentum-space properties and showed that increasing the number of moments improves the accuracy of nonrelativistic Compton profile calculations [20]. Wan et al. (2023) focused on accurate computation of nonrelativistic Compton profiles of orbitals in hydrogen-like ions. Their procedure agreed with analytical solutions and overcame numerical difficulties associated with complex integrals, allowing highly accurate Compton profiles to be computed over a wide range of momentum values [21]. Mohammed (2024) calculated the Compton profile of aluminum using the renormalized free-atom (RFA) model. The theoretical profiles were compared over the momentum range $p_z = 0 - 7$ a.u. and showed good agreement with experimental measurements [22]. Wan et al. (2025) used the generalized pseudospectral (GPS) method to solve the radial Dirac equation and optimize relativistic wavefunctions through hydrogenic fitting. This approach enabled accurate calculation of relativistic Compton profiles and detailed analysis of relativistic and nuclear-charge-distribution effects on the 1s orbital [23].

Most previous studies have focused on total atomic Compton profiles or experimentally based analyses supported by theoretical methods. However, the individual contributions of each shell and the interactions between different shells in momentum space have received less

attention, despite their importance for understanding how ionization affects orbital overlap and momentum distribution.

In this work, the ground-state Compton profiles of carbon are analyzed using the Roothaan-Hartree-Fock method for selected intra- and inter-shell contributions: $1s_\alpha 1s_\beta$, $2s_\alpha 2s_\beta$, $2p_{x\alpha} 2p_{y\alpha}$, $1s_\alpha 2s_\alpha$, $1s_\alpha 2p_{x\alpha}$ and $2s_\alpha 2p_{x\alpha}$. The atomic data reported by Clementi and Roetti were used [24]. The study was further extended to carbon-like ions, including N^+ , O^{2+} , and F^{3+} . A Wolfram Language code was developed to perform the calculations [25]. Both intra and inter-shell profiles were compared in detail to track profile evolution across the carbon isoelectronic series.

2 THEORETICAL FORMALISM

It is impossible to solve the exact Schrödinger equation for multi-electron atomic systems because of the complexity of electron-electron interactions [26]. To overcome this problem, an approximate approach is used in which the total wavefunction of the system is expressed as follows [27]:

$$\Psi(r_1, r_2, \dots, r_N) = \prod_{i=1}^N \varphi_i(r_i), \quad (1)$$

where,

$$\Pi(r_1, r_2, \dots, r_N) = \varphi_1(r_1) \varphi_2(r_2) \dots \varphi_N(r_N). \quad (2)$$

In this case, r_i will be a space coordinate to electrons and N is the number of electrons. The $\prod_{i=1}^N \varphi(r)$ denotes the multiple-product of the wave function of every electron. However, the Pauli exclusion has been violated in Eq (1). Moreover, the antisymmetric nature of the wavefunction has not been considered [28]. Thus, the antisymmetrized product of occupied spin-orbitals can be used to define the HF wavefunction of a many-electron system [29]:

$$\Psi_{HF}(r_1, r_2, \dots, r_N) = \hat{A} \prod_{i=1}^N \varphi_i(r_i), \quad (3)$$

where, $\hat{A}$ is an antisymmetric operator or antisymmetrizer, written as [30]:

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

Here, $\{\varphi_i(r_i)\}$ are a set of orthogonal spin-orbitals, and $\hat{A}$ is the antisymmetrizing operator. The factor N refers to the number of electrons in the system. The factor $(-1)^P$ takes +1 once the operator $\hat{P}$ conducts even permutations and -1 for odd ones. The Slater-type orbitals (STO) are called spin-orbitals:

$$\varphi_{nlm}(r, \theta, \phi) = N r^{n-1} e^{-\zeta r} Y_{l,m_l}(\theta, \phi), \quad (5)$$

where N is the normalisation factor and equal [31]:

$$N = \frac{(2\zeta)^{n+\frac{1}{2}}}{((2n)!)^{\frac{1}{2}}}. \quad (6)$$

In this case, n is the principal quantum number, r is the distance of the electron from the atomic nucleus, Y_{l,m_l} is spherical harmonic. The orbital exponent ζ is a constant. The Hartree-Fock spin orbital can be described as a linear combination of (STOs). This procedure was suggested by Roothaan in the 1950s [32], so the linear combination of STOs is defined as:

$$\Psi_{HF} = \sum_{i=0}^k c_i \frac{(2\zeta_i)^{n_i+\frac{1}{2}}}{((2n_i)!)^{\frac{1}{2}}} r_i^{n_i-1} e^{-\zeta_i r_i} Y_{l,m_l}(\theta, \phi) \quad (7)$$

It may be expressed in momentum space by the transformation of the position space wavefunction by the Dirac-Fourier technique, which provides the connection between the two representations [33]:

$$\Phi(y_1, y_2, \dots, y_N) = (2\pi)^{-3N/2} \int \Psi_{HF} e^{-i \sum_{k=1}^N p_k \cdot r_k} dr_1 dr_2 \dots dr_N \quad (8)$$

The wavefunction in momentum space $\Phi(y_1, y_2, \dots, y_N)$ is a function of momentum-spin coordinates $y_k = (p_k, \sigma_k)$ in which p_k is the linear momentum of the k^{th} electron. In short, Ψ and Φ are related by $3N$ -dimensional, norm-preserving, Fourier transform. If the r -space wavefunction is constructed from one-electron functions, an isomorphism exists between Ψ and Φ [34].

Density reduced two-particles to obtain physical properties it is determined [35], [36]:

$$\Gamma_{HF}(y_1, y_2) = \binom{N}{2} \int \Phi(y_1, y_2, y_p, \dots, y_q) dy_p, \dots, dy_q \Phi^*(y_1, y_2, y_p, \dots, y_q), \quad (9)$$

where, (N2) is the multiplicative binomial factor. The one-electron momentum density distribution for an atom or ions given by:

$$I(p) = \int \Gamma_{HF}(y_1, y_2) p_1^2 p_2^2 dp_2 d\Omega_1 d\Omega_2 d\sigma_1 d\sigma_2. \quad (10)$$

Here, $d\Omega_k$ represents the angular part of the volume element, whereas $d\sigma_k$ indicates the spin element. The isotropic component of the Compton profile $J(q)$ reads [10]:

$$J(q) = \frac{1}{2} \int_q^\infty \frac{I(p)}{p} dp \quad (11)$$

where, q denotes the momentum transfer vector and $I(p)$ is the spherically averaged one-electron radial momentum distribution [11]. Here, q represents the regular Compton parameter q , which defines the expansion of the Compton line according to the motion of the electron target. It is equal to $q = \frac{cl}{2\lambda_i \sin(\theta)}$. Here l denotes the wavelength distance from the line center, λ represents the incident photon wavelength, and θ is one-half the scattering angle [37]. The wave function normalization leads to an additional condition [20]:

$$\int_{-\infty}^{\infty} J(q) dq = 1 \quad (12)$$

In this paper, Compton profiles were computed using the Hartree-Fock (HF) method. Although HF provides a good first-order approximation, it has certain limitations. The HF method does not explicitly account for electron correlation, which may affect the accuracy of the central peak and the low-momentum region of the Compton profile. In addition, relativistic effects are neglected, although they become more significant with increasing nuclear charge [38]. Therefore, while the main features are well represented by the HF results, more advanced post-HF methods, such as configuration interaction (CI), multiconfiguration Hartree-Fock (MCHF), or Dirac-Fock approaches, could provide improved accuracy [3].

3 RESULTS AND DISCUSSION

In this section, the Compton profiles curves of some elements in the carbon isoelectronic: C, N^{+1}, O^{+2} and F^{+3} . will be discussed. The contributions considered in the analysis include contributions of intra-shells: $1s_\alpha 1s_\beta, 2s_\alpha 2s_\beta$, and $2p_{x\alpha} 2p_{y\alpha}$, and inter-shell: $1s_\alpha 2s_\alpha, 1s_\alpha 2p_{x\alpha}$, and $2s_\alpha 2p_{x\alpha}$. The individual profiles

are studied according to the peak height and the entire shape and tail behavior at increased momentum values. Figure 1 shows the theoretical Compton profiles of the $1s_\alpha 1s_\beta$ shell of a series of isoelectric systems: neutral carbon, and the positively charged ions N^{+1}, O^{+2} , and F^{+3} . As it is evidently shown, the Compton profile peaks at $q = 0$ decrease with increasing ionic charge in a progressive manner. The trend is indicative of the increasing nuclear attraction of the 1s electrons with increasing nuclear charge, leading to increased localization of the radial charge density in position space and, therefore, a wider distribution in the momentum space. As can be seen, in the case of carbon, which has a relatively lower nuclear attraction, the 1s electrons have a higher probability density at low momenta, which produces a sharper and stronger central peak. However, in the case of the F^{+3} ion, the electrons are much more firmly bound resulting in a reduced central peak and a long tail in the high momentum parts. This observation coincides with the overall finding of a past study by Alzubadi et.al [17]: that core electrons play an important role in the high-momentum regime, and that their enhanced binding is reflected in a profile shift towards higher values of q . In addition, the overlap of the profiles at the intermediate momentum range (approximately 3 a. u.) implies the existence of a transitional region where both the characteristics of the valence and the core are identifiable. This discussion supports the results of Alzubadi et al., who found that the large-momentum components of the Compton profile are dominated mainly by core-electron contributions, especially in systems with rising nuclear charge. Thus, the broadening and suppression of the peak with ionization are a clear indication of increasing central electron behavior in the momentum density distribution.

Figure 2 shows the Compton profiles of the $2s_\alpha - 2s_\beta$ shell electrons in C, N^{+1}, O^{+2} , and F^{+3} , indicating how nuclear charge influences the momentum-density distribution of valence electrons. Unlike the 1s orbital, the 2s electrons are more weakly bound and more spatially diffuse. Therefore, changes in nuclear charge strongly affect their momentum distribution.

The neutral carbon profile shows the highest value at $q = 0$, which reflects the generally diffuse nature of the 2s electrons in this system. A noticeable crossover point is observed in the middle momentum region near $q \approx 0.6$ a.u. This crossover represents the point at which the 2s electron momentum densities intersect across the ionic series. It indicates competition between the broader low-momentum distribution of neutral carbon and the more

localized, high-momentum character of the more highly charged ions. The existence of this crossover supports the redistribution of momentum caused by increasing nuclear charge. This interpretation is further supported by the profiles of the more positively charged ions, O^{2+} and F^{3+} , which show lower low- q amplitudes and progressively longer high-momentum tails.

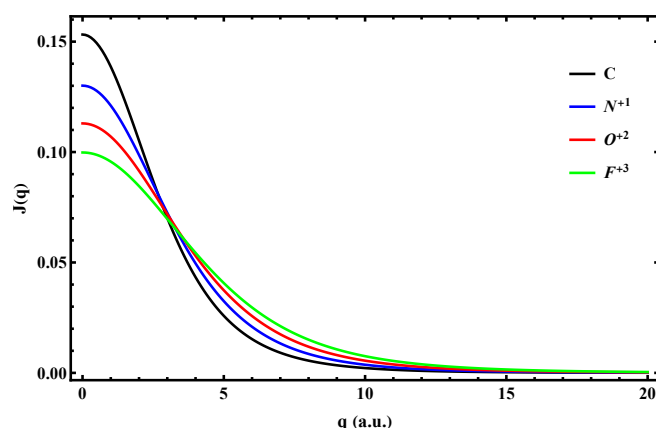


Fig. 1 Compton profile $J(q)$ for the $1s_\alpha 1s_\beta$ intra shell within C-like ions: C , N^{+1} , O^{+2} and F^{+3} .

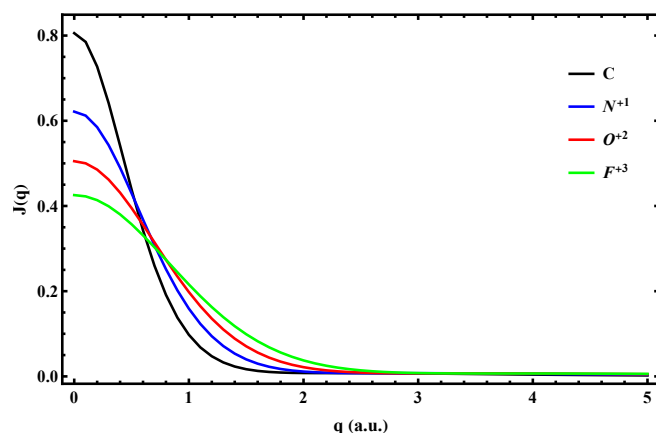


Fig. 2 Compton profile $J(q)$ for the $2s_\alpha 2s_\beta$ intra shell within C-like ions: C , N^{+1} , O^{+2} and F^{+3} .

With increasing nuclear charge from C to F^{3+} , broadening of the momentum distribution is observed, along with a significant decrease in central peak height. This behavior is caused by the stronger electrostatic attraction of the nucleus, which contracts the $2s$ orbital in real space and redistributes electron momentum toward higher values.

Figure 3 shows the Compton profiles of the $2p_x 2p_y$ shell contribution in C , N^{+} , O^{2+} , and F^{3+} . As expected for valence electrons, the profiles exhibit strong peaks in the low-momentum region, and the peak height decreases with increasing nuclear charge. The neutral carbon atom shows the highest central peak, reflecting the relatively delocalized nature of its $2p$ electrons in coordinate space.

Upon ionization, the increased electrostatic potential of the nucleus contracts the $2p$ orbitals, resulting in redistribution of electron momentum. Consequently, broadening of the Compton profile is evident from C to F^{3+} , accompanied by a reduction in peak height. This behavior is typical of valence electrons subjected to stronger binding, where higher kinetic energy leads to longer momentum tails in the $J(q)$ distribution. A crossover region is observed at approximately $q \approx 1.3 - 1.5$ a.u., further confirming the broadening and shift of the Compton profiles with increasing nuclear charge.

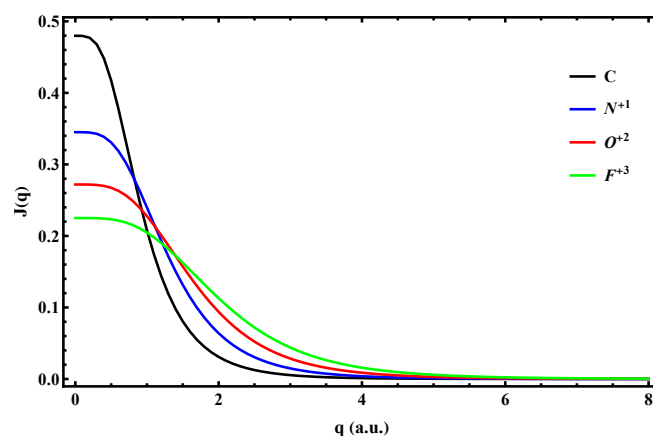


Fig. 3 Compton profile $J(q)$ for the $2p_x 2p_y$ intra shell within C-like ions: C , N^{+1} , O^{+2} and F^{+3} .

Figure 4 illustrates the Compton profiles associated with the inter-shell contribution of the $1s_\alpha 2s_\alpha$ orbitals in the atomic systems C , N^{+} , O^{2+} , and F^{3+} . Inter-shell interactions represent the quantum-mechanical mixing of momentum-density contributions between different shells, and their profiles reflect exchange behavior between core and valence electrons.

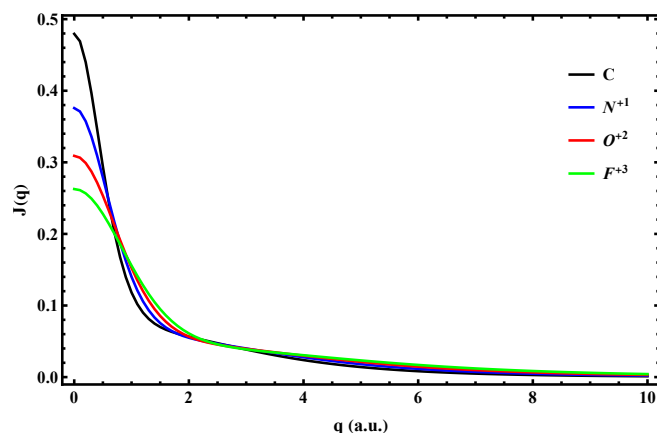


Fig. 4 Compton profile $J(q)$ for the $1s_\alpha 2s_\alpha$ inter shell within C-like ions: C , N^{+1} , O^{+2} and F^{+3} .

In the low-momentum region, $q < 1$ a.u., the central peak of neutral carbon is the highest, indicating a more diffuse spatial distribution of the electron cloud and weaker nuclear confinement. With further ionization, the peak amplitude decreases because of increased localization of the electronic states. The F^{3+} profile is strongly enhanced in the intermediate momentum range, $1 < q < 4$ a.u., indicating significant redistribution of overlapping momentum components. This behavior suggests enhanced inter-shell coupling and contraction of the orbital structure under the stronger nuclear potential. Toward high momentum values, $q > 5$ a.u., the curves gradually converge; however, F^{3+} continues to dominate, indicating a more persistent high-momentum contribution from tightly bound electrons in both shells.

Figure 5 shows the Compton profiles of the inter-shell $1s_\alpha 2p_{x\alpha}$ contribution in the isoelectronic series C , N^+ , O^{2+} , and F^{3+} . The profiles show a clear shift with increasing nuclear charge across the series. The carbon atom exhibits the highest Compton intensity at low momentum, $q = 0$ a.u., whereas F^{3+} shows the lowest intensity in this region. This behavior indicates the larger spatial extent of the electronic wavefunctions in lighter systems, which appears as a more localized momentum distribution around $q \approx 0$.

As nuclear charge increases, both the $1s$ and $2p$ orbitals contract because of stronger electrostatic attraction. This contraction increases the average electron momentum, shifting the Compton profile toward higher momentum values and broadening it in the intermediate- q region. Consequently, the F^{3+} curve overtakes the other profiles in the range $q \approx 0.8 - 2.5$ a.u., indicating stronger momentum components associated with more localized

real-space orbitals.

Interestingly, the curves show two crossover points: one in the low-momentum region, $q < 1.0$ a.u., and another near $q \approx 2.6$ a.u. These crossings mark the boundaries between spatial dominance, where lighter systems dominate near $q \approx 0$, and momentum-space dominance, where the more highly charged ions dominate because of stronger confinement. At the end of the distribution, $q > 3$ a.u., a slight inversion is observed, where the F^{3+} profile falls slightly below the others. This minor effect may be attributed to strong nuclear confinement altering the balance of momentum components at high q values. However, this interpretation should be treated cautiously and verified against the numerical accuracy of the calculated profiles.

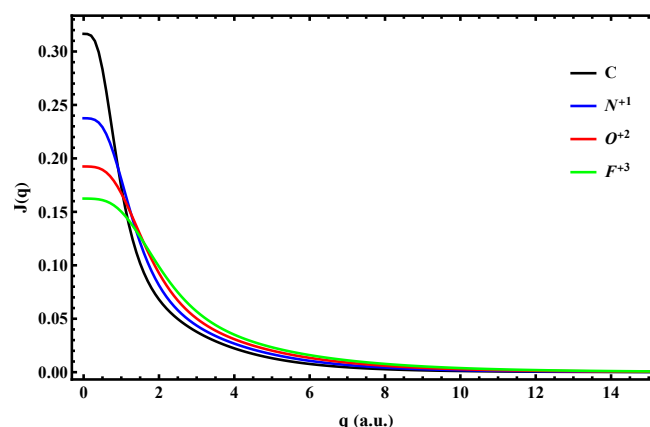


Fig. 5 Compton profile $J(q)$ for the $1s_\alpha 2p_{x\alpha}$ inter shell within C-like ions: C , N^{+1} , O^{+2} and F^{+3} .

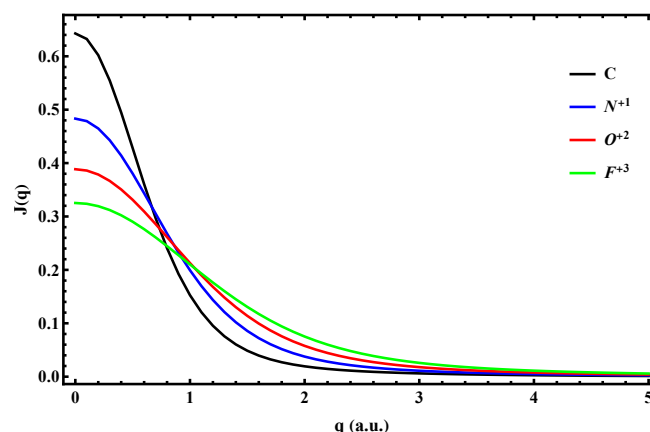


Fig. 6 Compton profile $J(q)$ for the $2s_\alpha 2p_{x\alpha}$ inter shell within C-like ions: C , N^{+1} , O^{+2} and F^{+3} .

The Compton profiles shown in Figure 6 represent the inter-shell interaction between the $2s_\alpha$ and $2p_{x\alpha}$ orbitals for C, N^+ , O^{2+} , and F^{3+} . This configuration represents an intra-valence interaction between orbitals with the same principal quantum number, $n = 2$, but different spatial symmetries, namely the spherically symmetric $2s$ orbital and the directional $2p_x$ orbital.

The carbon atom displays the highest central peak at $q = 0$, indicating a relatively diffuse spatial distribution and weaker nuclear confinement. As the ionic charge increases, the central peak gradually decreases and the Compton profile broadens, indicating redistribution of momentum density toward higher q values. This behavior occurs because the increased nuclear attraction spatially contracts both orbitals and redistributes the overlapping momentum components according to the uncertainty principle. A distinct crossover between the Compton profiles is observed in the intermediate momentum range, $q \approx 0.9 - 3.0$ a.u., where the low-momentum dominance of neutral carbon is gradually replaced by the higher-momentum contribution of more highly charged ions, especially F^{3+} .

The maximum Compton profile values at zero momentum, $J(q = 0)$, for the individual shells of the carbon atom and its isoelectronic series are presented in Table 1. The results show an overall gradual decrease in $J(q = 0)$ with increasing effective nuclear charge, reflecting contraction of the electron distributions in real space and broadening in momentum space. The inner $1s$ shell is less sensitive to increasing nuclear charge, as its $J(0)$ values change only slightly. In contrast, the outer $2s$ and $2p$ shells are more sensitive, showing more pronounced changes in peak values because of their diffuse nature and stronger response to the increased Coulomb attraction. The intermediate behavior observed for inter-shell cases, such as $1s_\alpha 2s_\alpha$ and $1s_\alpha 2p_{x\alpha}$, reflects combined core-valence characteristics and confirms that orbital interactions are also influenced by nuclear-charge effects.

To validate the calculated Compton profiles of the carbon atom, the values obtained for the $1s_\alpha 1s_\beta$, $2s_\alpha 2s_\beta$, and $2p_{x\alpha} 2p_{y\alpha}$ intra-shell contributions were compared with the results reported by Biggs et al. [10]. The comparative plots shown in Figure 7 demonstrate substantial agreement for each intra-shell profile.

It should be noted that, in the original work by Biggs et al., the subshell Compton profiles were calculated under the assumption of spherical symmetry. To ensure consistency with that reference and to provide a fair comparison, the same approximation was applied in

the present calculations for these intra-shell profiles. However, the present work extends the analysis further by including inter-shell contributions.

Table 1 Maximum values of the Compton profile at $q=0$ for individual shells in C-like ions.

Shells	C-like ions	$J(q = 0)$ (a.u.)
$1s_\alpha 1s_\beta$	C	0.153211
	N^{+1}	0.130072
	O^{+2}	0.112969
	F^{+3}	0.099803
$2s_\alpha 2s_\beta$	C	0.805634
	N^{+1}	0.621453
	O^{+2}	0.505117
	F^{+3}	0.425533
$2p_{x\alpha} 2p_{y\alpha}$	C	0.479818
	N^{+1}	0.345044
	O^{+2}	0.271909
	F^{+3}	0.22502
$1s_\alpha 2s_\alpha$	C	0.479422
	N^{+1}	0.375762
	O^{+2}	0.309043
	F^{+3}	0.262668
$1s_\alpha 2p_{x\alpha}$	C	0.316514
	N^{+1}	0.237558
	O^{+2}	0.192439
	F^{+3}	0.162411
$2s_\alpha 2p_{x\alpha}$	C	0.642726
	N^{+1}	0.483248
	O^{+2}	0.388513
	F^{+3}	0.325277

4 CONCLUSION

A theoretical study of the Compton profiles of individual shells of the carbon atom and selected ions in its isoelectronic series, namely N^+ , O^{2+} , and F^{3+} , was performed in the ground state using the Roothaan-Hartree-Fock (RHF) method. The study highlights the influence of ionization on orbital contraction and the redistribution of electron momentum. The clear distinction between intra-shell and inter-shell contributions allowed the observation of fine region-like structures that are not easily resolved in total Compton profiles. Good agreement with previously published data was also obtained, supporting the reliability of the present results. Since Compton profile analysis remains an active area of research, future

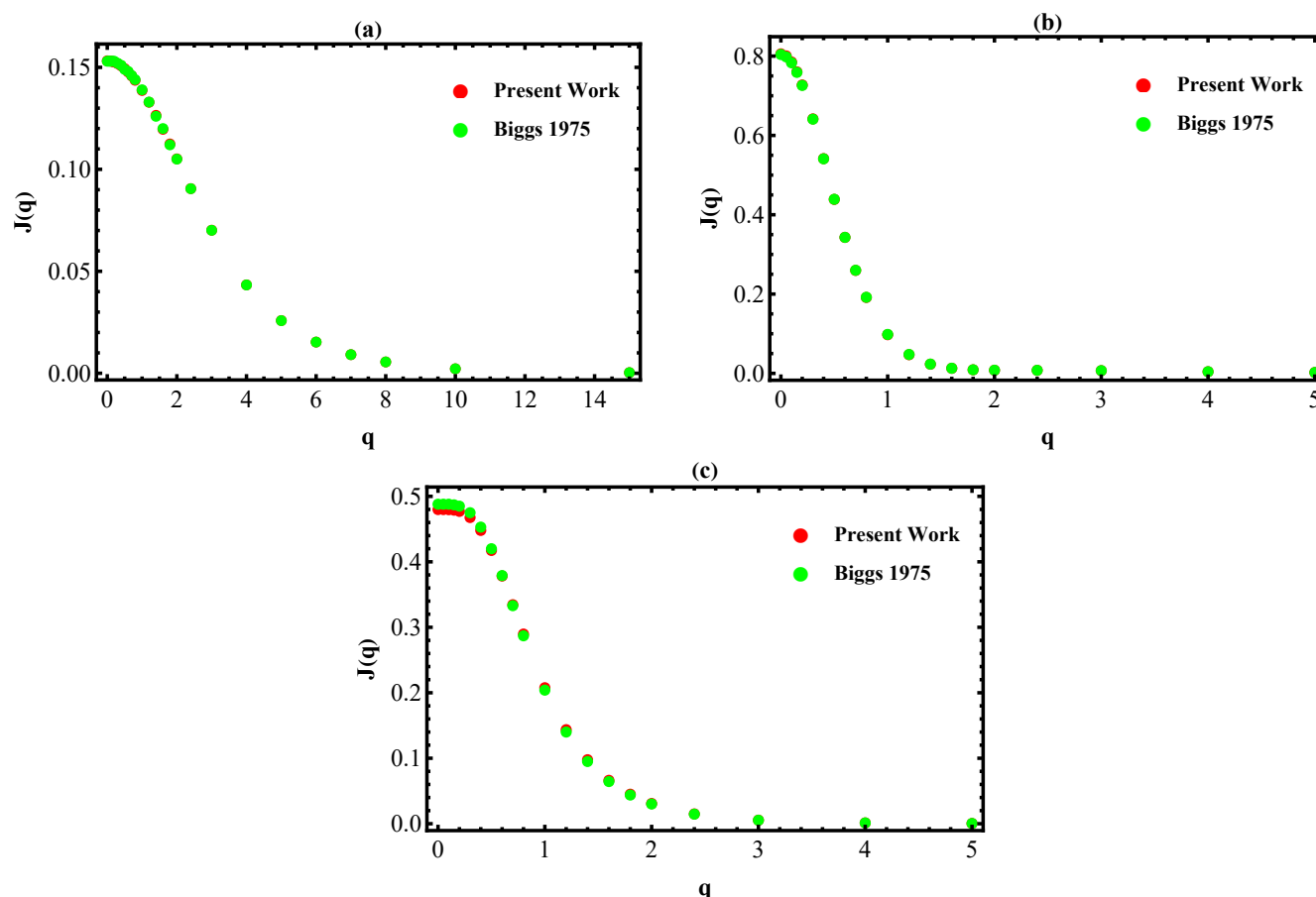


Fig. 7 Comparison between the Compton profile calculated in the present work for neutral carbon in the ground state for: (a) $1s_\alpha 1s_\beta$, (b) $2s_\alpha 2s_\beta$, (c) $2p_{x\alpha} 2p_{y\alpha}$ and those reported by Biggs (1975) [10].

work may extend this approach to excited states and individual-shell contributions in atomic systems using correlated wavefunctions.

Author contributions

R.A. performed the calculations, generated the figures, and wrote the manuscript. W.A. suggested the topic, developed the original codes, edited the manuscript, provided academic supervision and general guidance throughout the research process.

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Data availability

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DECLARATIONS

Conflict of interest

The authors declare no competing interests

Consent to publish

N/A

Ethical approval

N/A

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