



Compton Profile of $1s^2$ -State for $2 \leq Z \leq 10$

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Electron momentum distributions show a view of electronic structure that supplement the radial density function. The radial density function in momentum space, moments, and Compton profile of $1s^2$ -state for $2 \leq Z \leq 10$ are considered by configuration interaction (CI) wave function based on Coulomb Sturmian basis function. The realized results agree with the literature for Compton profiles of these atoms.

Keywords: Momentum space, Configuration interaction wave function, Compton profile

1 Introduction

Configuration interaction (CI) is the simplest method of describing electron-electron correlation in the theory of atoms and molecules¹. CI wave function can be mentioned linearly as an anti-symmetrized of one-electron combination function²⁻⁴. It considers the interaction of excited together with ground-state wave functions. However, the exciting wave function allows further useful independence to the total CI method that realizes the optimal energy⁵. Due to the electron's configuration in the orbital basis set, CI has two kinds. The first refers that all electrons are set in all possible ways (consistent with symmetry requirement) in a complete (infinite) orbital basis set (this is impossible). The second represents full CI that all electrons order in all possible ways for a finite orbital basis set.

The radial and angular expectation values investigated in Refs.^{6,7} for concerning configuration interaction wave function which based on Slater-type orbitals basis set for He-like ions. Ref.⁸ studied the configuration interaction calculations of the ground and excited states energy levels of He-isoelectronic series.

The Compton scattering operation in the electromagnetic field is the dissipation between the electron in bound state and an incident photon. It has paved the way of significant and peculiar electromagnetic processes in Physics. This approach was first investigated by Compton through which proven successfully by the nature of X-rays⁹. The experimental and theoretical studies of atomic

Compton scattering allow the details on the electron correlations, electron momentum distributions¹⁰. The physical properties of atoms recognized in momentum space and linked to the experimental studies.

Therefore, the momentum density $\Pi(\mathbf{p})$ and Compton profile estimated within CI¹¹⁻¹⁴, correlated¹⁵⁻¹⁸, Hartree-Fock^{14, 19-27}, density functional theory (DFT)²⁸, and Dirac-Hartree-Fock formalism²⁹ wave functions, respectively. The momentum density can be derived by the Fourier transformation of position space wave function. It has been analytically derived from a position wave function^{17, 30,31} and provided two-electron systems wave function in momentum space. The momentum radial density discussed in Ref.¹⁵ for He-like ions by adding the exponential correlation terms. Refs.^{32,33} have been studied the extracule density in different space for He-Ne atoms by considering correlated wave function. The electronic extracule expectation value in different spaces discussed in Ref.³⁴ within Hartree-Fock framework. The hydride examined and discussed in Ref.³⁵ by using the self-consistent field (SCF) and CI wave functions. It has found a tiny crucial discrepancy with the SCF as mentioned in Ref.³⁶. Within the Hartree-Fock wave function, the inter-electronic moments calculated in Ref.³⁷ for both position and momentum spaces of atomic systems. To this end, the momentum properties of the $1s^2$ -state for $2 \leq Z \leq 10$ atoms studied by considering the configuration interaction wave function in the momentum-space wave function that can be calculated via Fourier transformation of the position-space wave function. The paper is organized as

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follows, in Sec. 2, the position-space wave function discussed analyzing the wave function in momentum-space and studied the radial density function Π(p), the expectation values < pⁿ > as well as the Compton profile J(q). It discusses the findings results in Sec. 3 and compares them with the previous literature. Finally, Section 4 presents the concluded results.

2 Methodology

The CI wave function can be defined by Slater determinants,

$$\psi_{CI} = \sum_i C_i \Phi_i \quad \dots (1)$$

the constant C_i is measured by minimizing the energy, while Φ_i is the product of antisymmetrized one-electron functions³⁸⁻⁴⁰. For 1s²-state, the CI is considered linearly as a single Slater determinant combination with 15th term of s-states⁵, yielding,

$$\psi_{CI} = (\xi^2 \Psi) = \frac{1}{\sqrt{2}} |\xi(1)s_1 \Psi(2)s_2| \quad \dots (2)$$

$$|\xi(1)s_1 \Psi(2)s_2| = \xi(1)s_1 \Psi(2)s_2 - \xi(2)s_1 \Psi(1)s_2$$

The one-electron basis set is related to Coulomb Sturmian function^{41,42},

$$R(\eta, r) = \sqrt{\frac{\eta \Gamma(n-l)}{n \Gamma(n+l+1)}} (2\eta r) e^{-\eta r} (2\eta r)^l \mathcal{L}_{n-l-1}^{2l+1}(2\eta r), \dots (3)$$

with the associated Laguerre polynomial L, Γ(x) refers to gamma function, η is orbital exponent, while n and l are interrelated principal and angular quantum numbers, respectively. The s-functions were ultimately based on 1s, 2s, 1s', 2s', 3s', expect for 3s function, its identical Hartree-Fock basis set function for the helium isoelectronic series. By integrating Eq. (2) over all spins and inserting Eq. (3) into Eq. (2), it is obtained

$$\psi_{CI} = \frac{1}{\sqrt{2}} (R_\zeta(1)R_\psi(2) - R_\zeta(2)R_\psi(1)) \quad \dots (4)$$

The ψ(p) is obtained via

$$\psi(p) = (2\pi)^{-3/2} \int \psi(r)_{CI} e^{-ip \cdot r} dr \quad \dots (5)$$

By using Eq. (4), the radial momentum-space density function Π(p) of wave function ψ(p, p₂, ..., p_N) is given by

$$\Pi(p) = \int |\psi(p, p_2, \dots, p_N)|^2 ds_1 d\theta_1 d\phi_1 dp_2 \dots dp_N \quad \dots (6)$$

Indeed, the momentum moment is defined as

$$\langle p^n \rangle = \int dp p^n \Pi(p) \quad \dots (7)$$

Compton profile is concerning to the radial density function in momentum-space^{43,44} and is defined by

$$\mathcal{J}(q) = \frac{1}{2} \int_q^\infty \Pi(p) p^{-1} dp \quad \dots (8)$$

J(q) represents by the regular Compton parameter q, which defined the expanding of the Compton line according to the motion of the electron target. Its equal to q = cl/2λisin(θ). Here l denotes the wavelength distance from the line center, λ represents the incident photon wavelength with θ one-half the scattering angle. The wave function normalization leads to additional condition

$$\int_{-\infty}^\infty dq \mathcal{J}(q) = 1 \quad \dots (10)$$

3 Result and Discussion

The analysis of 1s²-state for 2 ≤ Z ≤ 10 is performed using 15th term of CI wave function.

Π(p), < pⁿ >, and J(q) examined by CI wave function based on Coulomb Sturmian basis function.

Figure 1 shows the radial density function Π(p) as a function of p of 1s²-state for 2 ≤ Z ≤ 10. black, blue, green curves represent the CI in Eq. (1), correlated trial, and RHF⁴⁵ wave functions, respectively. It is read that for a large value of p the maxima shifting gradually by increasing the electron's kinetic energy. This is clear as one realizes that the electron has tiny potential energy and a lot of kinetic energy close to the nucleus, while the state is inverted far away. In the case of He atom, the Π(p)

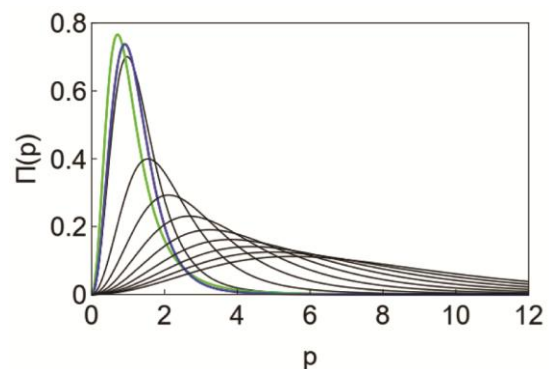


Fig. 1 — The radial density functions Π(p) of 1s²-state for 2 ≤ Z ≤ 10. black, blue, green curves are corresponded to CI Eq. (1), correlated trial of Ref.³⁰ and RHF of Ref.⁴⁵ wave functions, respectively.

is smaller in CI wave function than correlated trial wave function of Ref.³⁰ (black curve) and HFR obtained via of Ref.⁴⁵ basis set (green curve) due to the electron correlation and the separation between two electrons of this shell by setting each electron in a virtual state (configuration).

Table 1 discusses the expectation value $\langle p^n \rangle$ of $1s^2$ -state for $2 \leq Z \leq 10$ for different n . Indeed, $\langle p^n \rangle$ presents how the probability distribution is closer to the nucleus at $n = 2$. Whereas at $n = -2$, shows the probability distribution in the outer region of the charge clouds. $\langle p^n \rangle$ increases at $n = 2$, 1 via increasing Z which refers to increase the probability of finding the electron near the nucleus. On the other hand, the value of $\langle p^n \rangle$ decreases by increasing Z according to the weak attraction force between the electrons and the nucleus in the outer shells. By increasing the effective nuclear charge, the average probability size of the electron in momentum space is increased. The results have a good agreement in comparison results of Ref.⁴⁶.

Compton profile $\mathcal{J}(q)$ had shown in Fig. 2 for $1s^2$ -state for $2 \leq Z \leq 10$ obtained from the spherically

Table — 1 The expectation value $\langle p^n \rangle$ for different n

$1s^2$	$\langle p^{-2} \rangle$	$\langle p^{-1} \rangle$	$\langle p^1 \rangle$	$\langle p^2 \rangle$
He	1.7558	1.0060	1.4323	2.8476
Li	0.7205	0.6381	2.2712	7.1730
Be	0.3808	0.4660	3.1028	13.3784
B	0.2355	0.3668	3.9396	21.5645
C	0.1603	0.3028	4.7713	31.6297
N	0.1158	0.2574	5.6112	43.7426
O	0.0877	0.2240	6.4469	57.7404
F	0.0687	0.1983	7.2823	73.6724
Ne	0.0552	0.1779	8.1174	91.5383

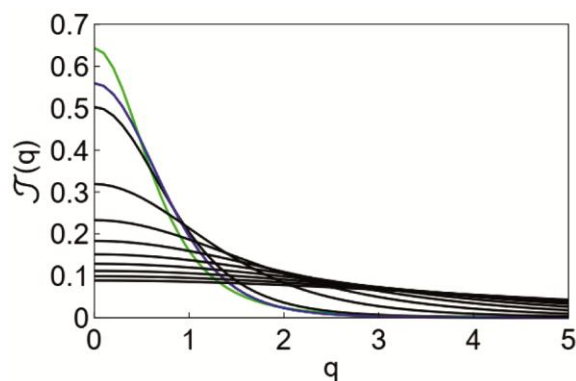


Fig. 2 — Compton profile of $1s^2$ -state for $2 \leq Z \leq 10$. black, blue, green curves correspond to CI Eq. (1), the correlated trial of Ref.³⁰ and RHF of Ref.⁴⁵ wave functions, respectively.

averaged CI wave function Eq. (1). To this end, it shows that the inner and valence electrons of atoms are involved by momentum ranges. The scattering behavior is incoherent which allows the electrons further representations to the cross-section of the scattering. Hence the $\mathcal{J}(q)$ is the sum of the profiles of different occupied states. One might look for the $\mathcal{J}(q)$ that showed how the electrons are strongly bounded, *i.e.*, almost a parabolic profile is provided by free electrons from the valence shell. Afterwards, a flat and wide profile is constructed by bound electrons from the core, as clearly appear in Fig. 2. Because of that, it is possible to gain much higher precision for the sharp momentum spectrum of the weakly bound electrons without worrying too much about a very accurate momentum distribution for the core electrons. It is noticed that the $\mathcal{J}(q)$ becomes sharper while it departs away from the nucleus.

Furthermore, it is useful to find out that almost all the contributions to $\mathcal{J}(q)$ are approached from the core electrons in the high momentum region wherever the electrons are closely confined to the nucleus. The maximum values of $\mathcal{J}(q)$ occur at $q = 0$, which indicates a maximum Compton scattering of X-ray read at $\theta = 90$. In particular, $\mathcal{J}(0) = 0.5 \langle p^{-1} \rangle$. For different q , the energy transferred is not quite larger than the binding energy, Eq. (8) is not reasonable and the $\mathcal{J}(q)$ in the Table 1 must be adjusted. Due to the electron correlation. It's clear that $\mathcal{J}(q)$ of He atom is smaller in CI wave function than the correlated trial wave function of Ref.³⁰ (black curve) and HFR obtained via of Ref.⁴⁵ basis set (green curve). The Compton profile results are agreed with the literature Refs.^{14,22}. It is pointed out that the orbital with quantum number Compton profile has a specific number such that $n - l$. The momentum distribution can be further scattered for the ion with larger Z for given n, l , which denotes that the orbitals subscribe extra momentum distribution for atom or ion with small Z close to $q = 0$ a.u., whereas larger Z the distribution in the high momentum is influenced

4 Conclusions

This paper studied the radial density function $\Pi(p)$ in momentum-space, the expectation values $\langle p^n \rangle$ as well as Compton profile $\mathcal{J}(q)$ of $1s^2$ -state for $2 \leq Z \leq 10$ by using CI wave function based on Coulomb Sturmian basis function. The electron

correlation effects are quite significant in achieving the precise radial density function. The most-reported correlation is formed in the vicinity of the valence region at tiny momentum values of Eq. (4), showing how the electron correlation is affected in momentum-space. One indicates the precision of the physical system used in our study by contrasting our theoretical data with the available literature. The information of $\langle p^n \rangle$ knowledge allowed for the realization of detailed upper and lower limits of momentum densities. It has also improved accuracy as the number of moments is raised. Since the Compton profile is stills a field of active research, the next step is to consider Compton profile for the ground state and excited state of some atomic system using multi-configuration interaction wave function.

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