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Study of the Information Content of He-Ne atoms

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1 Introduction

This report investigates the ground-state wavefunctions of the elements from helium (He, $Z = 2$) to neon (Ne, $Z = 10$) in the periodic table. These wavefunctions allow us to compute the position-space density $\rho(r)$ and momentum-space density $n(k)$, which serve as the basis for evaluating the system's information-theoretic properties using Shannon entropy and related measures (e.g., Onicescu and Fisher information). By analyzing these entropic quantities, we explore their correlation with experimentally measurable physical observables, such as the ionization potential. Additionally, we examine the radial electron probability distribution to further characterize the electronic structure of these atoms. This study aims to provide insights into the relationship between quantum-mechanical descriptions and information-theoretic metrics in atomic systems.

1.1 Roothaan-Hartree Fock Wave Functions

The Roothaan-Hartree-Fock method (RHF) [1] provides an analytical framework for solving the self-consistent-field (SCF) equations of atomic wave functions within the non-relativistic Schrödinger formalism. Unlike numerical Hartree-Fock approaches, RHF expands the radial part of each atomic orbital, $R_{nl}(r)$, as a finite linear combination of Slater-type orbitals (STOs), which serve as primitive basis functions. These STOs are defined by their exponential decay and power-law dependence on the radial coordinate, offering a balance between computational efficiency and physical accuracy. The expansion takes the form:

$$R_{nl}(r) = \sum_j C_{jnl} S_{jl}(r) \quad (1)$$

where C_{jnl} are the orbital expansion coefficients, determined by the Roothaan-Hartree-Fock calculations of Bunge et al. [1], and S_{jl} are the normalized Slater-type orbitals (STOs):

$$S_{jl}(r) = N_{jl} r^{n_{jl}-1} e^{-Z_{jl}r} \quad (2)$$

with n_{jl} as the principal quantum number, Z_{jl} the orbital exponent, l the azimuthal quantum number and N_{jl} the normalization constant:

$$N_{jl} = \frac{(2Z_{jl})^{n_{jl}+\frac{1}{2}}}{\sqrt{(2n_{jl})!}} \quad (3)$$

1.2 Momentum-Space Representation and Shannon Entropy

The Roothaan-Hartree-Fock wave functions, expressed in position space as:

$$\phi_i(r) = \phi_{nlm}(r) = R_{nl}(r) Y_{lm}(\Omega_r) \quad (4)$$

have a corresponding momentum-space representation obtained via Fourier transform [2]:

$$\tilde{\phi}_i(k) = \tilde{\phi}_{nlm}(k) = \tilde{R}_{nl}(k) Y_{lm}(\Omega_k) \quad (5)$$

where $\tilde{R}_{nl}(k)$ is the radial momentum wave function, related to $R_{nl}(r)$ through the spherical Bessel transform:

$$\tilde{R}_{nl}(r) = 4\pi \int_0^\infty r'^2 R_{nl}(r') j_l(kr) dr' \quad (6)$$

The electron density distributions in position and momentum spaces, $\rho(r)$ and $n(k)$, are derived from the squared moduli of $\phi(r)$ and $\tilde{\phi}_i(k)$, respectively. For spherically averaged systems, these reduce to:

$$\rho(r) = \frac{1}{4\pi Z} \sum_i A_i |R_{nl}(r)|^2, \quad n(k) = \frac{1}{4\pi Z} \sum_i A_i |\tilde{R}_{nl}(k)|^2 \quad (7)$$

1.3 Information-Theoretic Measures

To quantify the delocalization and information content of atomic systems, we employ the Shannon entropy in position space (S_r) and momentum space (S_k):

$$S_r = - \int \rho(r) \ln \rho(r) dr = -4\pi \int_0^\infty \rho(r) \ln \rho(r) r^2 dr \quad (8)$$

$$S_k = - \int n(k) \ln n(k) dk = -4\pi \int_0^\infty n(k) \ln n(k) k^2 dk \quad (9)$$

Here, S_r reflects the spatial localization of electrons (minimized for compact distributions, for example near the nucleus), while S_k characterizes momentum-space delocalization. The total Shannon entropy,

$$S_{\text{total}} = S_r + S_k \quad (10)$$

obeys rigorous inequalities $S_{\min} \leq S_{\text{total}} \leq S_{\max}$, where $S_{\min} = 3(1 + \ln \pi)$ and S_{\max} depends on $\langle r^2 \rangle$ and kinetic energy.

1.4 Connection to RHF Framework

The RHF expansion of $R_{nl}(r)$ in Slater-type orbitals (STOs) (Eq. 1) ensures high accuracy in calculating $\rho(r)$ and $n(k)$, enabling precise evaluation of S_r , S_k and S_{total} . Notably, the universal relation $S_{\text{total}} = a + b \ln Z$ is validated using RHF densities, with shell effects manifesting as local minima at closed-shell configurations.

1.5 Onicescu Information Energy and Landsberg's Order Parameter

The information-theoretic analysis extends beyond Shannon entropy to include Onicescu's information energy E , extended for a three-dimensional spherically symmetric density distribution $\rho(r)$ as

$$E_r = \int_0^\infty 4\pi r^2 \rho^2(r) dr \quad (\text{position space}) \quad (11)$$

$$E_k = \int_0^\infty 4\pi k^2 n^2(k) dk \quad (\text{momentum space}) \quad (12)$$

$$(13)$$

exhibits an inverse dimensional relationship between position and momentum spaces. While E_r carries dimensions of inverse volume, E_k has dimensions of volume, making their product $E_r E_k$ a dimensionless measure of total information concentration in the system. To compare this with Shannon entropy S , we use the inverse:

$$O = \frac{1}{E_r E_k} \quad (14)$$

Landsberg's order parameter Ω bridges entropy and complexity by comparing the actual Shannon entropy S to its maximum possible value S_{\max} for the system:

$$\Omega = 1 - \frac{S}{S_{\max}} \quad (15)$$

Here, $\Omega \rightarrow 1$ indicates perfect order, while $\Omega \rightarrow 0$ corresponds to complete disorder.

1.6 Ionization Potential Analysis

The first ionization potential (IP) represents the energy required to remove the outermost electron from an atom. The IP values used here (in eV for He–Ne) are from the NIST Atomic Spectra Database [3], which serves as the standard reference for atomic properties.

2 Computational Methodology - Results

The calculations begin with the Roothaan-Hartree-Fock wavefunctions expressed as linear combinations of Slater-type orbitals (STOs). For helium ($Z = 2$), the ground-state wavefunction is constructed from four STOs with optimized coefficients and exponents, as provided by Bunge et al. [1]. The electron density in position space, $\rho(r)$, and momentum space, $n(k)$, are derived by squaring the respective wavefunctions and accounting for the spherical symmetry and electron count (Eq. 7).

After ensuring $\int \rho(r)dr = \int n(k)dk = 1$ via numerical integration, we proceed to calculate the Shannon entropies in both position (S_r) and momentum spaces (S_k) and their sum (S_{total}). Finally, Onicescu's dimensionless information energy (O) and Landsberg's entropy deficiency (Ω) are calculated from the expectation values $\langle r^2 \rangle$ and $\langle k^2 \rangle$, linking information-theoretic measures to the spatial and momentum dispersion of the electron density.

Following the calculations, the $\rho(r)$ and $n(k)$ are plotted for r and k values in $\in [0, 4]$ atomic units, showcasing the characteristic decay profiles and momentum distributions for each element. While the core methodology remains consistent across all atoms, the orbital configurations introduce element-specific features in these distributions.

The derived Shannon entropies (S_r , S_k , S_{total}) are then analyzed as functions of atomic number Z , with their trends compared to experimental first ionization potentials.

The entropy data from Ref. [2] (Table I) was used to investigate the relationship between Shannon entropy S and atomic number Z . An exponential model $Z = ae^{bS} + c$ was fitted to the data, revealing a strong scaling trend.

2.1 He, $Z = 2$

Orbital configuration: $1s^2$

S_r	S_k	S	S_{max}	Ω	O
2.69851	3.91342	6.61193	7.04930	0.06204	100.36133

Table 1: Information Measures for Helium

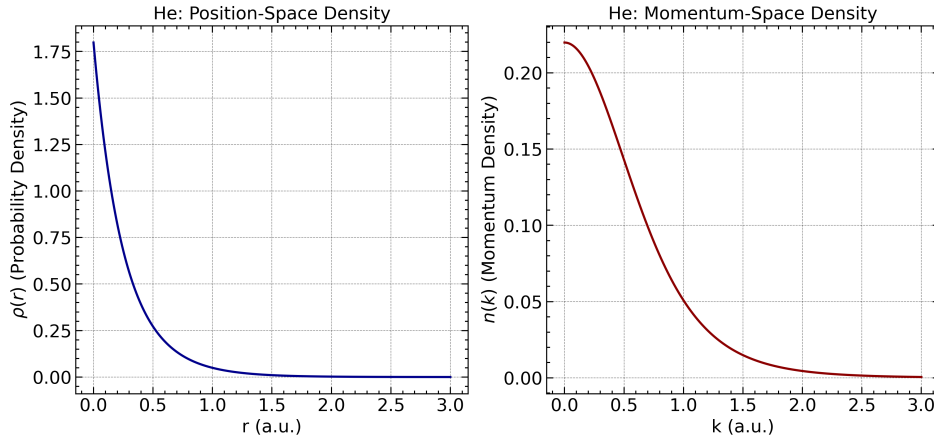


Figure 1: Density distribution of Helium, on position-space and momentum-space

2.2 Li, $Z = 3$

Orbital configuration: $1s^2 2s^1$

S_r	S_k	S	S_{max}	Ω	O
3.70144	3.99682	7.69826	10.35784	0.25677	9.15713

Table 2: Information Measures for Lithium

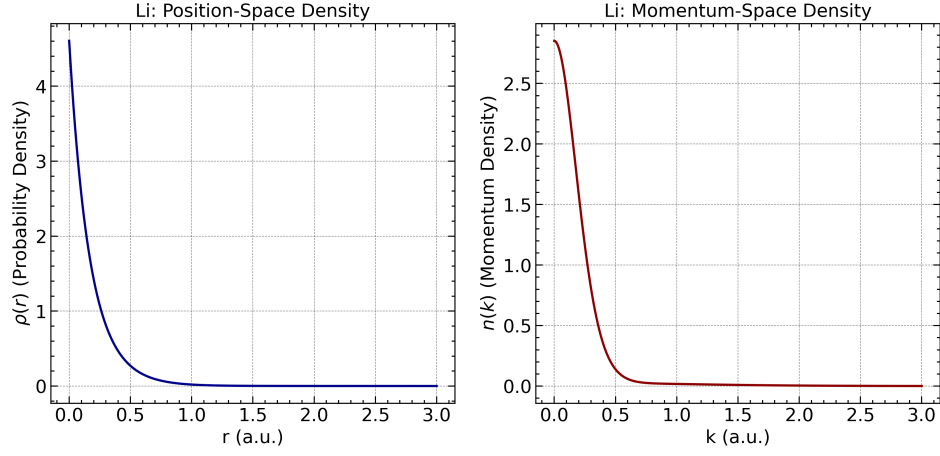


Figure 2: Density distribution of Lithium, on position-space and momentum-space

2.3 Be, $Z = 4$

Orbital configuration: $1s^2 2s^2$

S_r	S_k	S	S_{max}	Ω	O
3.6286	4.19019	7.81405	10.39503	0.24823	8.45434

Table 3: Information Measures for Beryllium

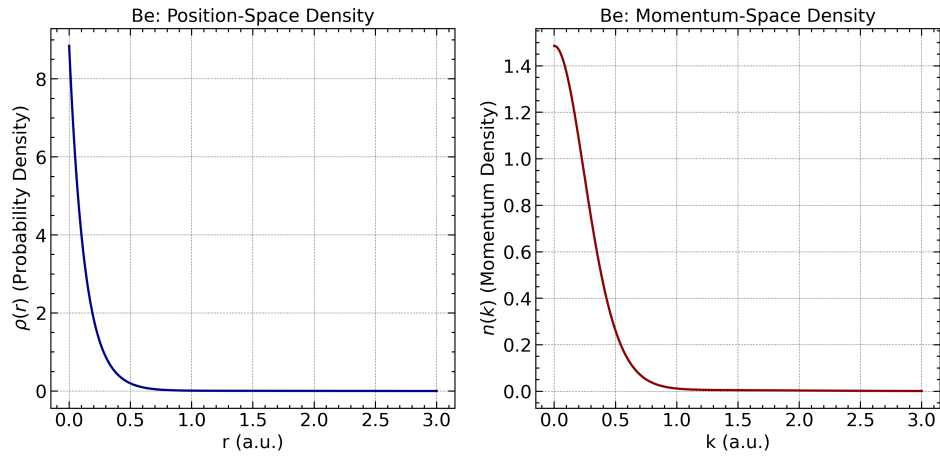


Figure 3: Density distribution of Beryllium, on position-space and momentum-space

2.4 B, $Z = 5$

Orbital configuration: $1s^2 2s^2 2p^1$

S_r	S_k	S	S_{max}	Ω	O
3.40545	4.70590	8.11135	10.37384	0.21810	15.96532

Table 4: Information Measures for Boron

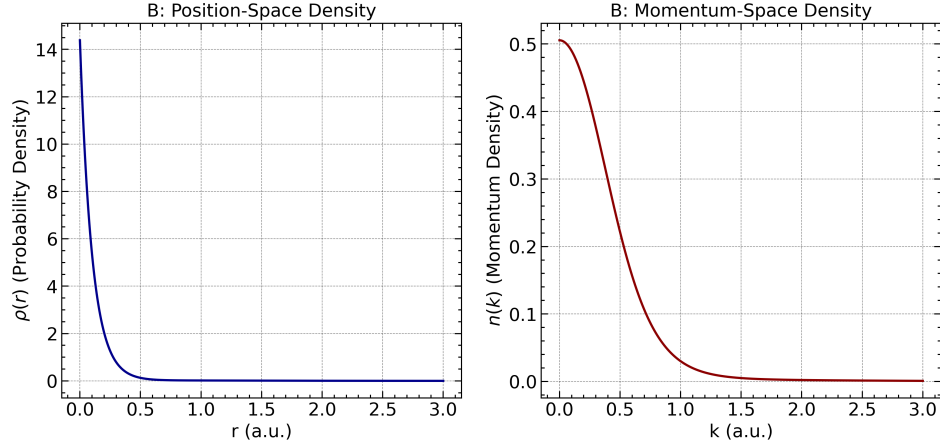


Figure 4: Density distribution of Boron, on position-space and momentum-space

2.5 C, $Z = 6$

Orbital configuration: $1s^2 2s^2 2p^2$

S_r	S_k	S	S_{max}	Ω	O
3.10602	5.15658	8.26260	10.26242	0.19487	25.71213

Table 5: Information Measures for Carbon

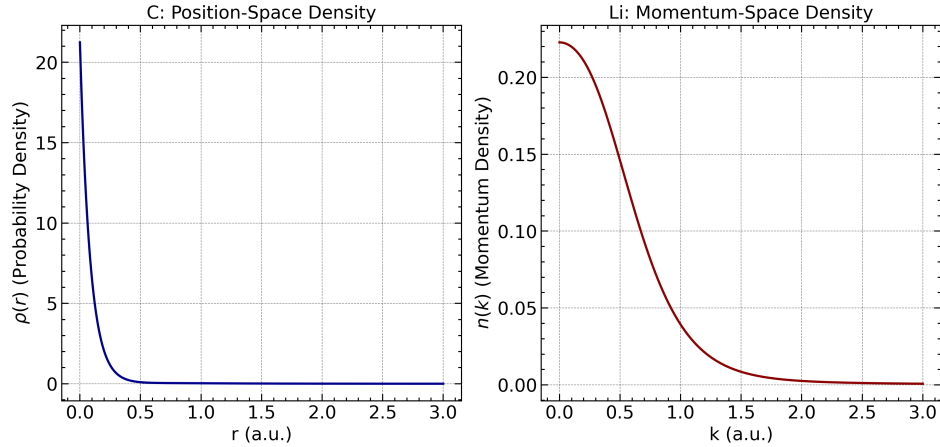


Figure 5: Density distribution of Carbon, on position-space and momentum-space

2.6 N, $Z = 7$

Orbital configuration: $1s^2 2s^2 2p^3$

S_r	S_k	S	S_{max}	Ω	O
2.80169	5.54934	8.35103	10.15197	0.17740	37.43198

Table 6: Information Measures for Nitrogen

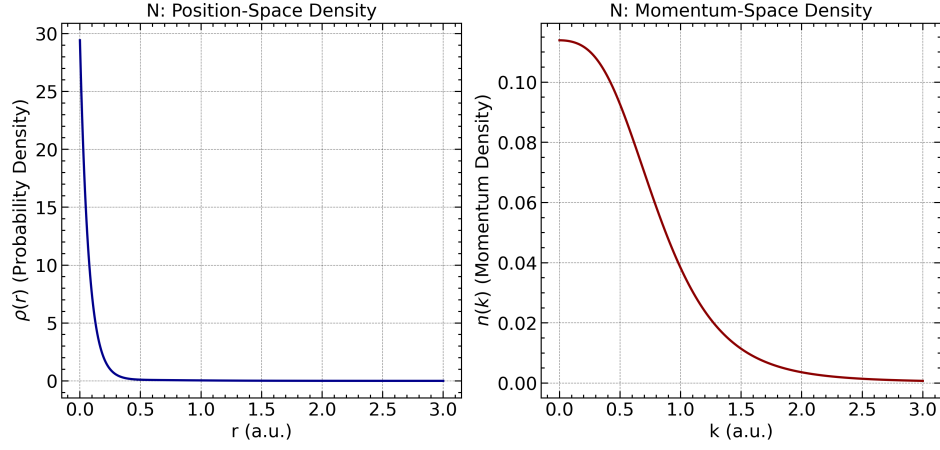


Figure 6: Density distribution of Nitrogen, on position-space and momentum-space

2.7 O, $Z = 8$

Orbital configuration: $1s^2 2s^2 2p^4$

S_r	S_k	S	S_{max}	Ω	O
2.55054	5.86735	8.41789	10.11127	0.16747	48.48377

Table 7: Information Measures for Oxygen

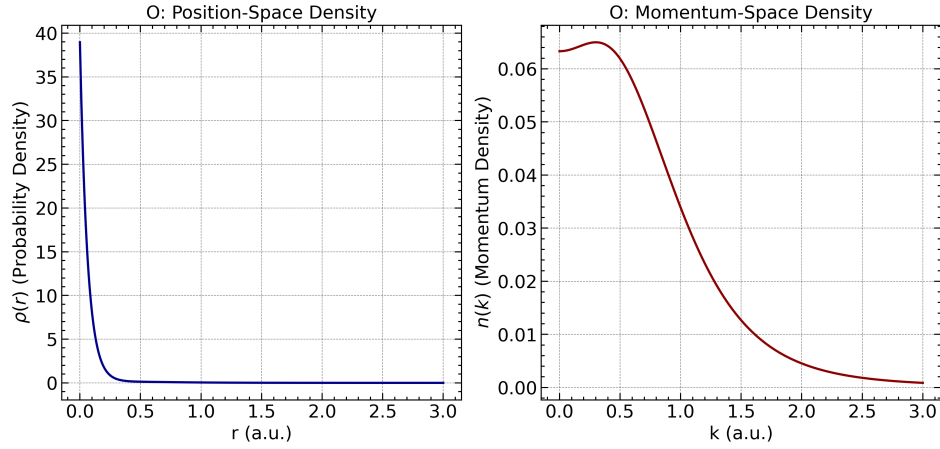


Figure 7: Density distribution of Oxygen, on position-space and momentum-space

2.8 F, $Z = 9$

Orbital configuration: $1s^2 2s^2 2p^5$

S_r	S_k	S	S_{max}	Ω	O
2.29883	6.16333	8.46215	10.05328	0.15827	61.14500

Table 8: Information Measures for Fluorine

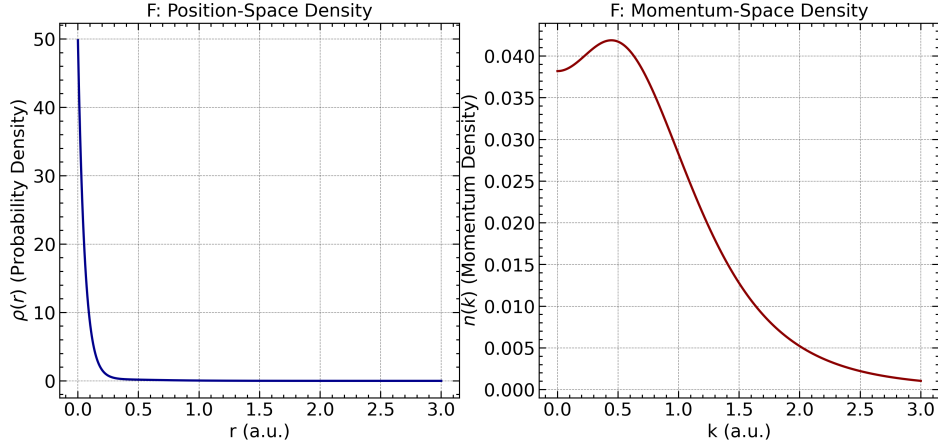


Figure 8: Density distribution of Fluorine, on position-space and momentum-space

2.9 Ne, $Z = 10$

Orbital configuration: $1s^2 2s^2 2p^6$

S_r	S_k	S	S_{max}	Ω	O
2.05514	6.43707	8.49221	9.99077	0.14999	75.24471

Table 9: Information Measures for Neon

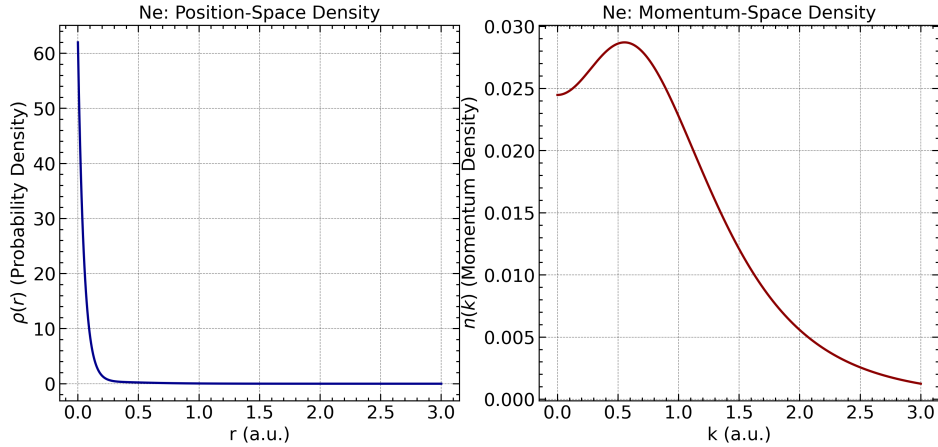


Figure 9: Density distribution of Neon, on position-space and momentum-space

2.10 Entropy Scaling with Atomic Number

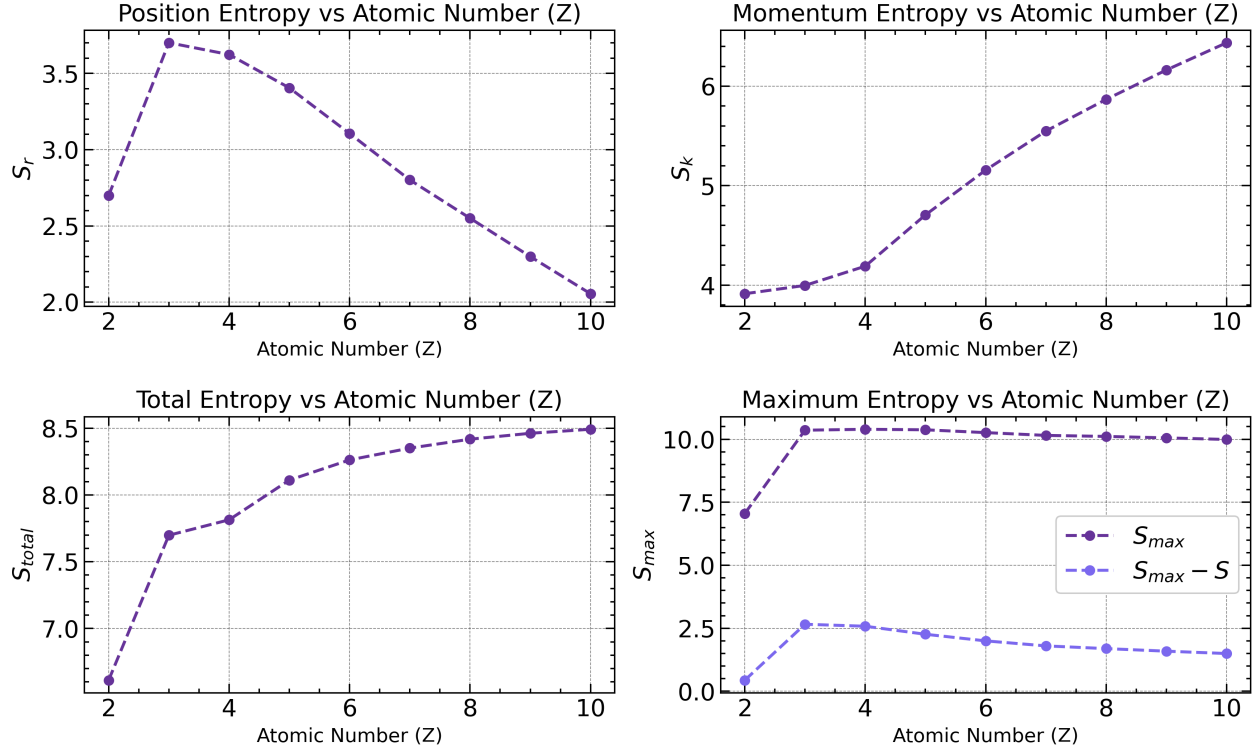


Figure 10: Systematic Trends in Shannon Entropies

The position-space entropy, S_r , generally decreases as atomic number Z increases, with an exception of increase when going from $Z = 2$ to $Z = 3$. The exception at $Z = 3$ reflects the transition from helium's compact $1s^2$ configuration to lithium's diffuse $2s$ electron. In contrast, momentum-space entropy, S_k , demonstrates a near-monotonic increase with Z . The total entropy $S = S_r + S_k$ reveals a logarithmic dependence on Z , validating the universal relation $S = a + b \ln Z$. The maximum entropy S_{max} represents the theoretical limit of electron delocalization. The difference $S_{max} - S$ measures how ordered an atom's electrons are.

2.11 Entropy vs. Ionization Potential Analysis

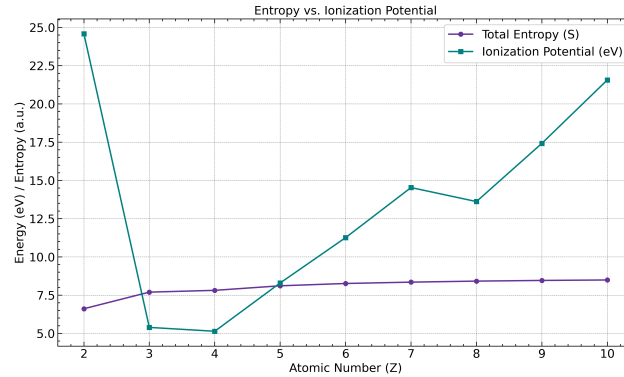


Figure 11: Total Entropy $S = S_r + S_k$ vs Energy Ionization Potential

The plot shows that as total entropy S increases from helium to neon, ionization potential (IP) drops sharply from helium’s high 24.6 eV to beryllium’s 9.3 eV, then climbs back up. This inverse relationship occurs because atoms with more delocalized electrons (higher S) lose them more easily (lower IP).

2.12 Exponential Fit Analysis

Using the entropy values S from Table 1 of Chatzisavvas et al. [2], we analyze the relationship between Shannon entropy and atomic number Z for elements $Z = 2$ –54. We model this trend with an exponential function to quantify the scaling behavior.

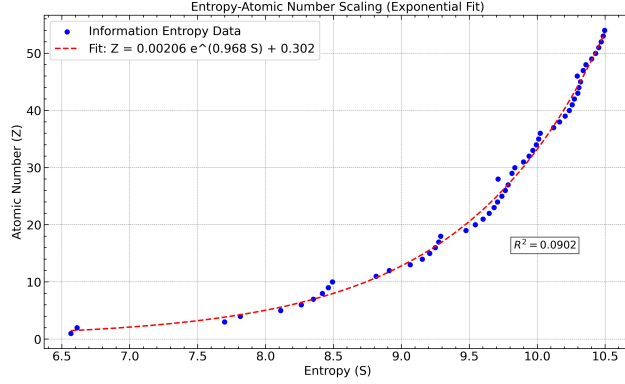


Figure 12: Exponential fit to entropy vs Atomic Number

The fit parameters $(a, b, c) = (0.00206, 0.968, 0.302)$ suggest a nonlinear dependence, with entropy growing sublinearly across the periodic table. This aligns with the expected increase in electron delocalization for heavier elements. The quality of the fit ($R^2 = 0.9952$) confirms the robustness of this empirical scaling and supports the suitability of the exponential model in capturing the observed trend. Minor deviations at low atomic numbers may be attributed to shell effects and electronic structure anomalies in lighter atoms.

3 Conclusions

This study explored the information-theoretic characteristics of He – Ne atoms by analyzing their electron density distributions in both position and momentum space using Roothaan-Hartree-Fock wavefunctions. The computed Shannon entropy, Onicescu energy, and Landsberg order parameter provide deep insight into the quantum structure of atoms and how it evolves with increasing atomic number Z . The results show that the Shannon entropy $S = S_r + S_k$ increases with Z , indicating more complex electron delocalization and a denser momentum-space structure for heavier atoms. The total entropy scales nearly logarithmically with Z , which aligns with earlier studies, while local dips at closed-shell configurations such as He and Ne highlight regions of higher internal order. Onicescu’s measure O drops sharply from He to Li , then fluctuates irregularly, suggesting that the density concentration in phase space does not vary smoothly with atomic number. Additionally, the Landsberg order parameter Ω decreases with increasing entropy, reinforcing the idea that atomic complexity and disorder grow with electron shell filling. A clear correlation was also observed between entropy-based measures and ionization potential: atoms with higher ionization energies tend to exhibit more localized electron distributions—reflected in lower S_r and higher Ω . Overall, these information-theoretic metrics emerge as powerful quantitative tools that go beyond traditional observables, effectively capturing shell structure, electron delocalization, and the intricate balance between order and disorder in atomic systems.

References

- [1] Carlos F. Bunge, José A. Barrientos, and Annik Vivier Bunge. Roothaan–hartree–fock ground-state atomic wave functions: Slater-type orbital expansions and expectation values for $z = 2$ –54. *Atomic Data and Nuclear Data Tables*, 53(1):113–162, 1993.
- [2] K. Ch. Chatzisavvas, Ch. C. Moustakidis, and C. P. Panos. Information entropy, information distances, and complexity in atoms. *The Journal of Chemical Physics*, 123(17):174111, 2005.
- [3] National Institute of Standards and Technology. Atomic spectra database - ionization energies, 2023. Version 5.10 (accessed: 2023-11-15).