

Ground State Wavefunctions for the First Ten Elements

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Abstract

This assignment delves into the construction of wavefunctions for the first ten elements of the periodic table. To achieve this, the spatial wavefunctions and momentum space wavefunctions are computed and visualized. From their analysis, the spatial, momentum, and maximum entropies are calculated and plotted against the atomic number. This comprehensive analysis enhances our understanding of quantum mechanical behavior in atomic systems, providing valuable insights into the electronic configurations and entropy characteristics of the first ten elements.

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1 Introduction

Describing the wavefunctions for elements represents a foundational endeavor in quantum mechanics, essential for comprehending and predicting quantum phenomena. While previous studies have explored these wavefunctions, their computation remains pivotal for advancing one's understanding and computational capabilities in quantum mechanics.

This project centers on computing the spatial and momentum space wavefunctions for the first ten elements of the periodic table. The spatial wavefunctions components R_{1s} , R_{2s} and R_{2p} are computed to elucidate the electron probability distributions around the nucleus. Accordingly, the momentum space wavefunctions components K_{1s} , K_{2s} and K_{2p} are calculated to describe the distributions of electron momentum. Plotting the final wavefunctions enhances our ability to comprehend these distributions.

Furthermore, to explore entropy in these quantum states, we compute S_r , S_k , S_{total} and S_{max} . These entropies are then plotted against the atomic number to analyze the relationship between atomic structure and entropy characteristics.

The primary objective of this project is to develop a Python code capable of universally computing the wavefunctions and entropies for the first ten elements, with potential applicability to subsequent elements. Additionally, the assignment aims to present and critically analyze the results, comparing them with existing research to validate their consistency.

2 Methodology

Due to its simplicity, the wavefunction of the first element H is omitted, focusing instead on the subsequent elements. The calculations are divided into three parts, as previously mentioned: computing the spatial wavefunction, the momentum space wavefunction, and finally the entropies.

2.1 Spatial and Momentum Wavefunctions

If $\phi_i(r)$ is a single particle wavefunction depicting the electrons in space and $\tilde{\phi}_i(k) = \int e^{-ik \cdot r} \phi_i(r) dr$ is the same wavefunction in the momentum space, then both the electron density and momentum density distributions are given by the following sums.

$$\rho(r) = \sum_i \phi_i^*(r) \phi_i(r) \quad n(k) = \sum_i \tilde{\phi}_i^*(k) \tilde{\phi}_i(k) \quad (1)$$

The wavefunctions can be expressed in the following form.

$$\phi_i(r) = \phi_{nlm}(r) = R_{nl}(r)Y_{lm}(\Omega_r) \quad \tilde{\phi}_i(k) = \tilde{\phi}_{nlm}(k) = K_{nl}(k)Y_{lm}(\Omega_k) \quad (2)$$

Where Ω represents the angular coordinates in spherical coordinates. The Roothaan-Hartree-Fock method computes analytical self-consistent-field atomic wave functions. By applying this method, the radial atomic orbital R_{nl} can be expressed as a finite sum of the primitive radial functions.

$$R_{nl}(r) = \sum_j C_{jnl} S_{jl}(r) \quad (3)$$

The Slater-type orbital set is given by the following equation:

$$S_{jl}(r) = N_{jl} r^{n_{jl}-1} e^{-Z_{jl}r} \quad (4)$$

And the normalization factor is N_{jl} is given by:

$$N_{jl} = (2Z_{jl})^{(n_{jl}+1/2)} / [(2n_{jl})!]^{1/2} \quad (5)$$

Where n_{jl} is the principal quantum number, Z_{jl} is the orbital exponent and l is the azimuthal quantum number. All the above formulas are derived from ref. [3], which provides the main foundational framework for our calculations and theoretical analysis.

From all the aforementioned formulas and calculations that are beyond the scope of this project, we can derive the following expressions for the distributions.

$$\rho(r) = \frac{1}{4\pi Z} \sum_i n_i R_{nl}(r) \quad n(k) = \frac{1}{4\pi Z} \sum_i n_i K_{nl}(k) \quad (6)$$

Where n_i is the number of electron in the nl orbital. These equations are normalized, meaning that the integral of $p(r) \cdot r^2$ multiplied by 4π should be equal to 1, and similarly for $n(k)$. These final versions of the formulas are sourced from ref. [2].

2.2 Entropy Calculation

To compute the entropies the electron distribution in space $\rho(r)$ and the momentum density distribution $n(k)$ are needed. The entropy S_r in position space is given by the Shannon information entropy formula, which is then expressed in terms of a mean square radius.

$$S_r = - \int \rho(r) \ln \rho(r) dr = -4\pi \int_0^\infty \rho(r) \ln \rho(r) r^2 dr \quad (7)$$

Accordingly, the entropy S_k in momentum space is expressed using the Shannon information entropy formula as follows, but is then revised to incorporate k^2 .

$$S_k = - \int n(k) \ln n(k) dk = -4\pi \int_0^\infty n(k) \ln n(k) k^2 dk \quad (8)$$

The total entropy is simply calculated by summing these two values, $S_{total} = S_r + S_k$. However, these values fluctuate between a minimum and maximum, so the maximum total entropy is determined using the following formula.

$$S_{max} = 3(1 + \ln \pi) + \frac{3}{2} \ln \left(\frac{8}{9} \langle r^2 \rangle T \right) \quad (9)$$

Where $\langle r^2 \rangle$ is the mean square radius and T the kinetic energy. This formula can be reformulated by calculating the mean square momentum $\langle k^2 \rangle$ instead of T . Then the previous formula takes the form:

$$S_{max} = 3(1 + \ln \pi) + \frac{3}{2} \ln \left(\frac{4}{9} \langle r^2 \rangle \langle k^2 \rangle \right) \quad (10)$$

The mean square values are easily calculated using the following integrals.

$$\langle r^2 \rangle = \int_0^\infty p(r) r^4 dr \quad \langle k^2 \rangle = \int_0^\infty n(k) k^4 dk \quad (11)$$

The general version of each entropy formula is derived from ref. [3], while the revised version is based on ref. [2].

3 Code Implementation

For the computational aspect of the project, a Python code has been implemented to compute the electron density distribution, momentum density distribution and the entropies. The first step is to define the functions for the $S(r)$ and $S(k)$ orbitals, with independent variables Z, r and Z, k respectively. The calculations for each orbital are preformed using the equation (4), with the finalized function results derived from ref. [2]. To compute the functions $R_{nl}(r)$ and $K_{nl}(k)$, the coefficients and factors of the $S(r)$ and $S(k)$ orbital functions are sourced from ref. [1] and organized into matrices.

All the necessary calculations are performed using a 'wavefunction' function, which takes as inputs matrices for the s orbital coefficients, p orbital coefficients, and the atomic number Z . Initially, the $R_{nl}(r)$ and $K_{nl}(k)$ functions are computed by beginning at 0 and successively adding each orbital $S(r)$ or $S(k)$, multiplied by its respective factor, with the corresponding independent variables. For $R_{nl}(r)$ and $K_{nl}(k)$ functions that have been defined but not used, they remain 0 and do not interfere with the rest of the calculations.

To ensure correctness of the $R_{nl}(r)$ and $K_{nl}(k)$ functions' calculations, each function is squared, multiplied by r^2 or k^2 and integrated from 0 to infinity. The result is then rounded to the 5th decimal place and checked to see if it equals 1. This extra step is added because computations inherently contain small errors. Subsequently, a message is displayed to the user indicating whether the calculations were successful or not.

The next step is to compute the $\rho(r)$ and $n(k)$ functions. The functions are initialized to 0, and utilizing the atomic number, as we iterate through each electron, the corresponding $R_{nl}(r)$ for $\rho(r)$ and $K_{nl}(k)$ for $n(k)$ are added with a factor that satisfies equation (6). Once again, to ensure the accuracy of the calculation, we verify if the integral of $\rho(r) \cdot r^2$ from 0 to infinity, multiplied by 4π , equals 1 after rounding. The analogous procedure is applied for $n(k)$. The appropriate message about the success of the calculations is then presented to the user. Afterwards, the $\rho(r)$ and $n(k)$ are plotted for r and k values in range of 0 to 4.

Lastly, the 'wavefunction' function calculates the entropies S_r , S_k , S_{total} and S_{max} , utilizing the equations (7), (8), (10) and (11). The function returns the entropy results in the form of an array. By executing the 'wavefunction' function for all specified elements, we gather all entropy results into a matrix. The matrix is then divided, and we plot all entropies S_r , S_k , S_{total} , and S_{max} against the atomic number Z .

4 Results

4.1 Helium (He)

For the Helium element, where $Z = 2$, the function generates the plots shown in Figure 1 for the $\rho(r)$ and $n(k)$ distributions. The entropy results are $S_r = 2.6985$, $S_k = 3.9134$, $S_{total} = 6.6119$ and $S_{max} = 7.0493$.

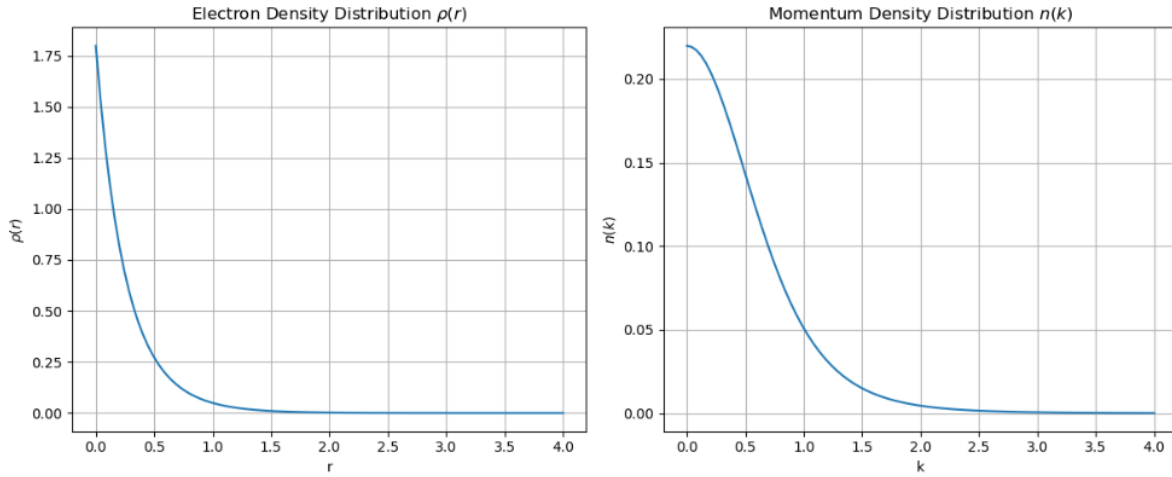


Figure 1: The distributions for the element **He**. On the left is the electron density distribution $\rho(r)$ against the distance r . On the right is the momentum density distribution $n(k)$ against the momentum k .

4.2 Lithium (Li)

Lithium, with $Z = 3$, has the plots depicted in Figure 2. Its entropy results are $S_r = 3.7014$, $S_k = 3.9968$, $S_{total} = 7.6983$ and $S_{max} = 10.3578$.

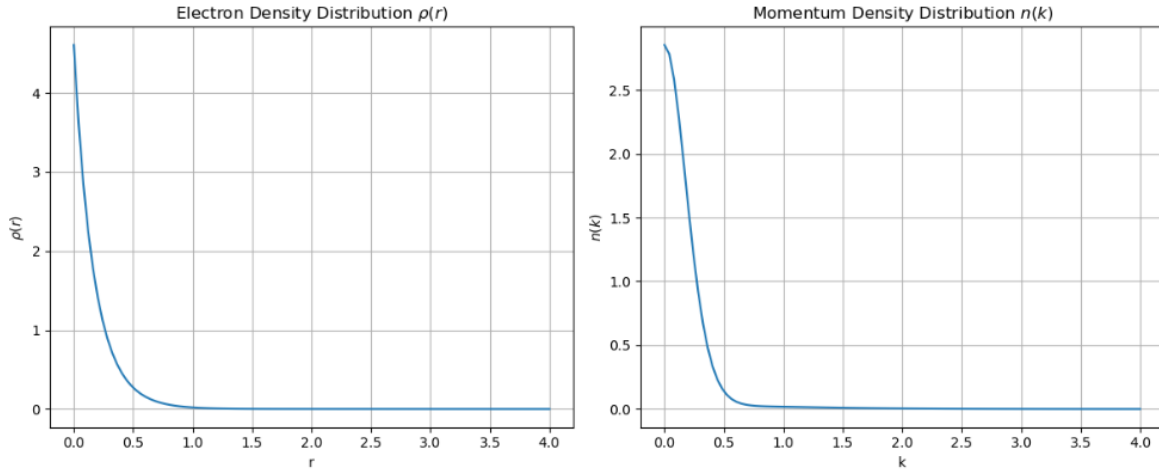


Figure 2: The distributions for the element **Li**. On the left is the electron density distribution $\rho(r)$ against the distance r . On the right is the momentum density distribution $n(k)$ against the momentum k .

4.3 Beryllium (Be)

In Figure 3 we see the plots of the distributions for Beryllium, which has an atomic number of $Z = 4$. The entropies are $S_r = 3.6239$, $S_k = 4.1902$, $S_{total} = 7.8140$ and $S_{max} = 10.3950$.

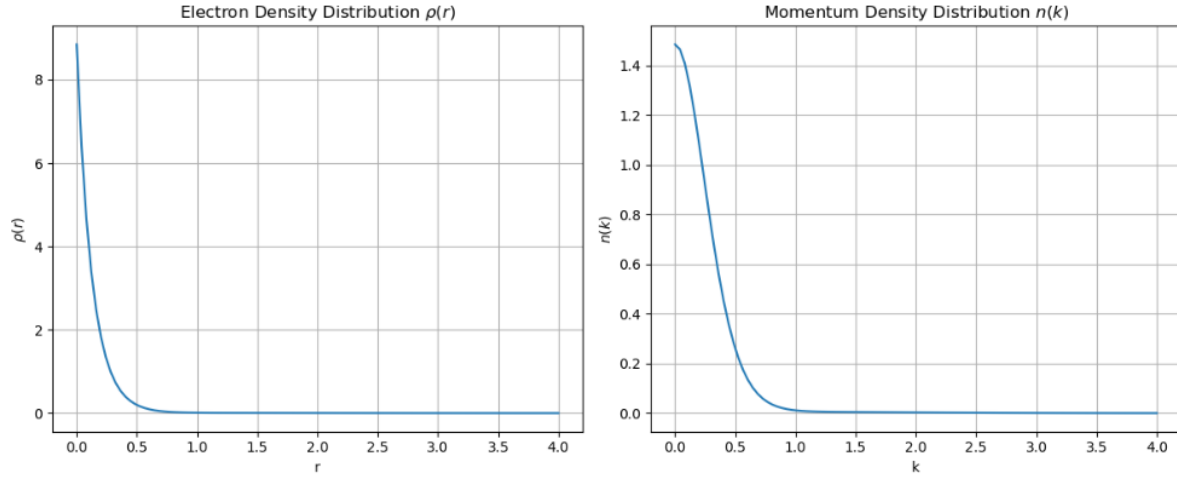


Figure 3: The distributions for the element **Be**. On the left is the electron density distribution $\rho(r)$ against the distance r . On the right is the momentum density distribution $n(k)$ against the momentum k .

4.4 Boron (B)

Boron has an atomic number of $Z = 5$. The results of the plots are presented in Figure 4 and the entropies are the following: $S_r = 3.4054$, $S_k = 4.7059$, $S_{total} = 8.1113$ and $S_{max} = 10.3738$.

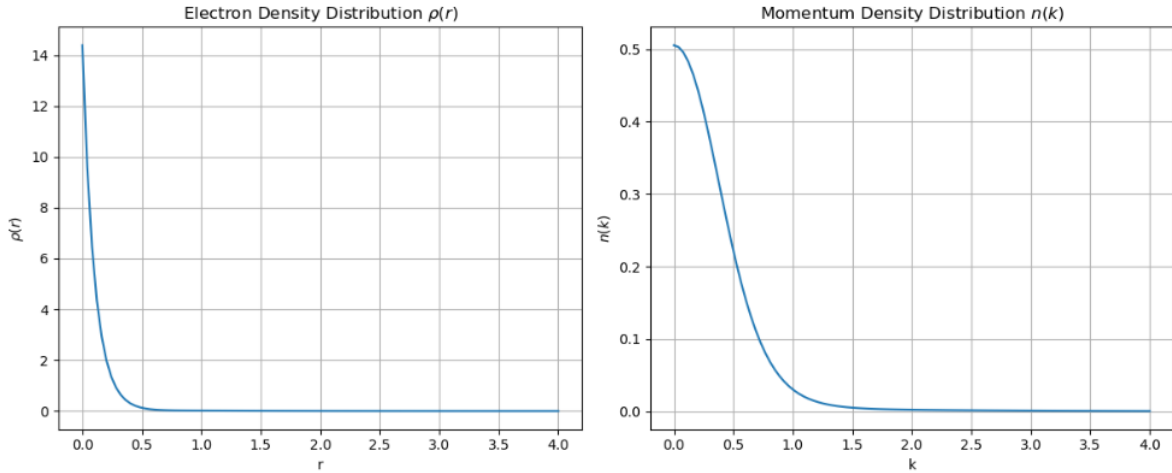


Figure 4: The distributions for the element **B**. On the left is the electron density distribution $\rho(r)$ against the distance r . On the right is the momentum density distribution $n(k)$ against the momentum k .

4.5 Carbon (C)

Next on the list is Carbon, with an atomic number of $Z = 6$. The distribution plots are shown in Figure 5, and the entropies are $S_r = 3.1060$, $S_k = 5.1566$, $S_{total} = 8.2626$ and $S_{max} = 10.2624$.

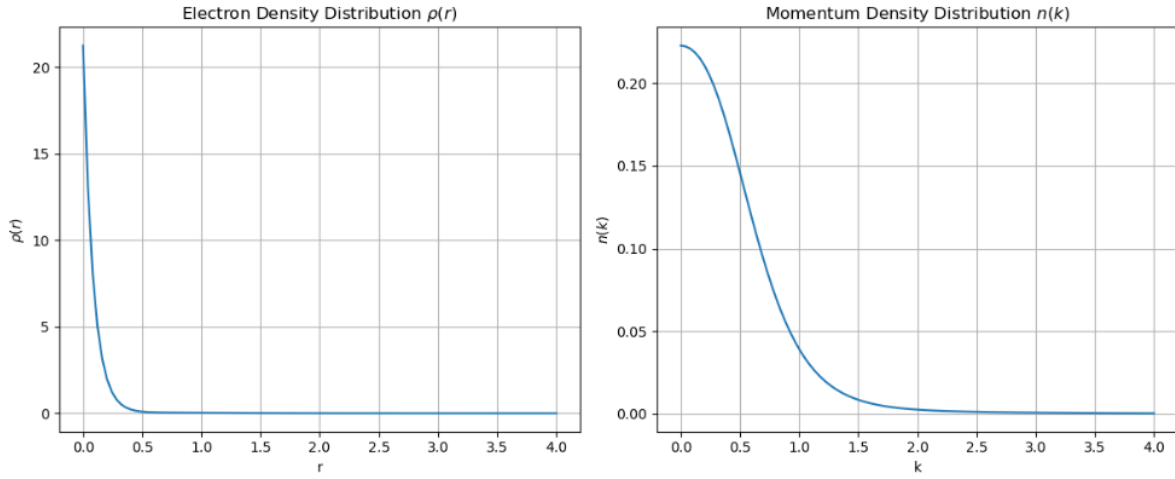


Figure 5: The distributions for the element **C**. On the left is the electron density distribution $\rho(r)$ against the distance r . On the right is the momentum density distribution $n(k)$ against the momentum k .

4.6 Nitrogen (N)

For Nitrogen, with $Z = 7$, the plots are depicted in Figure 6. The entropy results are $S_r = 2.8017$, $S_k = 5.5493$, $S_{total} = 8.3510$ and $S_{max} = 10.1520$.

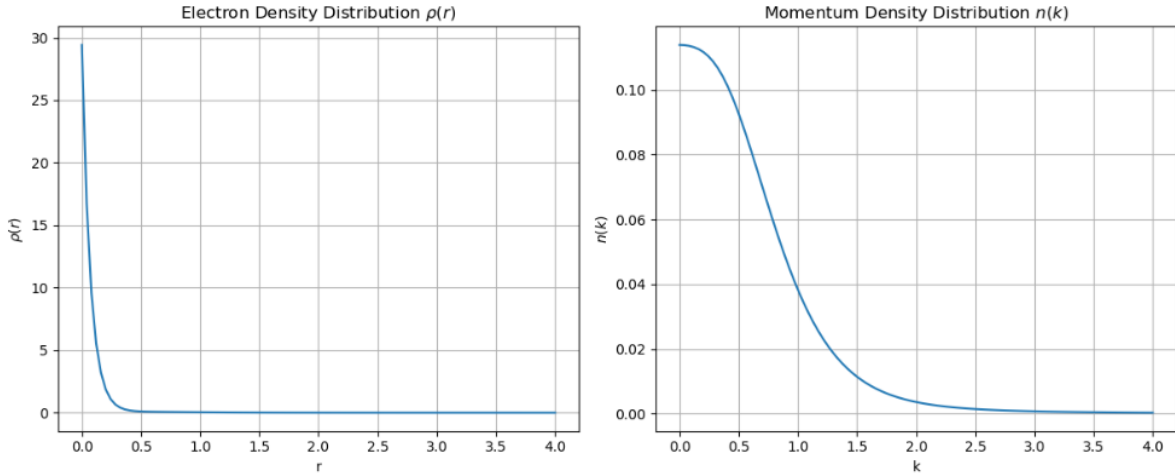


Figure 6: The distributions for the element **N**. On the left is the electron density distribution $\rho(r)$ against the distance r . On the right is the momentum density distribution $n(k)$ against the momentum k .

4.7 Oxygen (O)

For the next element, Oxygen, the atomic number is $Z = 8$. The plots for the distributions are shown in Figure and the entropies are $S_r = 2.5505$, $S_k = 5.8674$, $S_{total} = 8.4179$ and $S_{max} = 10.1113$.

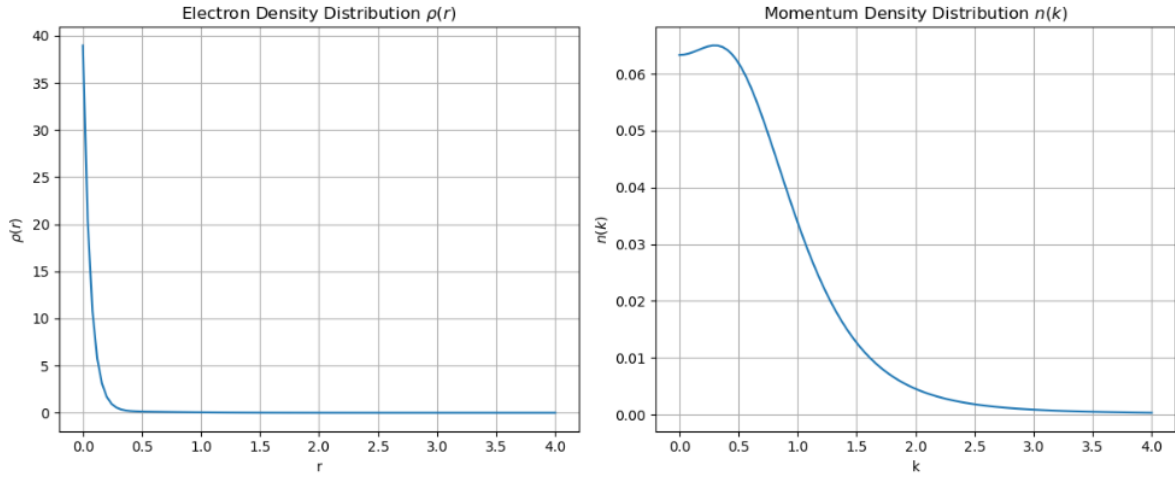


Figure 7: The distributions for the element **O**. On the left is the electron density distribution $\rho(r)$ against the distance r . On the right is the momentum density distribution $n(k)$ against the momentum k .

4.8 Fluorine (F)

The Fluorine element has $Z = 9$ and its plot results are presented in Figure 8. The results of the entropy calculations are $S_r = 2.2988$, $S_k = 6.1633$, $S_{total} = 8.4622$ and $S_{max} = 10.0533$.

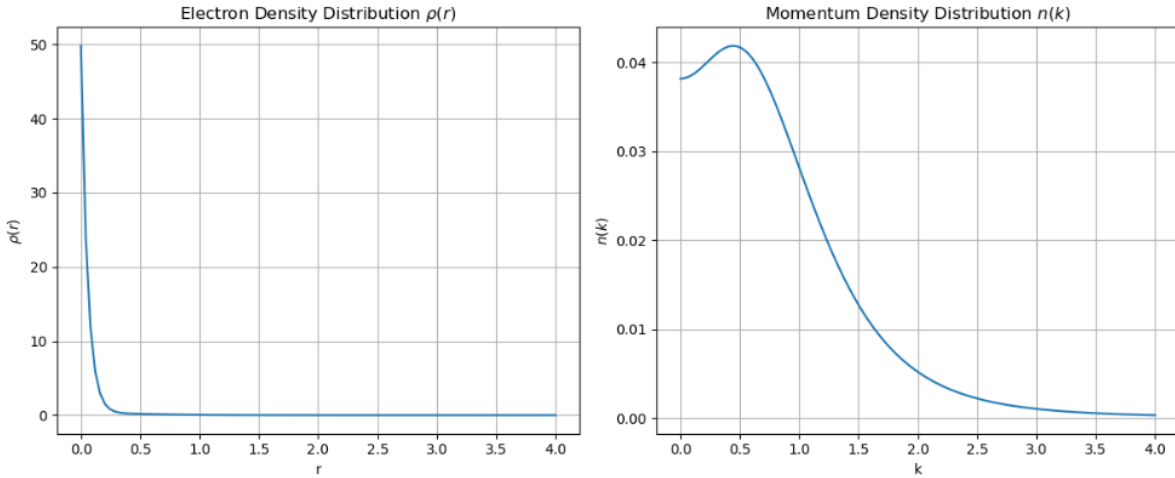


Figure 8: The distributions for the element **F**. On the left is the electron density distribution $\rho(r)$ against the distance r . On the right is the momentum density distribution $n(k)$ against the momentum k .

4.9 Neon (Ne)

The final element on our list for analysis is Neon, which has an atomic number of $Z = 10$. The distribution plots are presented in Figure 9 and the entropies are $S_r = 2.0551$, $S_k = 6.4371$, $S_{total} = 8.4922$ and $S_{max} = 9.9908$.

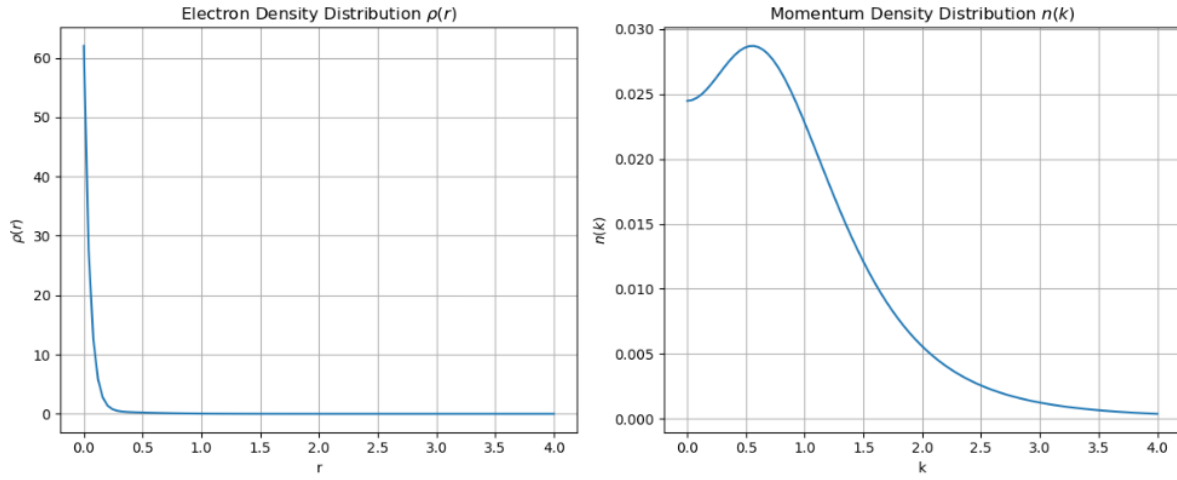


Figure 9: The distributions for the element **Ne**. On the left is the electron density distribution $\rho(r)$ against the distance r . On the right is the momentum density distribution $n(k)$ against the momentum k .

4.10 Entropy Results

For convenience, we compile all the aforementioned entropy results and present them in Table 1.

Z	Atom	S_r	S_k	S_{total}	S_{max}
2	He	2.69851	3.91342	6.61193	7.04930
3	Li	3.70144	3.99682	7.69826	10.35784
4	Be	3.62386	4.19019	7.81405	10.39503
5	B	3.40545	4.70590	8.11135	10.37384
6	C	3.10602	5.15658	8.26260	10.26242
7	N	2.80169	5.54934	8.35103	10.15197
8	O	2.55054	5.86735	8.41789	10.11127
9	F	2.29883	6.16333	8.46215	10.05328
10	Ne	2.05514	6.43707	8.49221	9.99077

Table 1: Collected values of entropies S_r , S_k , S_{total} and S_{max} for all studied atoms

We generate a graph for each entropy value plotted against the atomic number to observe the behavior of entropy across elements. The entropy in position space S_r is displayed in Figure 10. Meanwhile, the entropy in momentum space S_k is shown in Figure 11. Their combined total S_{total} is illustrated in Figure 12 and the maximum entropy value S_{max} is presented in Figure 13.

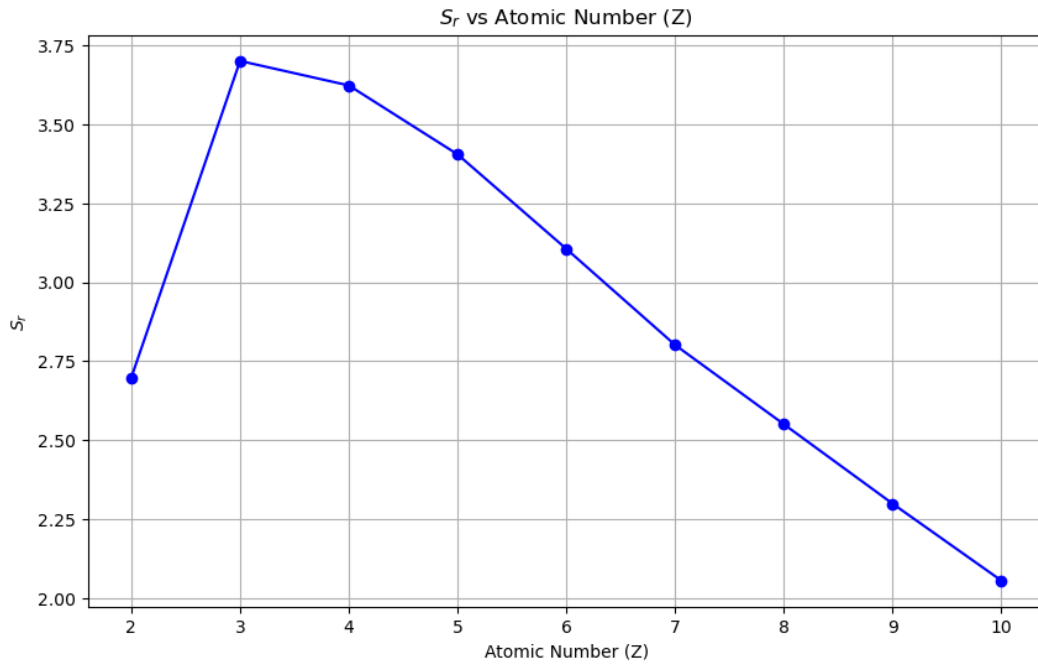


Figure 10: The entropy in position space S_r versus the atomic number Z

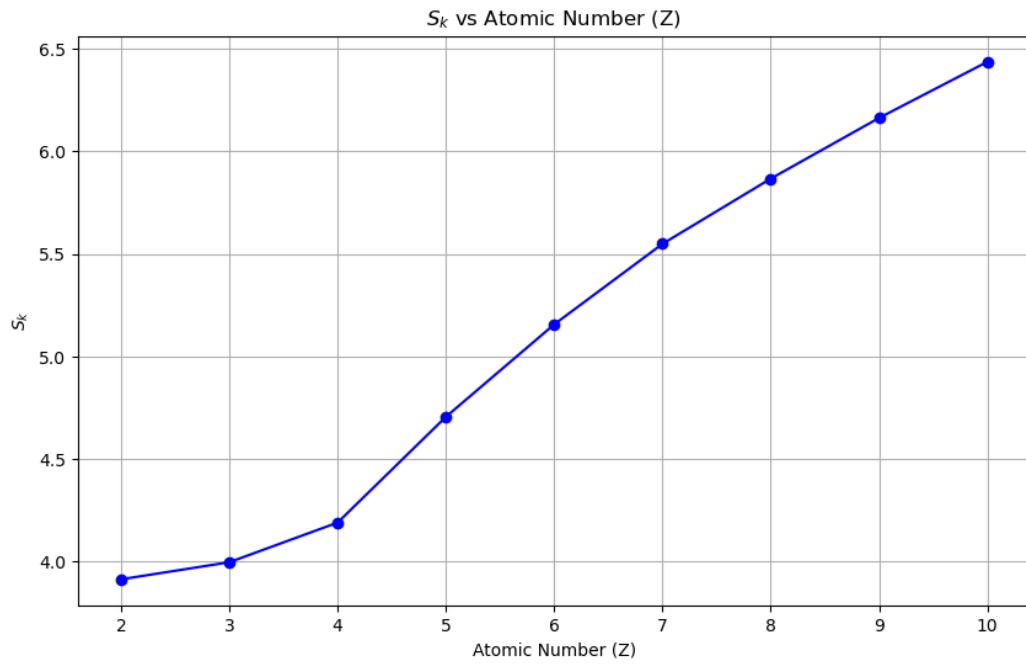


Figure 11: The entropy in momentum space S_k versus the atomic number Z

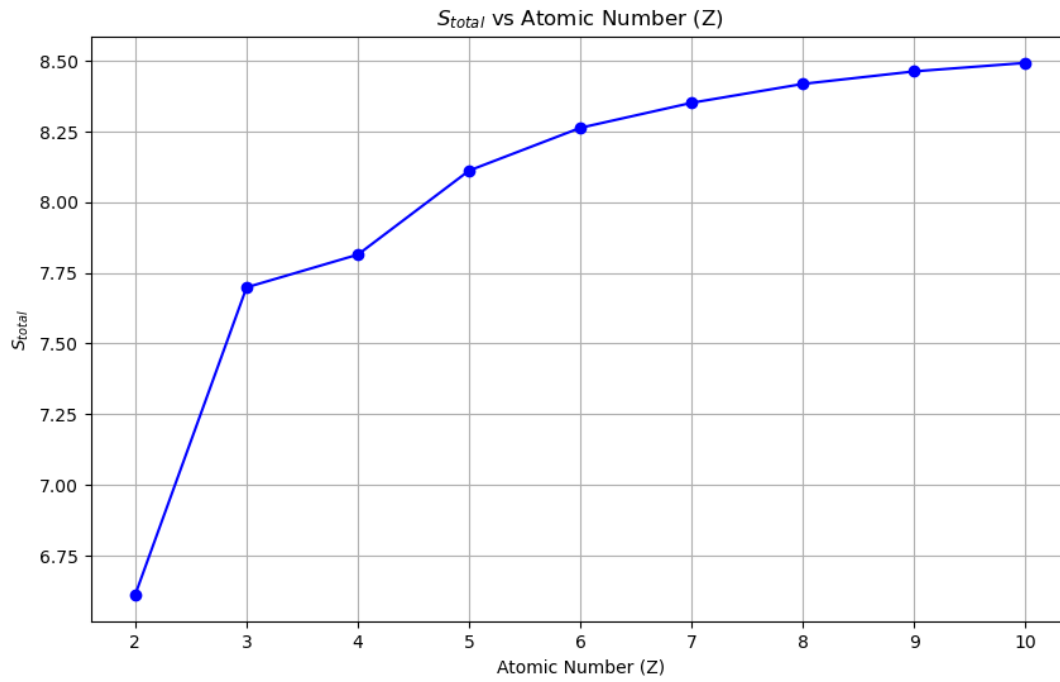


Figure 12: The total sum of position space and momentum space entropies S_{total} versus the atomic number Z

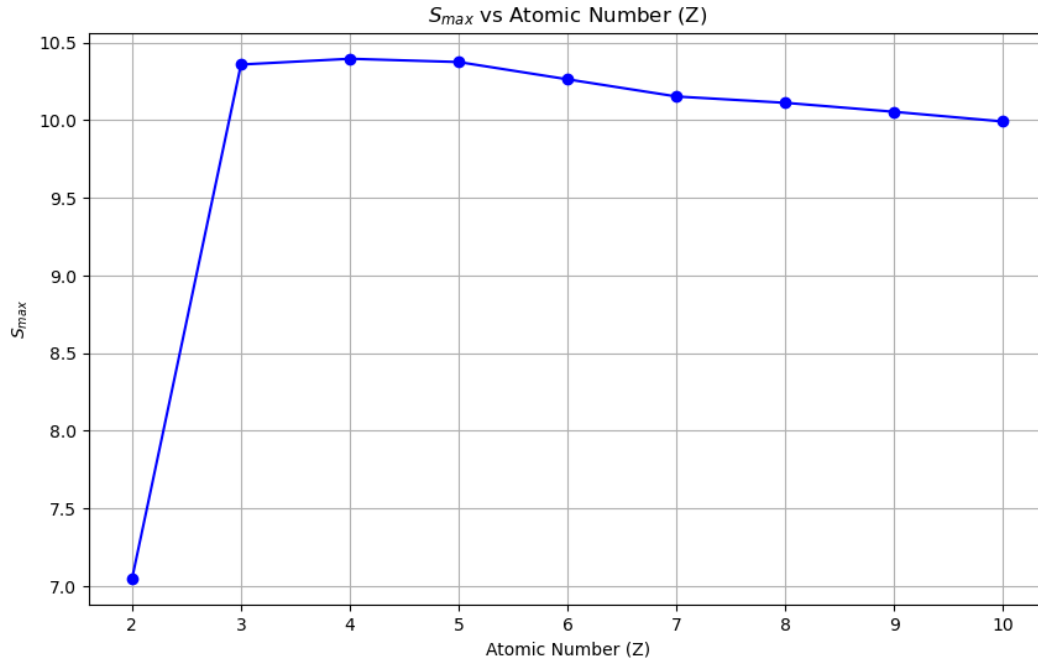


Figure 13: The maximum entropy S_{max} versus the atomic number Z

5 Discussion

5.1 Electron Density and Momentum Density Distribution Patterns

As evident from the plots, the distributions exhibit a similar shape across all studied elements, with minor variations from one element to the next.

The electron density distribution $\rho(r)$ decreases exponentially with distance r . As the atomic number increases, the curve decreases more rapidly and the initial point of the decline becomes higher. Overall, the electron density plots for all elements have the same form: the curve starts high at a distance of 0 and decreases swiftly to 0 as the distance increases. The rapid exponential decrease with increasing atomic number is expected, because electrons are more strongly attracted to the nucleus, resulting in a higher electron density near the nucleus.

The momentum space distribution $n(k)$ exhibits a more intriguing shape. As we progress from lower to higher atomic numbers, the shape of the curve changes significantly. The momentum space distribution initially exhibits an almost exponential decrease with a slight sinusoidal-like curve at the top. At Nitrogen, this curve becomes more rounded at the peak, and at Oxygen, a small rounded peak begins to form, becoming more prominent as we reach Neon. This change in shape indicates variations in quantum states, with electrons acquiring higher quantum numbers as atomic numbers increase.

5.2 Entropy Analysis

The entropy values we have calculated appear to correspond precisely to the results reported in ref. [3]. Each entropy quantity shows a unique relationships with the atomic number.

The position space entropy S_r starts at a mid-range value. It reaches a peak for the second element, Li, and then decreases evenly for the remaining elements. On the contrary, the momentum space entropy S_k starts low and then rises, as the atomic number increases. After a slight increase for the next two elements, Li and Be, the subsequent increases in entropy per element are slightly higher and remain consistent across the rest of the elements.

The sum of these two S_{total} starts low, sees a rapid increase in the next element, Li, and then each subsequent increase diminishes, somewhat reaching a plateau in the last two elements, F and Ne. The maximum entropy S_{max} is low for the first element, He, experiences a significant increase to near maximum in the next element, Li, and then remains relatively constant for the following two elements, Be and B. After that, the maximum entropy starts to decrease, but very slightly.

6 Conclusion

This project focused on computing spatial and momentum space wavefunctions for the first ten elements of the periodic table. By computing the spatial and momentum orbitals R_{nl} and K_{nl} , we were able to calculate and visualize both the electron density distribution $\rho(r)$ and the momentum density distribution $n(k)$. Our findings revealed that the electron density distribution $\rho(r)$ consistently decreased exponentially with distance r . This decrease became more rapid as the atomic number increased. The momentum space distribution $n(k)$ showed a more complex behavior, evolving from an almost exponential decrease

with a slight sinusoidal curve at the top, to a more rounded peak as atomic number increased. This behavior indicated changes in the electrons' quantum states.

Additionally, we explored the entropies of these quantum states by calculating the entropy in position space S_r , the entropy in momentum space S_k , their sum S_{total} and the maximum entropy S_{max} . Plotting these entropies against the atomic number allowed us to analyze the relationship between them. The results of the entropies' calculations aligned precisely with existing research, confirming their accuracy. The S_r peaked at Li, and then steadily decreased. For S_k the value started low and increased with each next element. The S_{total} began low, experienced a sharp increase at Li, and subsequent increments tapered off, approaching a plateau by the end. The S_{max} began low, underwent a significant increase nearing maximum and then gradually decreased slightly.

The Python code created for the computation of these wavefunctions and entropies has the potential to be expanded for a broader applicability, beyond the first ten elements.

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