
Atomic Number and Information

COMPUTATIONAL QUANTUM MECHANICS



Aristotle University of Thessaloniki
Physics Department
Msc Computational Physics
Bompotas Christos
AEM:4435
19/06/2024

Contents

I	Abstract	1
1	Theoretical Introduction	2
1.1	Wave Functions and Probability Densities	2
1.1.1	Position Space Wave Functions	2
1.1.2	Probability Density Functions	2
1.2	Momentum Space Representation	3
1.3	Probability Density Functions in Momentum Space	3
1.4	Integration for Information Entropy	3
1.4.1	Position Space Entropy S_r	3
1.4.2	Momentum Space Entropy S_k	3
2	Results	4
2.1	Helium (He)	4
2.1.1	Probability Densities	4
2.1.2	Shannon Entropies	5
2.2	Lithium (Li)	6
2.2.1	Probability Densities	6
2.2.2	Shannon Entropies	7
2.3	Beryllium (Be)	8
2.3.1	Probability Densities	8
2.3.2	Shannon Entropies	9
2.4	Boron (B)	10
2.4.1	Probability Densities	10
2.4.2	Shannon Entropies	11
2.5	Carbon (C)	12
2.5.1	Probability Densities	12
2.5.2	Shannon Entropies	13
2.6	Nitrogen (N)	14
2.6.1	Probability Densities	14
2.6.2	Shannon Entropies	15
2.7	Oxygen (O)	16
2.7.1	Probability Densities	16
2.7.2	Shannon Entropies	17
2.8	Fluorine (F)	18
2.8.1	Probability Densities	18
2.8.2	Shannon Entropies	19
2.9	Neon (Ne)	20
2.9.1	Probability Densities	20
2.9.2	Shannon Entropies	21
2.10	Entropy as a function of Z	22
3	Conclusions	24
	Bibliography	25

I Abstract

The purpose of this study is the exploration of information loss associated with the quantum mechanical description of atoms. Following strictly the given computational algorithm, the calculation of the Shannon information entropy was achieved, for both the position r and the momentum k . For each atom under consideration, we constructed its wave functions, which were subsequently used in the calculations of electron densities for both position and momentum spaces. Finally, these densities were employed in the computation of the required entropy quantities. So, in the sections below, the entropies are presented for each element and finally we plot the entropies as a function of the atomic number S .

1 Theoretical Introduction

In this section we analyze the theoretical background, necessary for understanding the process that was followed in this study to reach the results for the information entropy. In atomic and quantum systems, information entropy is derived from the spatial and momentum electron distributions. This duality stems from the Heisenberg uncertainty principle, which dictates that precise knowledge of an electron's position implies greater uncertainty in its momentum and vice versa.

1.1 Wave Functions and Probability Densities

To compute S_r and S_k , we start with the wave functions of electrons in their respective orbitals. These wave functions are solutions to the Schrödinger equation for the hydrogen-like atoms, adjusted for more complex atoms using approximation methods such as the Roothaan-Hartree-Fock (RHF) method.

1.1.1 Position Space Wave Functions

The position space wave functions for the 1s, 2s, 3s and 2p orbitals, since only these orbitals are occupied for the atoms involved, are given by:

- 1s Orbital:

$$\psi_{1s}(r) = 2z^{3/2}e^{-zr} \quad (1.1)$$

- 2s Orbital:

$$\psi_{2s}(r) = \frac{2}{\sqrt{3}}z^{5/2}re^{-zr} \quad (1.2)$$

- 3s Orbital:

$$\psi_{3s}(r) = \frac{2^{3/2}}{3\sqrt{5}}z^{7/2}r^2e^{-zr} \quad (1.3)$$

- 2p Orbital:

$$\psi_{2p}(r) = \frac{2}{\sqrt{3}}z^{5/2}re^{-zr} \quad (1.4)$$

1.1.2 Probability Density Functions

The probability density functions in position space, $p(r)$, are derived from the wave functions:

$$p(r) = \psi^*(r)\psi(r) \quad (1.5)$$

For a multi-electron atom, the total wave function is a combination of the individual wave functions weighted by their coefficients, leading to:

$$p(r) = \frac{1}{4\pi Z} (a\psi_{1s}^2 + b\psi_{2s}^2 + c\psi_{2p}^2) \quad (1.6)$$

where a is the number of electrons in the 1s orbital, b the number of electrons in the 2s orbital, and c the number of electrons in the 2p orbital.

1.2 Momentum Space Representation

The momentum space wave functions are obtained by taking the Fourier transform of the position space wave functions:

- 1s Orbital:

$$\tilde{\psi}_{1s}(k) = \frac{16\pi z^{5/2}}{(z^2 + k^2)^2} \quad (1.7)$$

- 2s Orbital:

$$\tilde{\psi}_{2s}(k) = \frac{16\pi z^{5/2}(3z^2 - k^2)}{\sqrt{3}(z^2 + k^2)^3} \quad (1.8)$$

- 3s Orbital:

$$\tilde{\psi}_{3s}(k) = \frac{64\sqrt{10}\pi z^{9/2}(z^2 - k^2)}{5(z^2 + k^2)^4} \quad (1.9)$$

- 2p Orbital:

$$\tilde{\psi}_{2p}(k) = \frac{64\pi k z^{7/2}}{\sqrt{3}(z^2 + k^2)^3} \quad (1.10)$$

1.3 Probability Density Functions in Momentum Space

The probability density functions in momentum space, $n(k)$, are derived similarly:

$$n(k) = \tilde{\psi}^*(k)\tilde{\psi}(k) \quad (1.11)$$

For a multi-electron atom, the total wave function in momentum space is also a combination of the individual wave functions weighted by their coefficients:

$$n(k) = \frac{1}{4\pi Z} \left(a\tilde{\psi}_{1s}^2 + b\tilde{\psi}_{2s}^2 + c\tilde{\psi}_{2p}^2 \right) \quad (1.12)$$

where again a is the number of electrons in the 1s orbital, b the number of electrons in the 2s orbital, and c the number of electrons in the 2p orbital.

1.4 Integration for Information Entropy

The integration of the probability density functions over all space yields the information entropy values.

1.4.1 Position Space Entropy S_r

The entropy in position space is computed by integrating:

$$S_r = - \int_0^\infty 4\pi r^2 p(r) \ln(p(r)) dr \quad (1.13)$$

1.4.2 Momentum Space Entropy S_k

Similarly, the entropy in momentum space is calculated as:

$$S_k = - \int_0^\infty 4\pi k^2 n(k) \ln(n(k)) dk \quad (1.14)$$

2 Results

Now for each element we plot its probability electron function in both the position and momentum space, and we present its corresponding entropy values. Finally, we plot the Shannon entropies in position and momentum space, along with the total entropy.[1],[2],[4],[5]

2.1 Helium (He)

2.1.1 Probability Densities

The electron configuration of Helium is $1s^2$. We plot the densities from equations (1.6),(1.12) and we get:

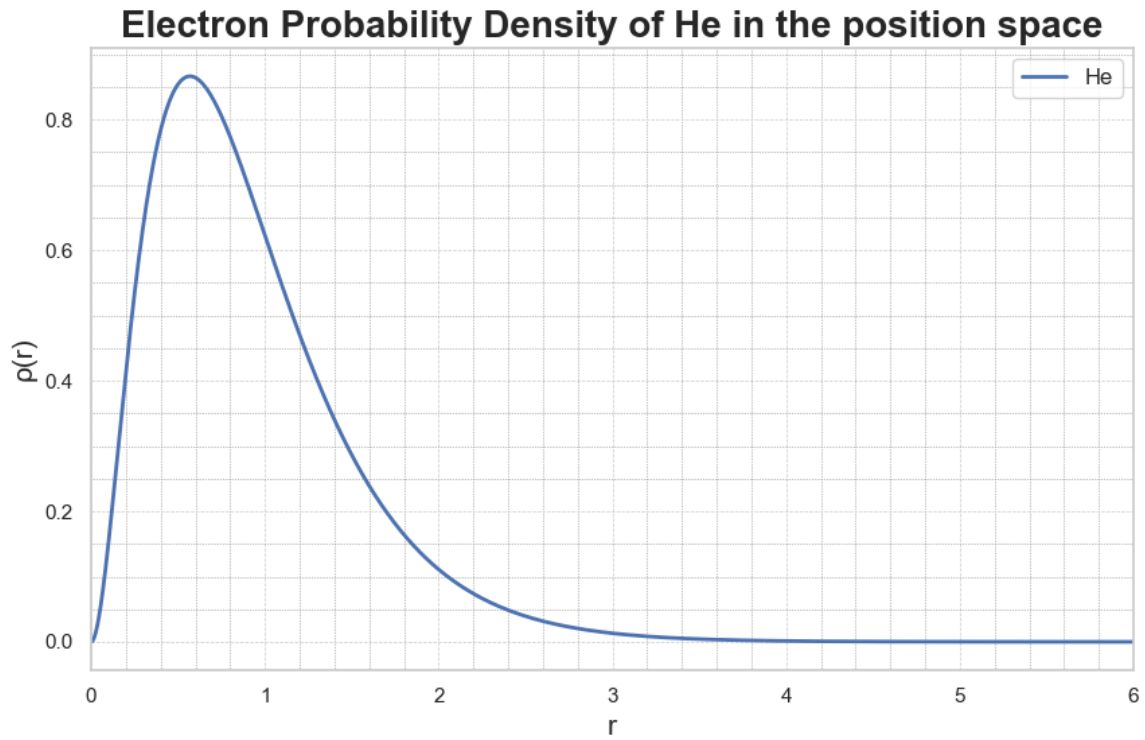


Figure 1: The electron probability density as a function of the distance from the center of the atom of He. We notice the maximum probability around $r=0.55$, and an asymptotic decline after that. So the most of the electrons are gonna be close to the nucleus.

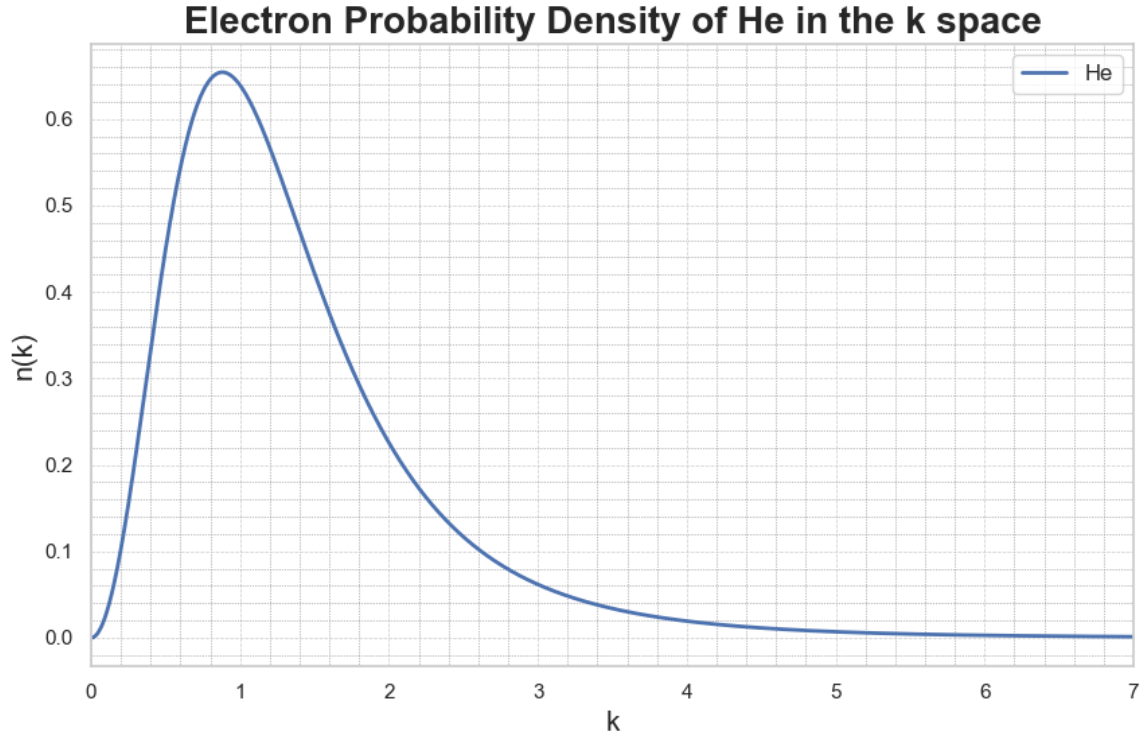


Figure 2: The electron probability density as a function of momentum for the atom of He. We notice that we will mostly find low kinetic energy electrons, with a small momentum.

2.1.2 Shannon Entropies

Table 1: Entropies Calculation for Helium (He)

Entropies	Calculation
S_r	2.6985109837
S_k	3.91341875979
S_{total}	6.61192974349

We notice that the entropy in position space is smaller than that of momentum space. Expected since the k-space peak of the probability density is wider than that of the r-space.

2.2 Lithium (Li)

2.2.1 Probability Densities

The electron configuration of Lithium is $1s^2 2s^1$. We plot the densities and we get:

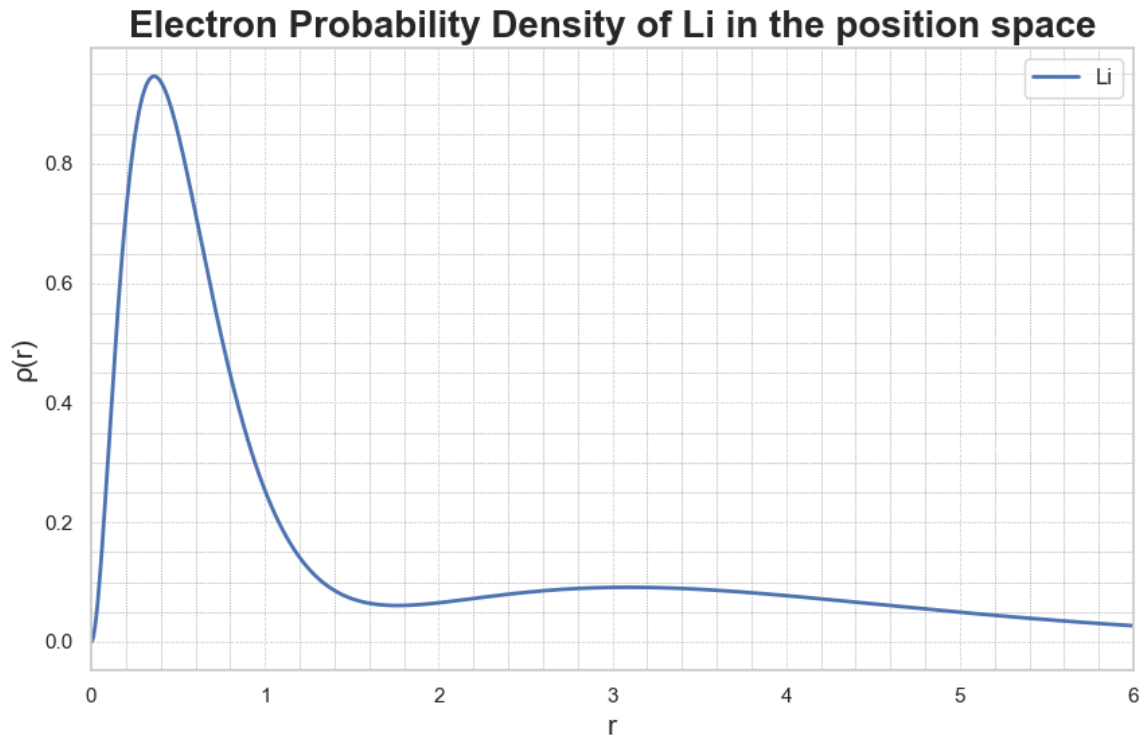


Figure 3: The electron probability density as a function of the distance from the center of the atom of Li. We notice again a peak similar to Helium, but this time we also have a bump near $r=3.2$, which is justified since Lithium also has an electron in an $2s$ orbital, thus we can find an electron further away from the nucleus

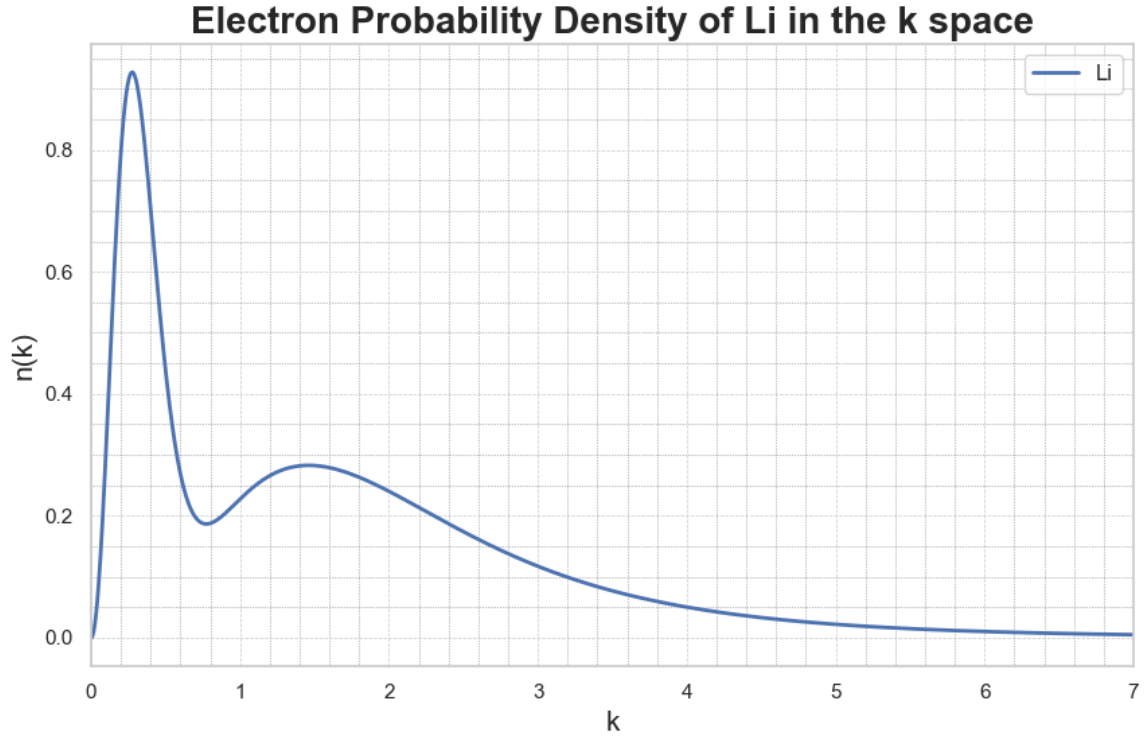


Figure 4: The electron probability density as a function of momentum for the atom of Li. We see a peak narrower than that of Helium, but also a bump a little further away from the nucleus, meaning we have a high chance of finding electrons with different kinetic energy.

2.2.2 Shannon Entropies

Table 2: Entropies Calculation for Lithium (Li)

Entropies	Calculation
S_r	3.70143692041
S_k	3.99681902691
S_{total}	7.69825594732

We notice that the entropies are similar, because of the similarity in behavior of their densities

2.3 Beryllium (Be)

2.3.1 Probability Densities

The electron configuration of Beryllium is $1s^2 2s^2$. We plot the densities and we get:

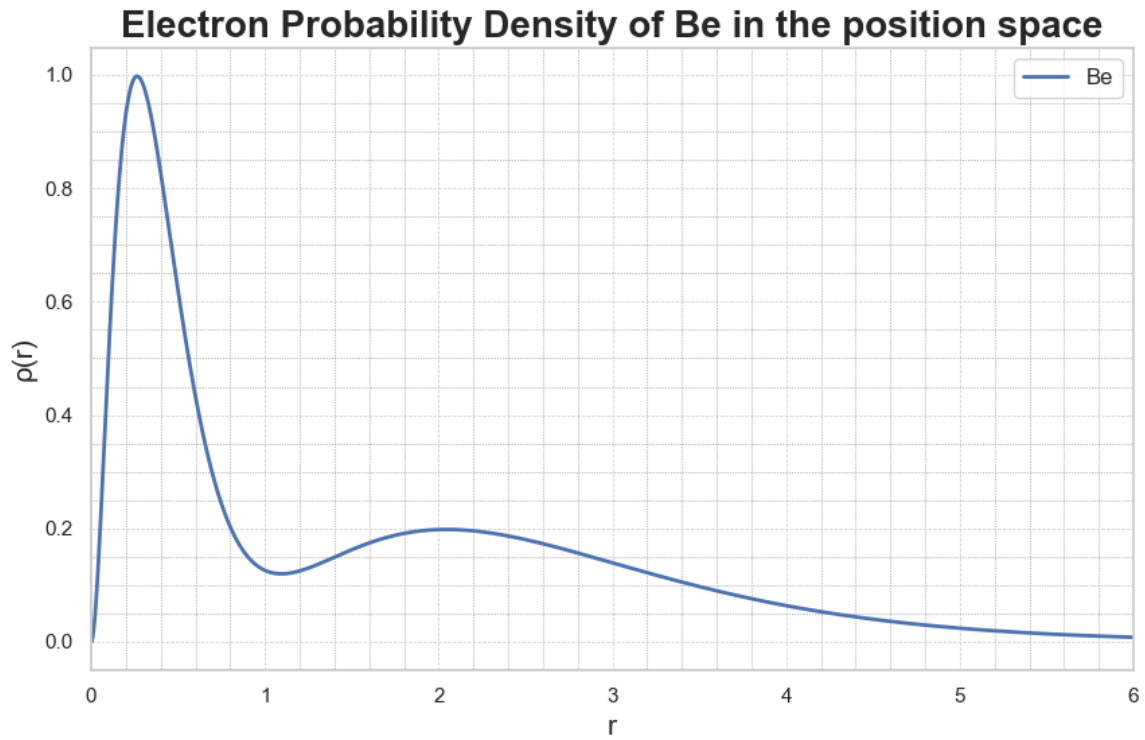


Figure 5: The electron probability density as a function of the distance from the center of the atom of Be. We notice its shape is similar to that of Lithium, expected since both of these elements have electrons in orbitals only up to $n=2$.

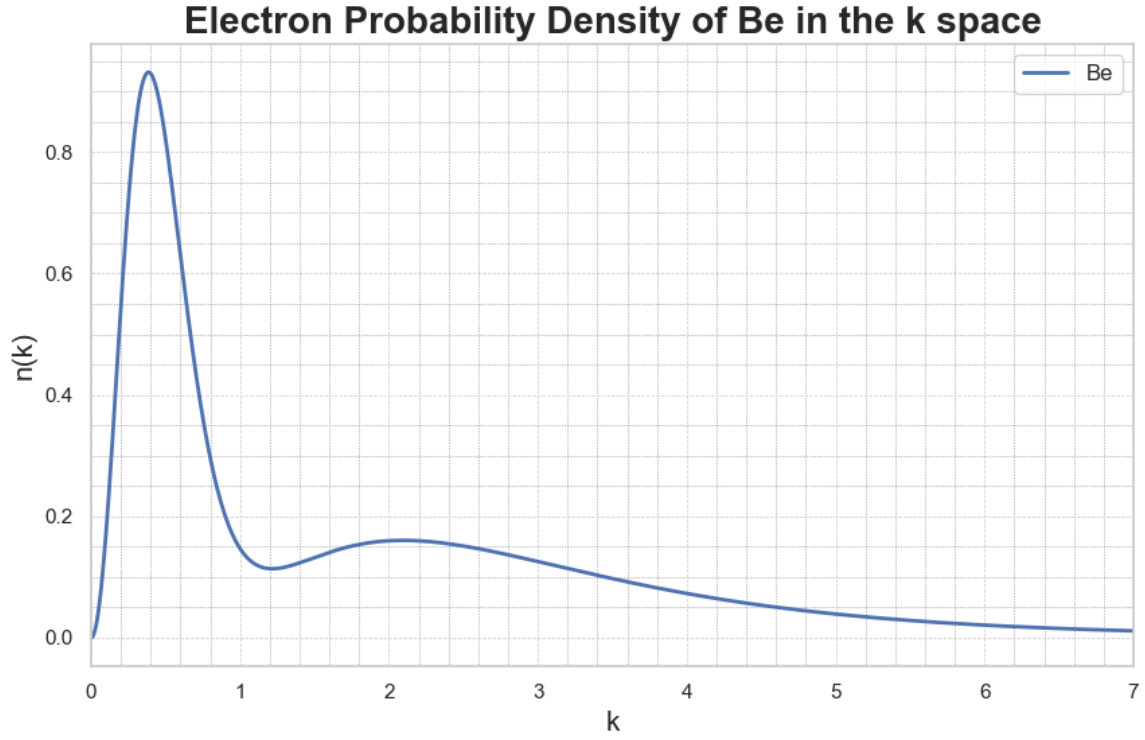


Figure 6: The electron probability density as a function of momentum for the atom of Li. Again, just like in position space, we notice the similarity with Lithium.

2.3.2 Shannon Entropies

Table 3: Entropies Calculation for Beryllium (Be)

Entropies	Calculation
S_r	3.62385902268
S_k	4.19018755678
S_{total}	7.81404657946

Again the same behavior and "width" of the densities leads in the similar entropy values.

2.4 Boron (B)

2.4.1 Probability Densities

The electron configuration of Boron is $1s^2 2s^2 2p^1$. We plot the densities and we get:

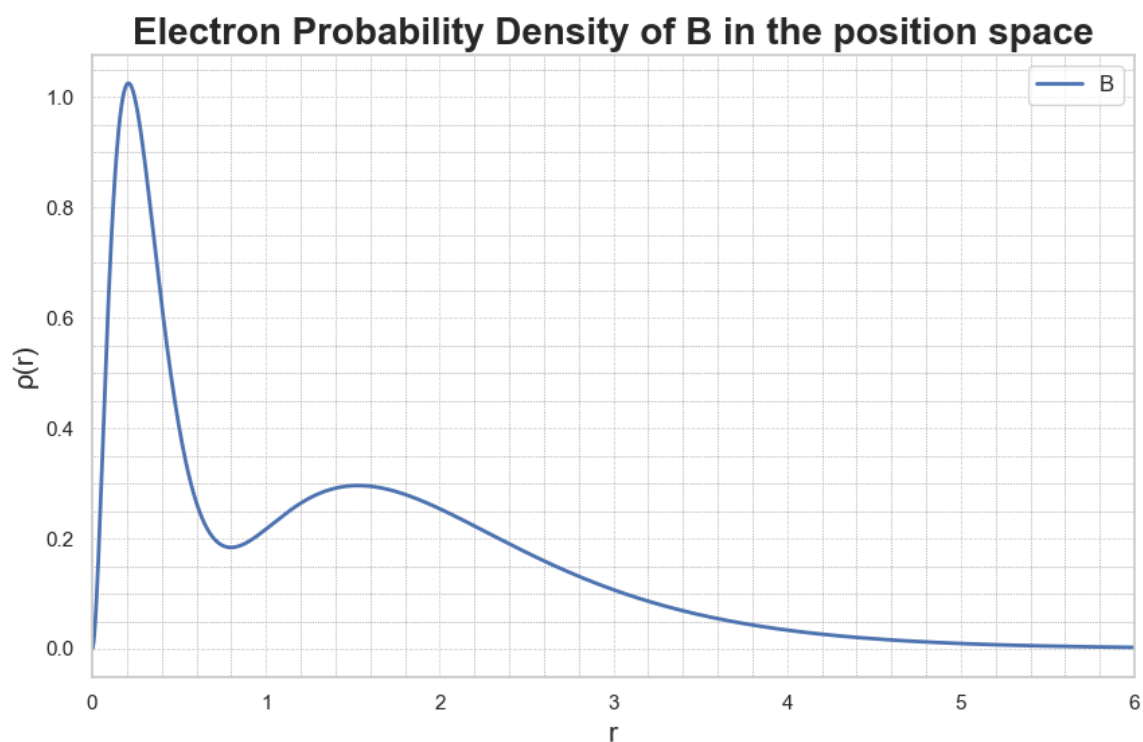


Figure 7: The electron probability density as a function of the distance from the center of the atom of B. We notice that the second bump has a higher probability in comparison to Be, along with a smaller decline, justified from the existence of the $2p$ electron.

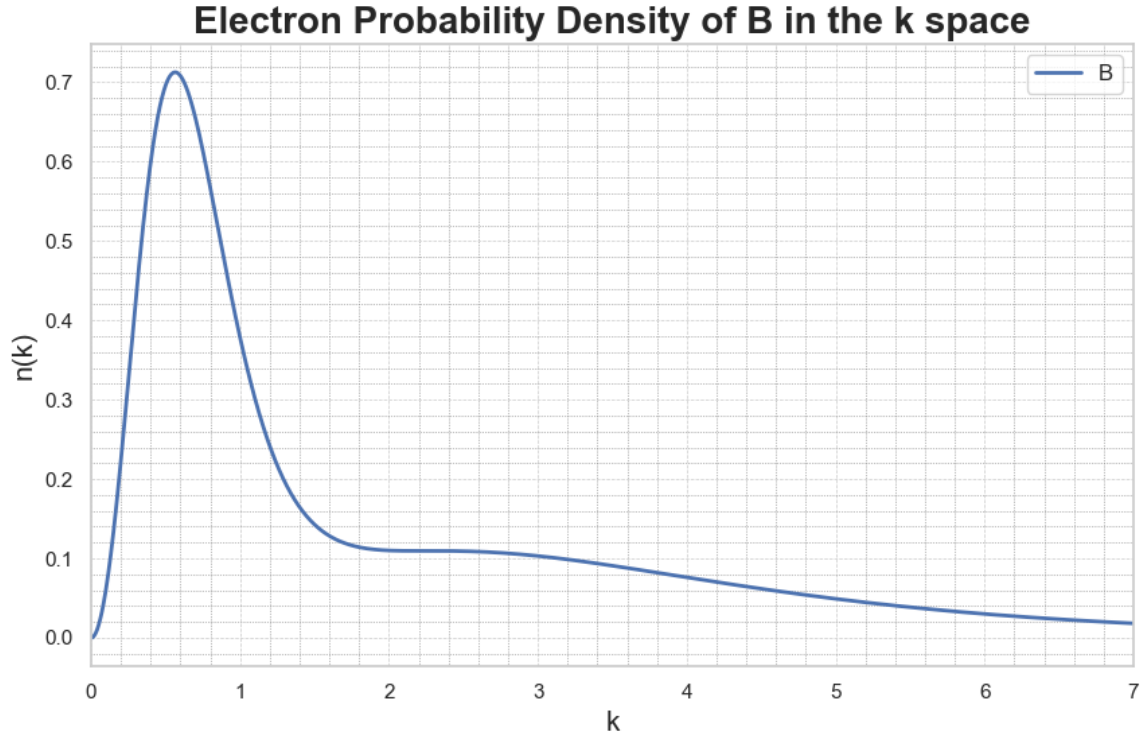


Figure 8: The electron probability density as a function of momentum for the atom of B. Clearly higher probability in finding higher energy electrons because of the slower decline.

2.4.2 Shannon Entropies

Table 4: Entropies Calculation for Boron (B)

Entropies	Calculation
S_r	3.40544522715
S_k	4.70590178737
S_{total}	8.11134701452

Because the density in k-space doesn't have a second peak, its probability is more spread out and so its entropy is bigger.

2.5 Carbon (C)

2.5.1 Probability Densities

The electron configuration of Carbon is $1s^2 2s^2 2p^2$. We plot the densities and we get:

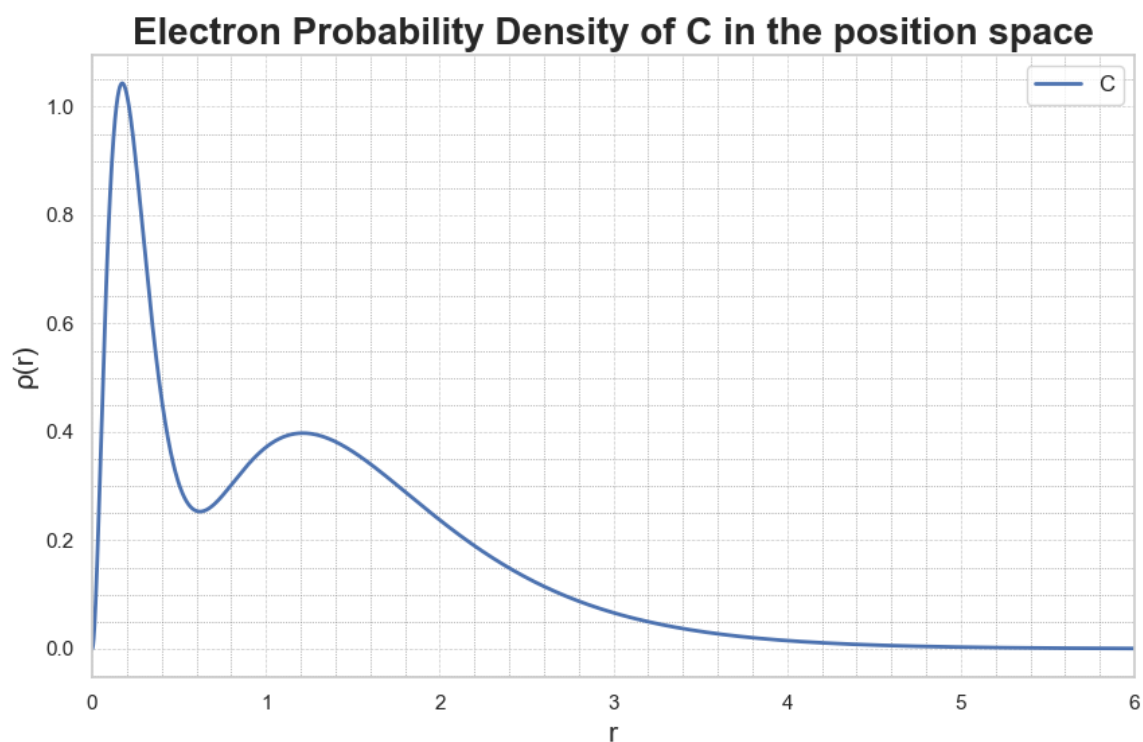


Figure 9: The electron probability density as a function of the distance from the center of the atom of C. We notice a higher probability than all the previous elements away from the nucleus.

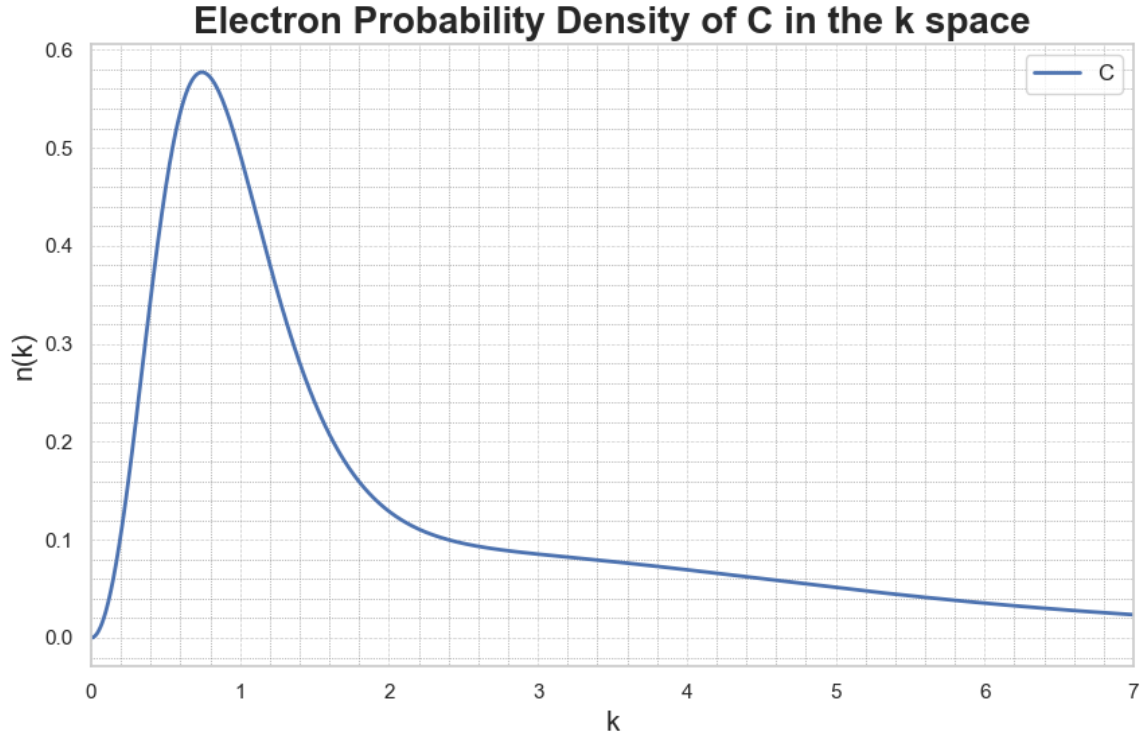


Figure 10: The electron probability density as a function of momentum for the atom of C. The decline is even slower now than that of B and so even higher energy electrons are found.

2.5.2 Shannon Entropies

Table 5: Entropies Calculation for Carbon (C)

Entropies	Calculation
S_r	3.1060249538
S_k	5.15657627645
S_{total}	8.26260123025

The entropy in k-space is bigger because of the slow, steady decline of the probability density in k-space, while the second bump of the corresponding one in r-space declines more rapidly and hence is narrower.

2.6 Nitrogen (N)

2.6.1 Probability Densities

The electron configuration of Nitrogen is $1s^2 2s^2 2p^3$. We plot the densities and we get:

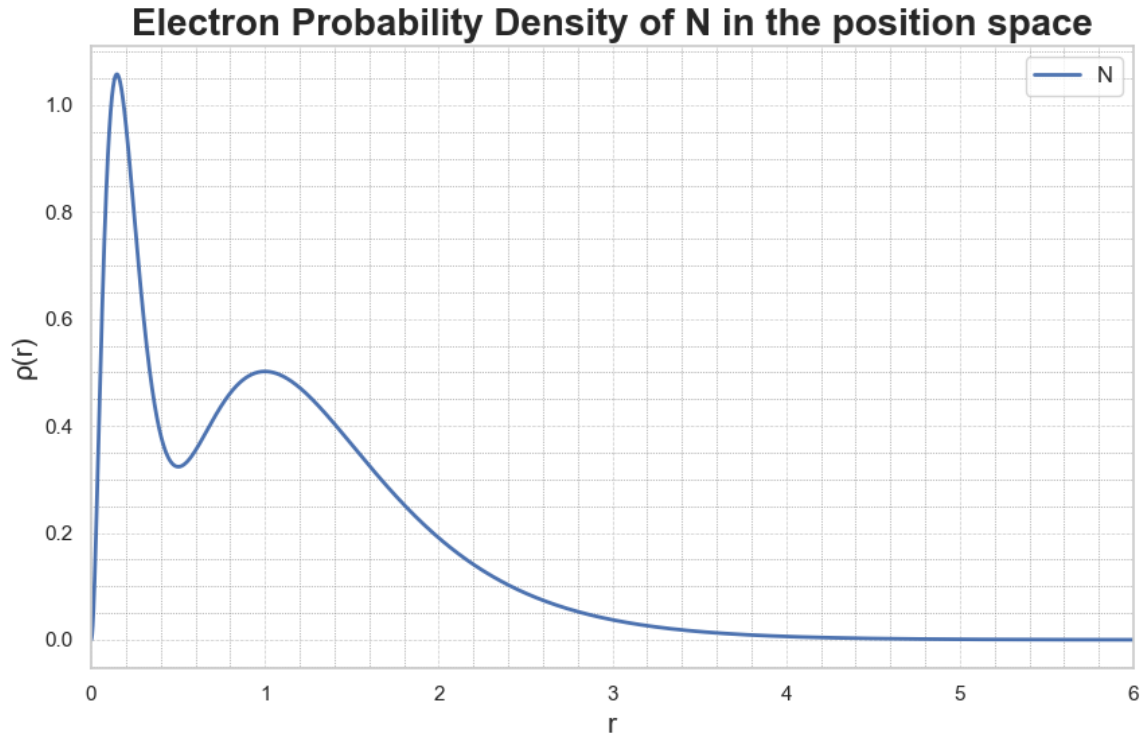


Figure 11: The electron probability density as a function of the distance from the center of the atom of N.

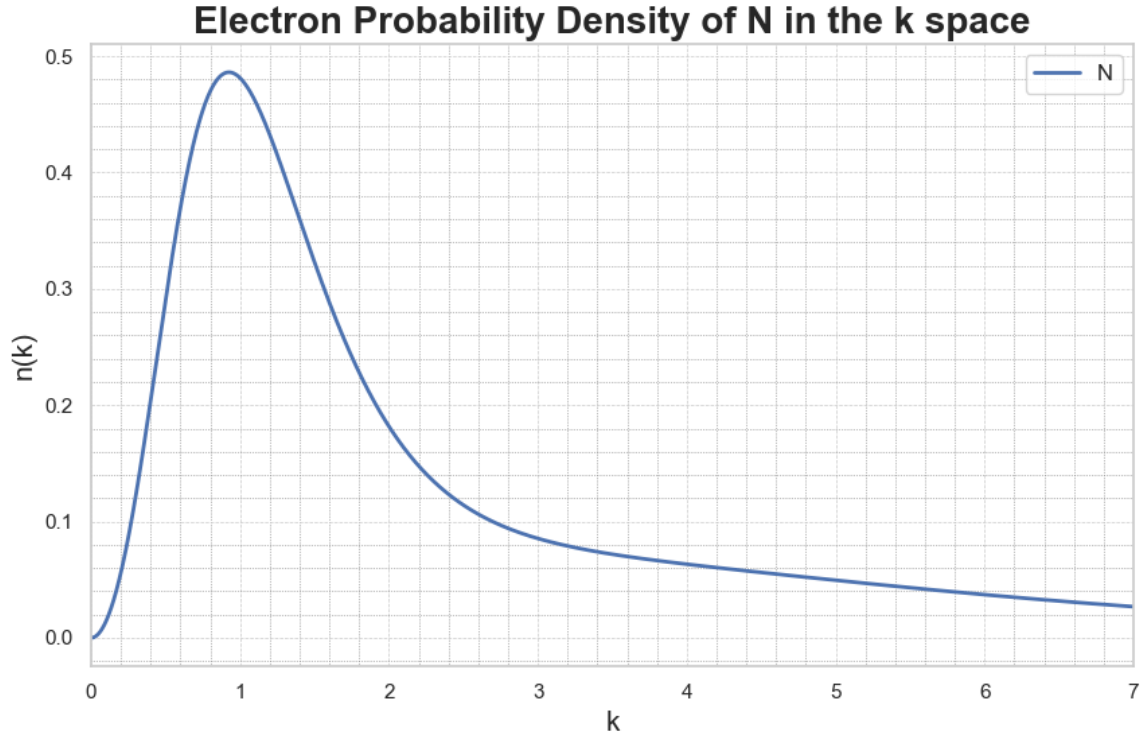


Figure 12: The electron probability density as a function of momentum for the atom of N.

2.6.2 Shannon Entropies

Table 6: Entropies Calculation for Nitrogen (N)

Entropies	Calculation
S_r	2.80168815405
S_k	5.54933715739
S_{total}	8.35102531144

The pattern is now clear that when the density plot is wider, since it will be harder to define the characteristics of the electrons, the corresponding entropy will be bigger.

2.7 Oxygen (O)

2.7.1 Probability Densities

The electron configuration of Oxygen is $1s^2 2s^2 2p^4$. We plot the densities and we get:

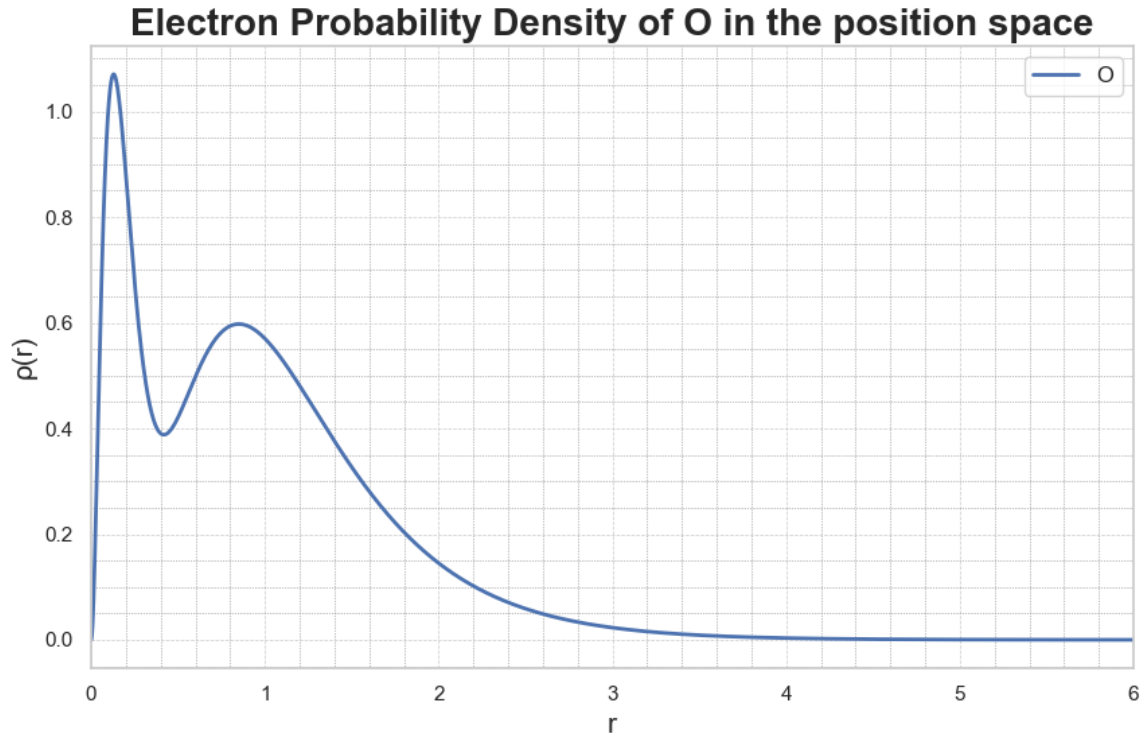


Figure 13: The electron probability density as a function of the distance from the center of the atom of O. The second bump is coming closer to the nucleus, since the number of protons inside it is bigger, and of course its probability gets bigger while the peak gets narrower.

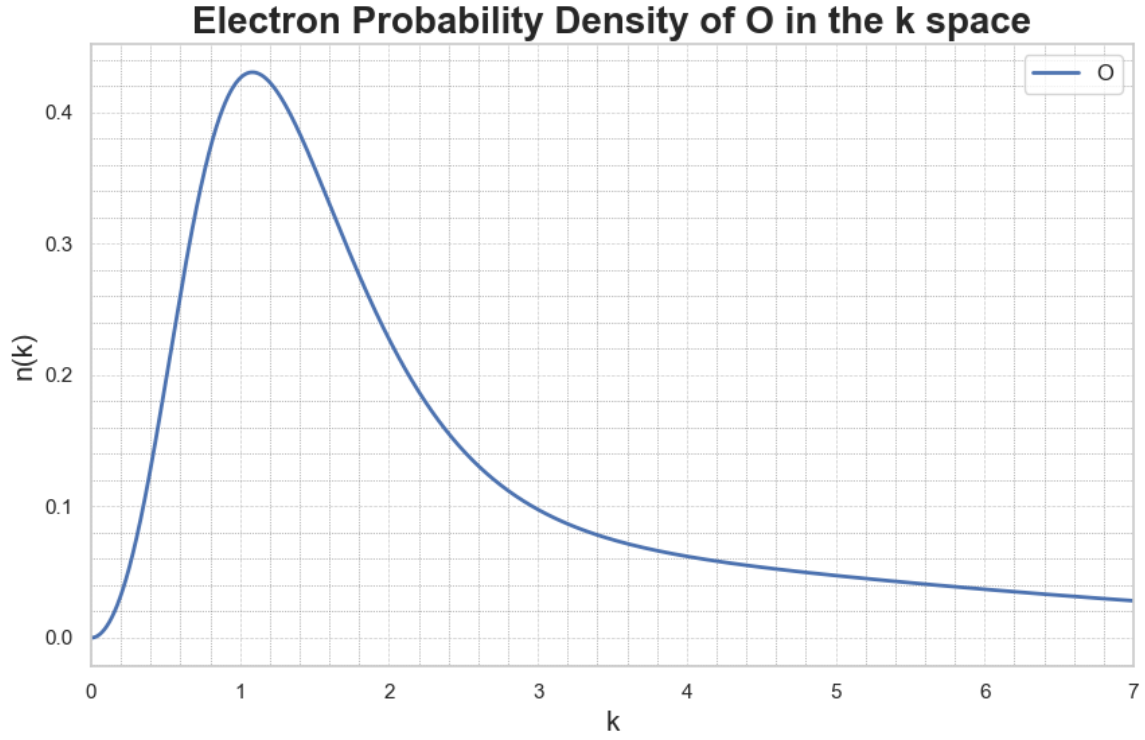


Figure 14: The electron probability density as a function of momentum for the atom of O. We notice the peak getting away from zero, meaning more and more found electrons are going to be found with higher energies.

2.7.2 Shannon Entropies

Table 7: Entropies Calculation for Oxygen (O)

Entropies	Calculation
S_r	2.55053873396
S_k	5.86735360143
S_{total}	8.41789233539

Again the k-space peaks are wider than those of the r-space.

2.8 Fluorine (F)

2.8.1 Probability Densities

The electron configuration of Fluorine is $1s^2 2s^2 2p^5$. We plot the densities and we get:

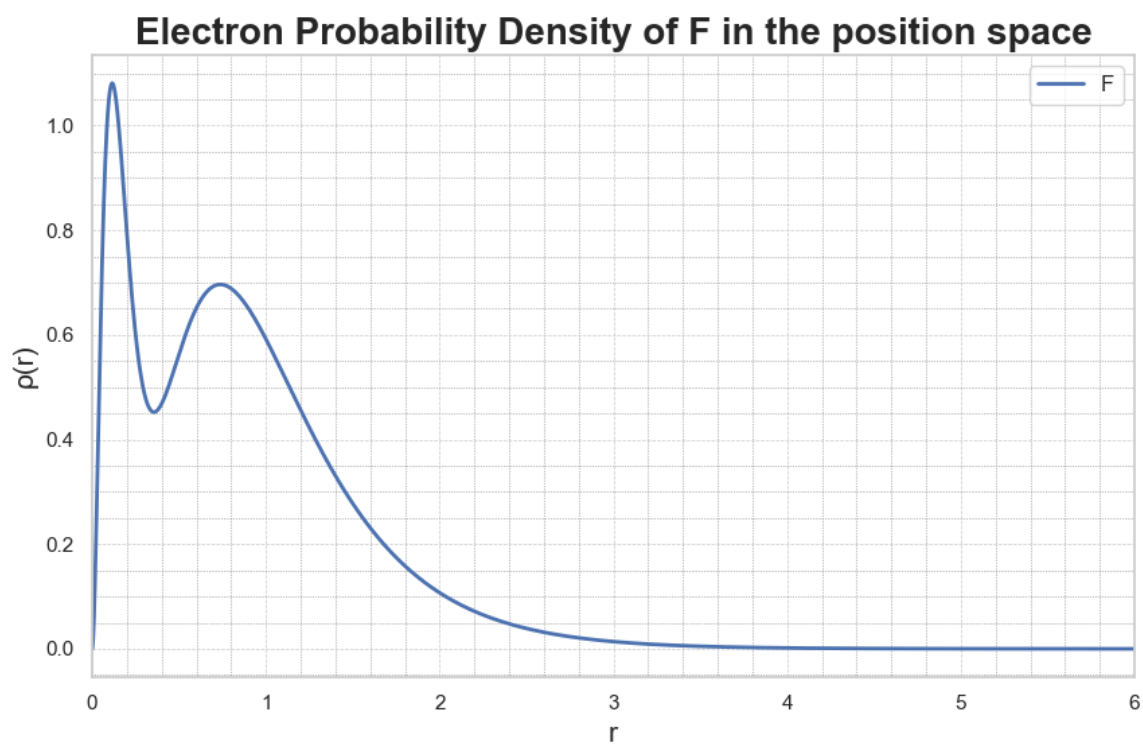


Figure 15: The electron probability density as a function of the distance from the center of the atom of F.

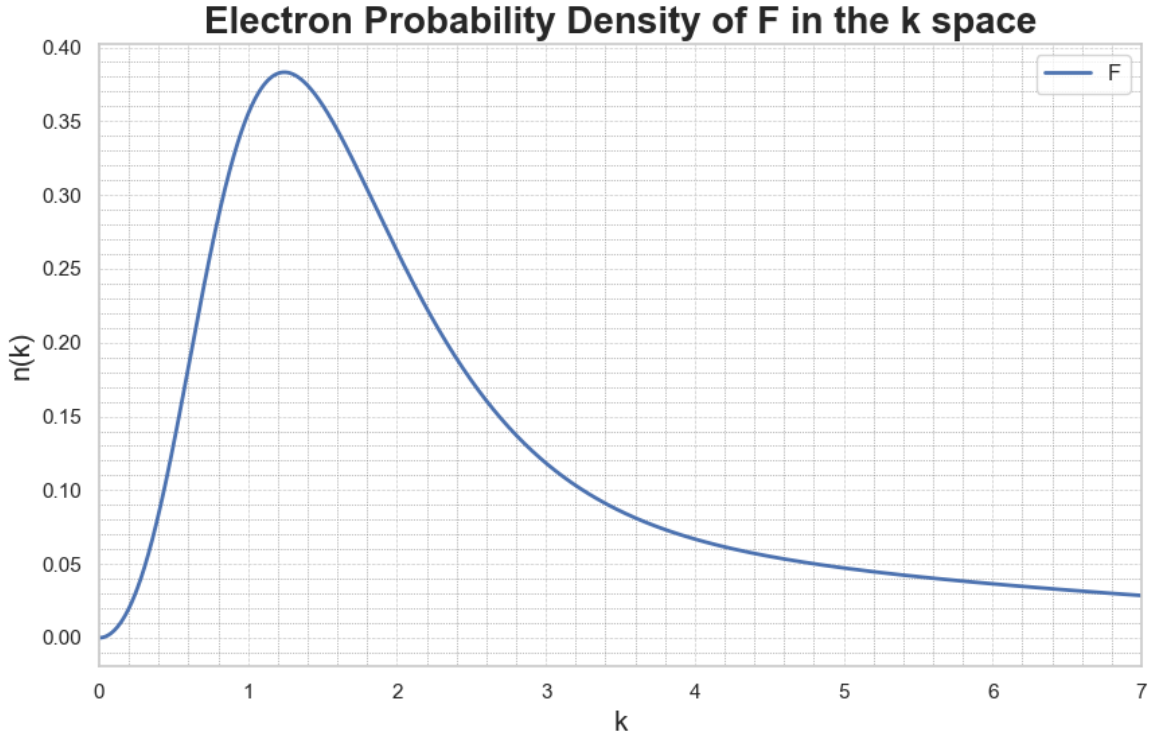


Figure 16: The electron probability density as a function of momentum for the atom of F.

2.8.2 Shannon Entropies

Table 8: Entropies Calculation for Fluorine (F)

Entropies	Calculation
S_r	2.29882699944
S_k	6.16332518286
S_{total}	8.46215218231

We see that the entropy values for the r-space exhibit minimal variation, while the k-space values get constantly bigger.

2.9 Neon (Ne)

2.9.1 Probability Densities

The electron configuration of Neon is $1s^2 2s^2 2p^6$. We plot the densities and we get:

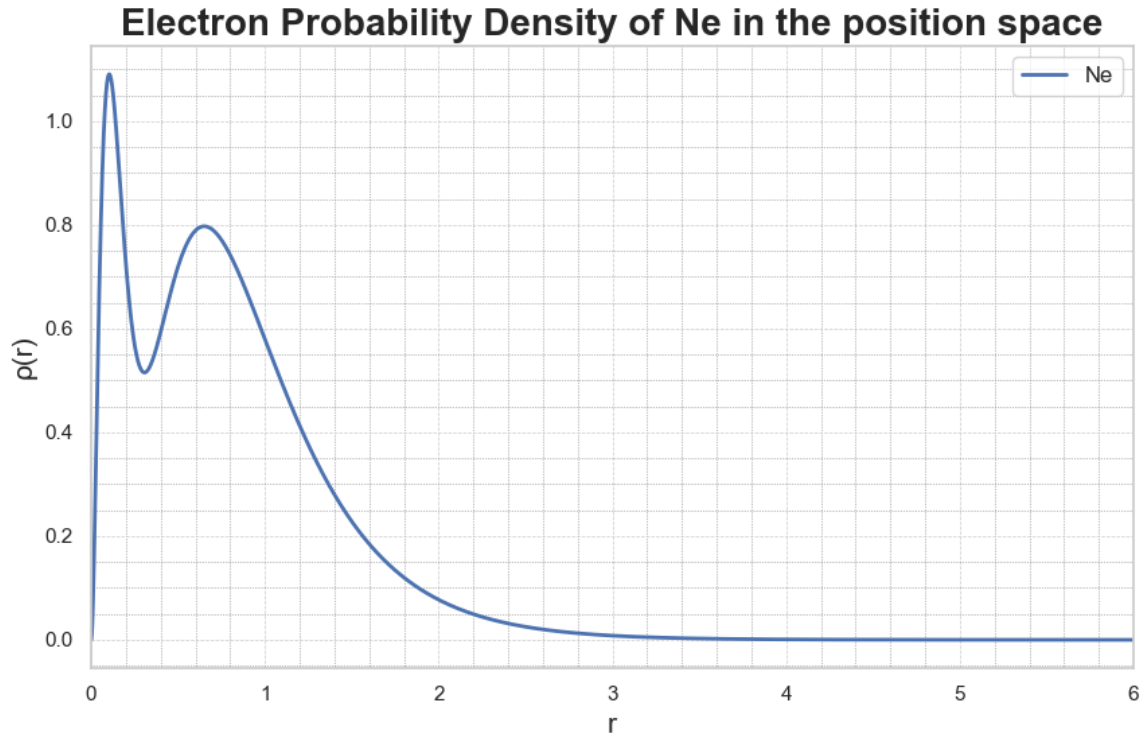


Figure 17: The electron probability density as a function of the distance from the center of the atom of Ne. We see that slowly the second bump merges into the peak because of the strong pull of the nucleus.

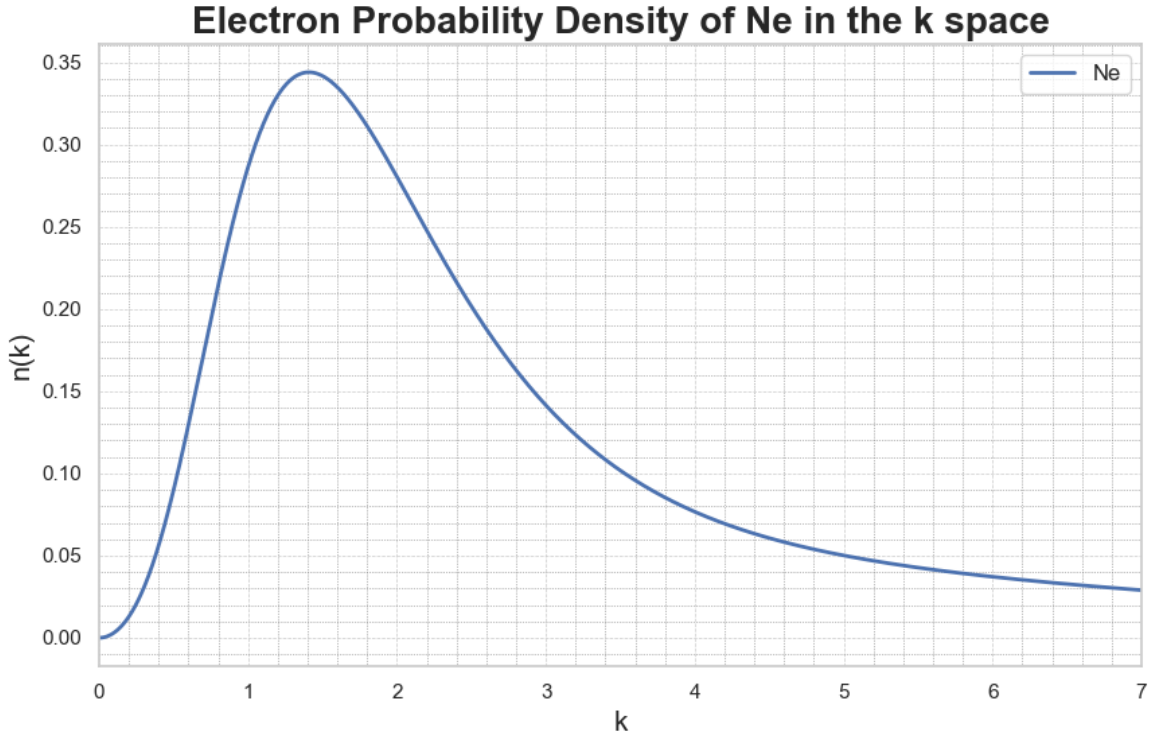


Figure 18: The electron probability density as a function of momentum for the atom of Ne. It is clear that the peak is again moving away from 0.

2.9.2 Shannon Entropies

Table 9: Entropies Calculation for Neon (Ne)

Entropies	Calculation
S_r	2.05513774324
S_k	6.43706852125
S_{total}	8.49220626449

We see that the difficulty in predicting the momentum of an electron results in a high entropy value in the corresponding space.

2.10 Entropy as a function of Z

Now we collected the values of S_r , S_k and S_{total} and plotted them along the atomic number Z to analyze the correlation between the two quantities.

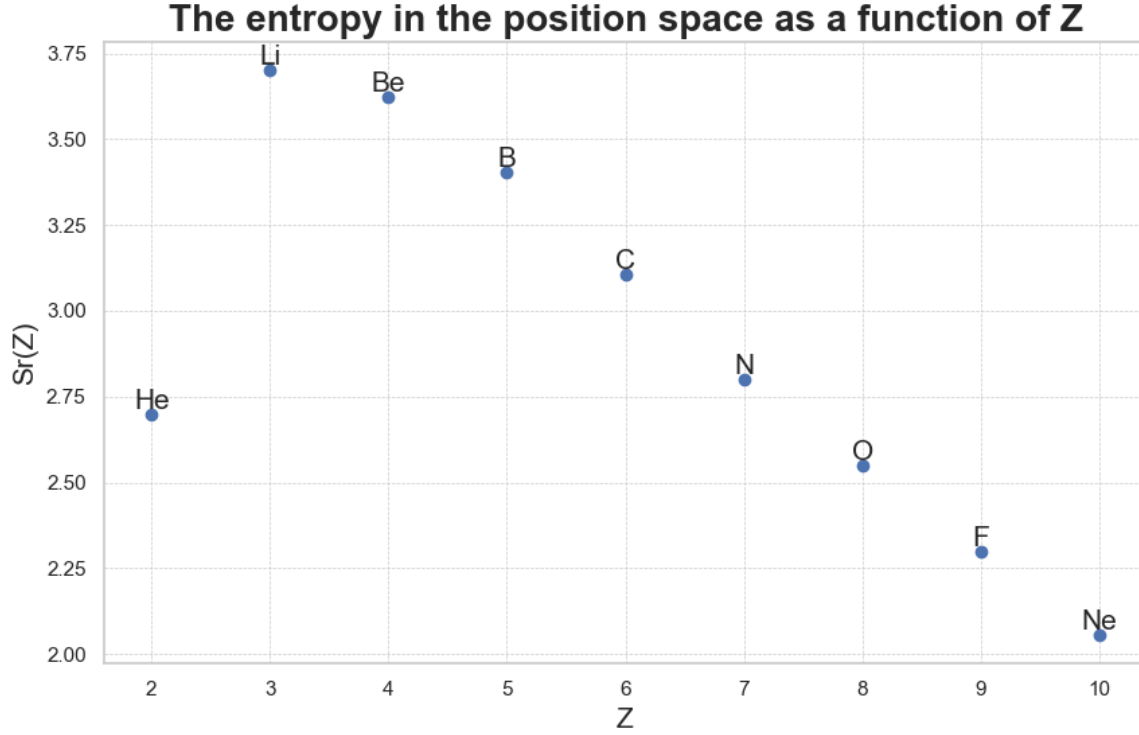


Figure 19: The entropy in the position space as a function of the atomic number Z . We notice the relatively linear decline as we go up to heavier nuclei.

We observe that Helium does not stand on top of the line from Lithium to Neon. This could be justified from the fact that it has its electron only in orbitals with $n=1$, and so it can be found in a small sphere around its nucleus, resulting in a smaller entropy than the rest of the elements.

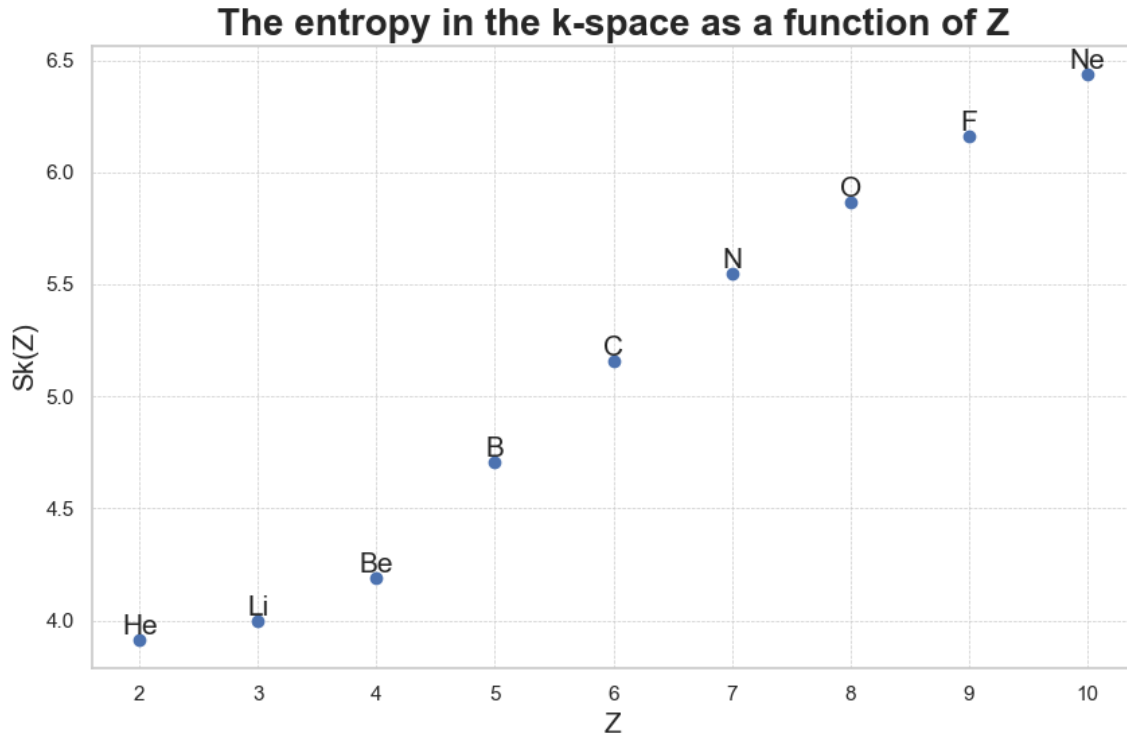


Figure 20: The entropy in the momentum space as a function of the atomic number Z . It is clear that the entropy increases almost linearly as Z increases.

The higher energy of electrons at the outermost shells of the atom makes them harder to be specified exactly and so we have a bigger entropy value.

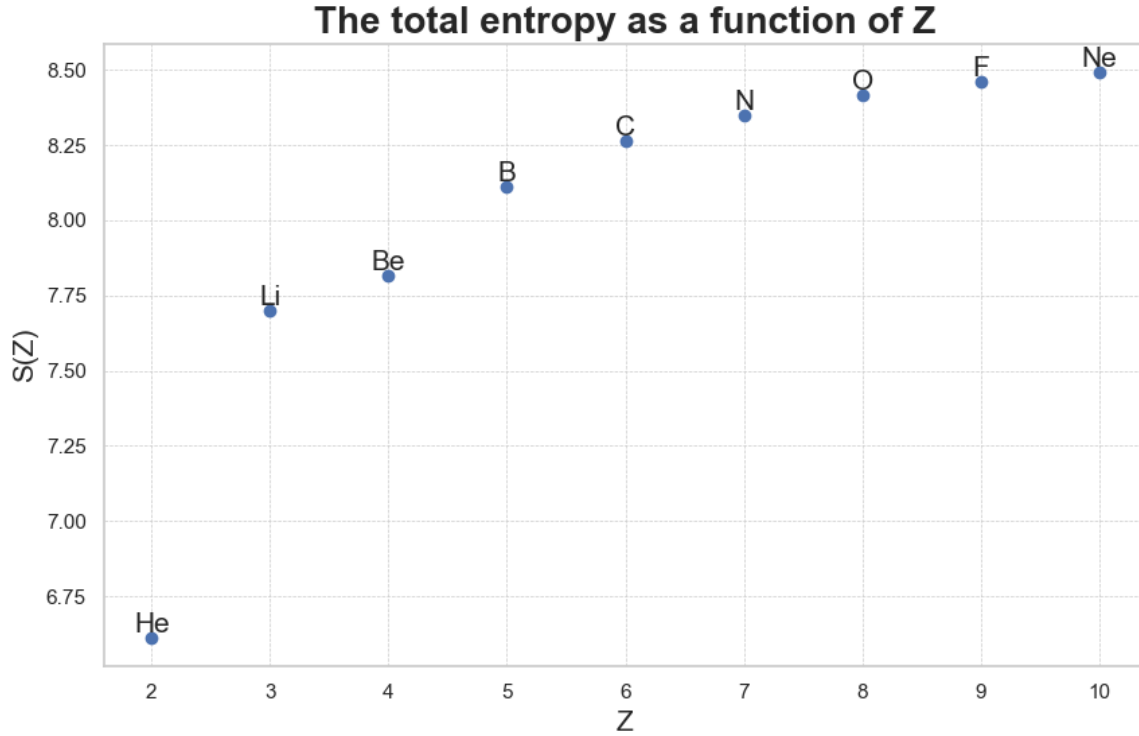


Figure 21: The total entropy as a function of the atomic number Z . It is clear that the entropy increases almost linearly as Z increases.

Apparently, the low values of entropy in position space for helium significantly impact its total entropy, resulting in a substantially lower total entropy compared to rest of the elements that we studied. [3]

3 Conclusions

From the aggregate of the probability density plots, we conclude that the second peak in the radial distribution function, corresponding to electrons with the principal quantum number $n = 2$, shifts closer to the nucleus as the atomic number Z increases. This indicates that as the number of protons in the nucleus increases, the electrostatic attraction on these electrons becomes stronger, causing them to be drawn closer to the nucleus. Furthermore, the fact that the two peaks of r -space probability density tend to merge, reduces the r -space entropy, resulting in its decrease, as Z increases. Additionally, as the atomic number increases, the peak of the k -space distribution for each element shifts further from the origin, reflecting the increasing energy of the outer electrons. With this shift, we also observe the peak broadening, which accounts for the continuous increase in k -space entropy as we move to elements with higher atomic numbers.

Bibliography

- [1] Claudio Amovilli and Franca Maria Floris. “Shannon entropy in atoms: a test for the assessment of density functionals in Kohn-Sham theory”. In: *Computation* 6.2 (2018), p. 36.
- [2] Angel Ballesteros and Ivan Gutierrez-Sagredo. “Shannon information entropy for a quantum nonlinear oscillator on a space of non-constant curvature”. In: *Physica D: Nonlinear Phenomena* 445 (2023), p. 133618.
- [3] Carlos F Bunge, Jose A Barrientos, and A Vivier Bunge. “Roothaan-Hartree-Fock ground-state atomic wave functions: Slater-type orbital expansions and expectation values for $Z=2-54$ ”. In: *Atomic data and nuclear data tables* 53.1 (1993), pp. 113–162.
- [4] K Ch Chatzisavvas, Ch C Moustakidis, and CP Panos. “Information entropy, information distances, and complexity in atoms”. In: *The Journal of chemical physics* 123.17 (2005).
- [5] GJ Gounaris, EA Paschos, and PI Porfyriadis. “Electron spectra in the ionization of atoms by neutrinos”. In: *Physical Review D—Particles, Fields, Gravitation, and Cosmology* 70.11 (2004), p. 113008.