Aristotle University of Thessaloniki
Physics Department
MSc Computational Physics

Final Project 1:
Ground state atomic orbitals from *He* to *Ne*

Calculation and Visualization
Brief Shannon Information Entropy Analysis

Subject: Computational Quantum Physics
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1 Introduction

Calculating the wave functions for atomic orbitals can be a complex and exhaustive process. However, once the wave-functions are found, we can experiment on them by applying various metric operators or even plot them, in order to obtain useful information, about the state and behaviour of the atom. In this assignment, we will use `Python` as a programming tool for computation and visualization. Following the *Roothan-Hartree-Fock* approach, we will obtain the radial atomic orbitals from **He** ($Z = 2$) to **Ne** ($Z = 10$), both in position space and momentum space, and plot them. We will, also, calculate the *Shannon* information entropy for each atom, and perform a brief analysis of it.

2 Theoretical background

2.1 The *Roothan-Hartree-Fock* method

According to the *Roothan-Hartree-Fock* approach in [1] and [2], the radial atomic orbitals in position space $R_{nl}(r)$, are given as a finite linear combination (superposition) of primitive radial functions:

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

where C_{jln} are the coefficients of the combination and $\{S_{jl}\}$ the normalized primitive basis. The vectors $S_{jl}(r)$ are considered as *Slater*-type orbitals (STO)

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

where n_{jl} is the principal quantum number, l the azimuthal quantum number, Z_{jl} the orbital exponent and N_{jl} the normalization factor, given by

$$N_{jl} = (2Z_{jl})^{(n_{jl}+1/2)} / [(2n_{jl})!]^{1/2} \tag{3}$$

while, the normalization of $R_{nl}(r)$ demands that

$$\int_0^\infty |R_{nl}(r)|^2 r^2 dr = 1 \tag{4}$$

We move, now, to the momentum space. This can be done via the *Fourier* transformation below

$$\tilde{R}_{nl}(k) = 4\pi \int_0^\infty r^2 R_{nl}(r) j_l(kr) dr \tag{5}$$

where $j_l(kr)$ is a spherical *Bessel* function. Therefore, the radial momentum wave-functions can also be written as a finite superposition (see [3])

$$\tilde{R}_{nl}(k) = \sum_l C_{jnl} \tilde{S}_{jl}(k) \tag{6}$$

where the *Slater*-type orbitals $\tilde{S}_{jl}(k)$ in momentum space, are related to $S_{jl}(r)$ orbitals through the *Fourier* transformation below

$$\tilde{S}_{jl}(k) = 4\pi \int_0^\infty r^2 S_{jl}(r) j_l(kr) dr \tag{7}$$

The normalization of $\tilde{R}_{nl}(k)$ is such that

$$\int_0^\infty |\tilde{R}_{nl}(k)|^2 \frac{k^2 dk}{(2\pi)^3} = 1 \tag{8}$$

where the term $1/(2\pi)^3$ can be included in $\tilde{R}_{nl}(k)$ by multiplying each $\tilde{S}_{jl}(k)$ with a $1/(2\pi)^{3/2}$ factor.

2.2 Density distributions and *Shannon* information entropy

For the calculation of the *Shannon* information entropy of an atom with atomic number Z, two density distributions are needed: the electron density distribution $\rho(\mathbf{r})$, in position space, and the momentum density distribution $n(\mathbf{k})$, in momentum space, respectively. These are given by (see [2])

$$\rho(\mathbf{r}) = \frac{1}{Z} \sum_j \phi_j^*(\mathbf{r}) \phi_j(\mathbf{r})$$

$$\tag{9}$$

$$n(\mathbf{k}) = \frac{1}{Z} \sum_j \tilde{\phi}_j^*(\mathbf{k}) \tilde{\phi}_j(\mathbf{k})$$

with the index j running over all Z single-particle states and the division by Z ensures the normalization to unity. Also

$$\tilde{\phi}_j(\mathbf{k}) = \int e^{-i\mathbf{k}\mathbf{r}} \phi_j(\mathbf{r}) d\mathbf{r} \tag{10}$$

with both $\phi_j(\mathbf{r})$ and $\tilde{\phi}_j(\mathbf{k})$ be the single-particle wave functions describing the electron in an atom (in position and in momentum space respectively). They are decomposed in the usual form:

$$\phi_j(\mathbf{r}) = \phi_{nlm}(\mathbf{r}) = R_{nl}(r) Y_{lm}(\Omega_r)$$

$$\tag{11}$$

$$\tilde{\phi}_j(\mathbf{k}) = \tilde{\phi}_{nlm}(\mathbf{k}) = \tilde{R}_{nl}(k) Y_{lm}(\Omega_k)$$

where $R_n l(r)$, $\tilde{R}_n l(k)$ are the radial atomic orbitals, that take the *Roothan-Hartree-Fock* form we discussed in paragraph 2.1, and $Y_{lm}(\Omega_r)$, $Y_{lm}(\Omega_k)$ are the spherical harmonics.

In general $\rho(\mathbf{r})$ and $n(\mathbf{k})$ are not spherically symmetric but depend on the θ angle. However, in this project, we consider both $\rho(\mathbf{r})$ and $n(\mathbf{k})$ average spherically (i.e. independent from the spherical coordinates (θ, ϕ)). In this case, we can replace $Y_{lm}(\Omega_r)$ and $Y_{lm}(\Omega_k)$ in

11 with their form for $l = 0$ and $m = 0$ ($Y_{00} = 1/\sqrt{4\pi}$). That is

$$\phi_j(\mathbf{r}) = \phi_{nl}(r) = \frac{1}{\sqrt{4\pi}} R_{nl}(r)$$

$$\tilde{\phi}_j(\mathbf{k}) = \tilde{\phi}_{nl}(k) = \frac{1}{\sqrt{4\pi}} \tilde{R}_{nl}(k)$$

$$(12)$$

and the density distributions become

$$\rho(\mathbf{r}) = \rho(r) = \frac{1}{4\pi Z} \sum_{nl} A_{nl} |R_{nl}(r)|^2$$

$$n(\mathbf{k}) = n(k) = \frac{1}{4\pi Z} \sum_{nl} A_{nl} |\tilde{R}_{nl}(k)|^2$$

$$(13)$$

where the sum in 13 runs all over the atomic orbitals that are occupied by electrons and A_{nl} the number of electrons that occupy a certain orbital.

According to [2], now, the *Shannon* entropy S gives us information about the localization (or delocalization) of an atomic system. More, specifically in position space S_r determines the extent of electron delocalization, whereas S_k is an indicator of delocalized distribution in momentum space. The sum of both, gives us the total information entropy:

$$S = S_r + S_k \tag{14}$$

Up to this point, it is obvious, that S_r and S_k are directly related to the density distributions of 13. Indeed, we have the following formulas:

$$S_r = - \int \rho(\mathbf{r}) \ln \rho(\mathbf{r}) d\mathbf{r} = -4\pi \int r^2 \rho(r) \ln \rho(r) dr$$

$$S_k = - \int n(\mathbf{k}) \ln n(\mathbf{k}) d\mathbf{k} = -4\pi \int k^2 n(k) \ln n(k) dk$$

$$(15)$$

where the integrand functions

$$S_r^{loc}(\mathbf{r}) = -4\pi r^2 \rho(\mathbf{r}) \ln \rho(\mathbf{r}) = -4\pi r^2 \rho(r) \ln \rho(r)$$

$$S_k^{loc}(\mathbf{k}) = -4\pi k^2 n(\mathbf{k}) \ln n(\mathbf{k}) = -4\pi k^2 n(k) \ln n(k)$$

$$(16)$$

are the local Shannon entropies, in position and momentum spaces, respectively.

3 Methodology

We tried to make the algorithms as general as possible, so that the user can just give the atomic number of an element and some other parameters and get the desired result. To achieve this we followed the steps described in the following paragraphs.

3.1 Creating a data structure for the elements adn the orbitals

One thing that differs between the elements is of course the number of electrons in their atoms, and thus the contribution of *Slater*-type orbitals to the final shape of the radial orbitals. This difference is ensured by the changing values of the constants C_{jnl}, Z_{jl} and n_{jl}, in equations 1-3 and 6, as we move from one element to another. Thus, we define tables for each element and for each orbital with the same azimuthal quantum number l, and store the values of the principal quantum number n_{jl} (of the contributing *Slater*-type orbitals), the exponent Z_{jl} and the coefficient C_{jnl} in them (see section 1.2 in the attached `FinalProject1_RHF.ipynb` notebook).

For example, using the values listed in [1], the table for the s-orbitals of **He** $(Z = 2)$ is

$$He_s = \begin{pmatrix} n_{js} & Z_{js} & C_{j1s} \\ 1 & 1.4595 & 1.347900 \\ 3 & 5.3244 & -0.001613 \\ 2 & 2.6298 & -0.100506 \\ 2 & 1.7504 & -0.270779 \end{pmatrix} \tag{17}$$

and for the p-orbitals

$$He_p = \begin{pmatrix} n_{jp} & Z_{jp} & Cj_{2p} \\ - & - & - \end{pmatrix} \tag{18}$$

since only the $1s$ orbital is occupied by electrons in the ground state of **He**. On the other hand, the table for the s-orbitals of **Ne** $(Z = 10)$ is

$$\begin{pmatrix} n_{js} & Z_{js} & C_{j1s} & C_{j2s} \\ 1 & 13.9074 & 0.392290 & -0.053023 \\ 1 & 8.2187 & 0.425817 & 0.419502 \\ 3 & 26.0325 & -0.000702 & -0.000263 \\ 2 & 11.9249 & 0.217206 & -0.055723 \\ 2 & 4.2635 & 0.002300 & -0.349457 \\ 2 & 2.8357 & 0.000463 & -0.523070 \\ 2 & 2.0715 & 0.000147 & -0.246038 \end{pmatrix} \tag{19}$$

and for the p-orbitals

$$\begin{pmatrix} n_{jp} & Z_{jp} & C_{j2p} \\ 2 & 12.3239 & 0.004391 \\ 2 & 5.6525 & 0.133955 \\ 2 & 3.5570 & 0.342978 \\ 2 & 2.2056 & 0.395742 \\ 2 & 1.4948 & 0.221831 \end{pmatrix} \tag{20}$$

since in the ground state of **Ne** the electrons are distributed in the orbitals $1s$, $2s$ and $2p$. Notice, also, that we do not proceed further than the orbital $2p$, since **Ne** is the last element in our study.

We proceed by storaging the aforementioned tables into a general list for each element and, thus, forming a first layer of nested lists. That is

$$He = \begin{bmatrix} He_s, & He_p \end{bmatrix} \tag{21}$$

and

$$Ne = \begin{bmatrix} Ne_s, & Ne_p \end{bmatrix} \tag{22}$$

for **He** and **Ne**, respectively. Finally, we store these lists into a total list that contains, also, the atomic number Z of each element and its name. This is the second layer of nested lists in our algorithm, regarding the elements data structure and has the following form:

$$\text{elements} = \begin{bmatrix} 2 & He & \text{'He'} \\ 3 & Li & \text{'Li'} \\ 4 & Be & \text{'Be'} \\ 5 & B & \text{'B'} \\ 6 & C & \text{'C'} \\ 7 & N & \text{'N'} \\ 8 & O & \text{'O'} \\ 9 & F & \text{'F'} \\ 10 & Ne & \text{'Ne'} \end{bmatrix} \tag{23}$$

Our data structure is combined with two scanning functions, `find_elmt_data(Z)` and `find_elmt_name(Z)`, that search in the structure by entering the atomic number and return the corresponding element's data or name (if the atomic number is included on the structure).

As of the orbitals, we define a table that contains the azimuthal quantum number on the 1st column and the corresponding name in the 2th column. That is:

$$\begin{bmatrix} 0 & \text{'s'} \\ 1 & \text{'p'} \\ 2 & \text{'d'} \\ 3 & \text{'f'} \end{bmatrix} \tag{24}$$

We combine this list with the scanning function `find_orb_name(n,l)` that returns the orbital's name by entering its principal n and azimuthal l quantum numbers. For example, for $n = 2$ and $l = 1$ the algorithm will return '2p'.

3.2   Calculating the radial atomic orbitals in position space

Having the elements' and orbitals' data structures ready, we proceed to the calculation of the radial atomic orbitals $R_{nl}(r)$ in position space (see section 1.3 in the `FinalProject1_RHF.ipynb` notebook). We use the general formulas of 1–3 and define the respective functions `Njl(z,n)`, `Srjl(r,z,n)` and `Rnl(r,n,l,Z)`, with `n` the principal quantum number, `l` the azimuthal quantum number, `z` the orbital's exponent Z_{jl} and `Z` the atomic number.

Analyzing further, the operation of the `Rnl(r,n,l,Z)` function, that calculates the orbital $R_{nl}(r)$, its algorithm scans the elements' data structure of 23 provided the atomic number and obtains the respective element's list (like the ones in 21 and 22). Then, it obtains the orbital's data (like the ones of 17-20) with respect to the given value of azimuthal number l. Finally, it performs an iterative sequence (with j as the iterations index) for the linear combination that results to the final $R_{nl}(r)$ value. Notice, that we can input r as a symbol or as a number, and obtain the expression or a value of $R_{nl}(r)$, respectively.

Regarding, the *Slater*-type orbitals involved in the calculations of $R_{nl}(r)$ in our study, these are $1s$, $2s$, $3s$ and $2p$, according to [1], with

$$S_{1s}(r,z) = 2z^{3/2}e^{-zr}$$

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

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

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

(25)

their respective formulas. Finally, we include the function `I_Rnl(r,n,l,Z)`, that calculates the integral of 4, to confirm the correct normalization of $R_{nl}(r)$ and a plotting function `plot_Rnl(min_r,max_r,n,l,Z,axis)`.

3.3 Calculating the radial atomic orbitals in momentum space

Moving on to the calculation of the radial atomic orbitals $\tilde{R}_{nl}(\mathrm{k})$ in momentum space (see section 1.4 in the `FinalProject1_RHF.ipynb` notebook). This time we work differently. Since, we don't have a general formula, we have to write each of the contributing $\tilde{S}_{jl}(k)$ orbital's formula separately. That is, we have to define functions that are the *Fourier* transformations of the orbitals in 25, including the factor $1/(2\pi)^{3/2}$ we discussed in paragraph 2.1. Then we define a function that stores these transformations in a `Sympy` matrix. This matrix is going to be the general formula for our study, since it contains all the needed *Slater*-type orbitals in momentum space. We have

$$\tilde{S}_{jl}(k,z) = \begin{pmatrix} \tilde{S}_{1s}(k,z) & NaN \\ \tilde{S}_{2s}(k,z) & \tilde{S}_{2p}(k,z) \\ \tilde{S}_{3s}(k,z) & \tilde{S}_{3p}(k,z) \end{pmatrix}$$

(26)

with the formulas

$$\tilde{S}_{1s}(k, z) = \frac{1}{(2\pi)^{3/2}} \frac{16\pi z^{5/2}}{(z^2+k^2)^2}$$

$$\tilde{S}_{2s}(k, z) = \frac{1}{(2\pi)^{3/2}} \frac{16\pi z^{5/2}(3z^2-k^2)}{\sqrt{3}(z^2+k^2)^3}$$

$$\tilde{S}_{3s}(k, z) = \frac{1}{(2\pi)^{3/2}} \frac{64\sqrt{10}\pi z^{9/2}(z^2-k^2)}{5(z^2+k^2)^4} \tag{27}$$

$$\tilde{S}_{2p}(k, z) = \frac{1}{(2\pi)^{3/2}} \frac{64\pi k z^{7/2}}{\sqrt{3}(z^2+k^2)^3}$$

$$\tilde{S}_{3p}(k, z) = \frac{1}{(2\pi)^{3/2}} \frac{64\sqrt{10}\pi k z^{7/2}(5z^2-k^2)}{15(z^2+k^2)^4}$$

Notice that we put NaN in the position of $\tilde{S}_{1p}(k, z)$, since there is not an $1p$ orbital, and that the orbital $\tilde{S}_{3p}(k, z)$ is only defined to fill the matrix properly.

Then we define a function `Knl(k,n,l,Z)` that calculates the $\tilde{R}_{nl}(k)$ orbital. The operation of this function is identical to the one of the `Rnl(r,n,l,Z)` function we mentioned earlier, in paragraph 3.2. Here, we can input k as a symbol or as a number, and obtain the expression or a value of $\tilde{R}_{nl}(k)$, respectively. We also, include the function `I_Knl(k,n,l,Z)`, that calculates the integral of 8, to confirm the correct normalization of $\tilde{R}_{nl}(k)$ and a plotting function `plot_Knl(min_k,max_k,n,l,Z,axis)`.

3.4 Calculating the density distributions and *Shannon* entropies

We have arrived at the point of calculating the density distributions and the Shannon information entropy. As we showed in 13, it is necessary to know the distribution of electrons in the orbitals of an atom in the ground state. For this purpose we define a matrix containing the principal n and the azimuthal l quantum number of the orbitals, in the order in which they are occupied by electrons in the ground state (see section 1.5.1 in the `FinalProject1_RHF.ipynb`). That is

$$\begin{bmatrix} n & l \\ 1 & 0 \\ 2 & 0 \\ 2 & 1 \end{bmatrix} \tag{28}$$

since the filling queue is $1s, 2s, 2p$ for elements up to **Ne** (with $Z : 1 - 10$). Then, we define the function `e_orb_dist(Z)`, that returns the distribution of electrons by entering the atomic number of the element, in the form of a nested list. The first element of this list, contains an array of the number of electrons that occupy the orbitals (A_{nl} in 13) and the second element of the list the respective names of these orbitals. Thus, for $Z = 3$ we should get

$$[[2, 1], \quad ['1s', '2s']] \tag{29}$$

while for $Z = 10$ we get

$$[[2, 2, 6], \quad ['1s', '2s', '2p']] \tag{30}$$

Hence, we are ready to calculate the electron density distribution (r) (see section 1.5.2 in the `FinalProject1_RHF.ipynb`). We define the function `pr(r,Z)`, that provided an atomic number Z, finds the occupied orbitals $R_{nl}(r)$ and performs an iterative sequence, in order to include the contribution of each one of these orbitals. The final result is multiplied by $1/(4\pi Z)$ to ensure the proper normalization. To check this normalization, we define the function `I_pr(r,Z)` that calculates the integral

$$4\pi \int_0^\infty \rho(r) r^2 dr \tag{31}$$

that should return 1 (or a value very close to 1), once the normalization is correct. We also, define the functions `SR_loc(r,Z)` and `SR_tot(r,Z)`, that calculate the local $S_r^{loc}(\mathbf{r})$ and the total S_r information entropy in position space (see 15 and 16) and the plotting function `plot_pr(min_r,max_r,Z,axis)`.

The case is the same for the calculation of the momentum density distribution $n(k)$, with the definition of the function `nk(k,Z)` that operates exactly as `pr(r,Z)`, only for the $\tilde{R}_{nl}(k)$ orbitals that contribute. The function `I_nk(k,Z)`, checks the normalization by calculating the integral

$$4\pi \int_0^\infty n(k) k^2 dk \tag{32}$$

and returns 1 (or a value very close to 1), when $n(k)$ is correctly normalized. Finally, we inlclude the functions `SK_loc(k,Z)` and `SK_tot(k,Z)`, to find the local $S_k^{loc}(\mathbf{k})$ and the total S_k information entropy in momentum space (see 15 and 16) and the plotting function `plot_nk(min_k,max_k,Z,axis)`.

4 Results

Let's present and discuss, now, the results of our work. The behaviour of the electron cloud can be described through the plots of the probability $\phi_{nl}(r)$ function, in position space, and/or the plots of probability $\tilde{\phi}_{nl}(k)$ function in momentum space. To clarify, these functions are: $\phi_{nl}(r) = |r * R_{nl}(r)|^2$ and $\tilde{\phi}_{nl}(k) = |k * R_{nl}(k)|^2$, i.e. different from the ones we saw in paragraph 2.2. In Figure 1, we take the electron's behavior when occupy the 1s orbital. As we can see there is a total maximum, which becomes steeper and gets closer to the nucleus of the atom, as we move from **He** to **Ne**. This is because electrons are more attracted to the nucleus, as the atomic number Z increases, making them more likely to be closer to the center of the atom.
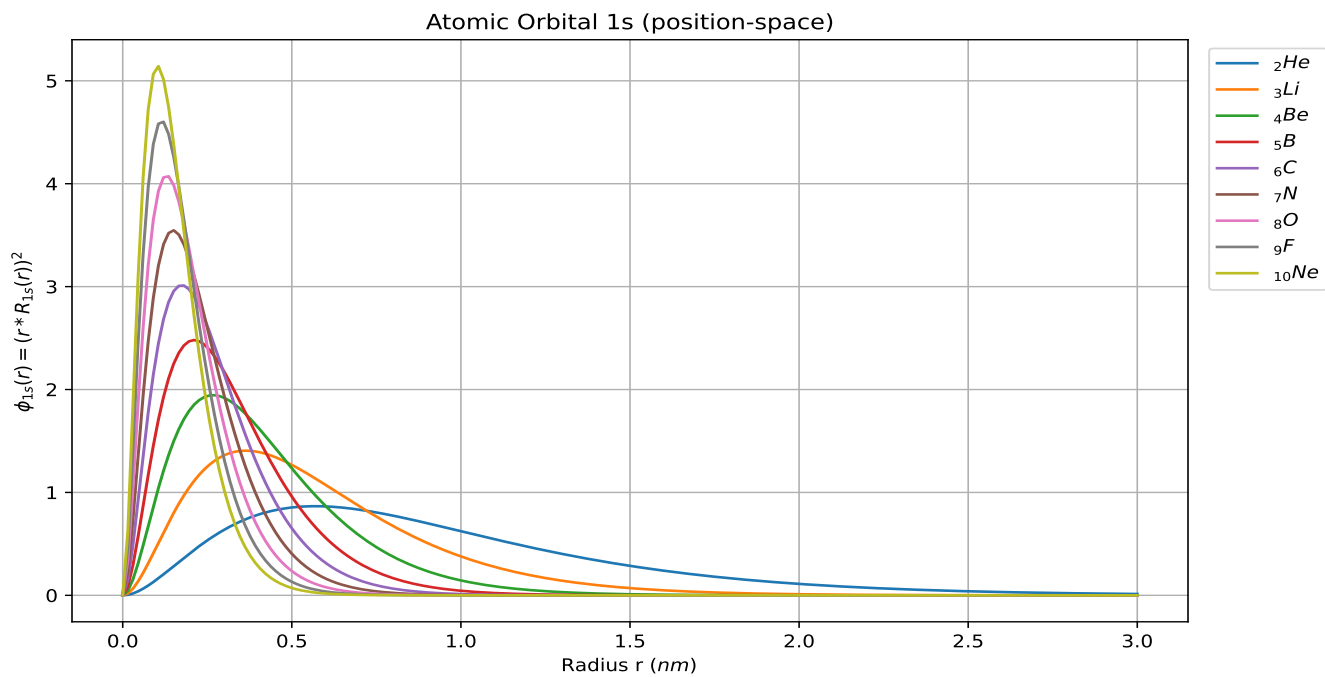
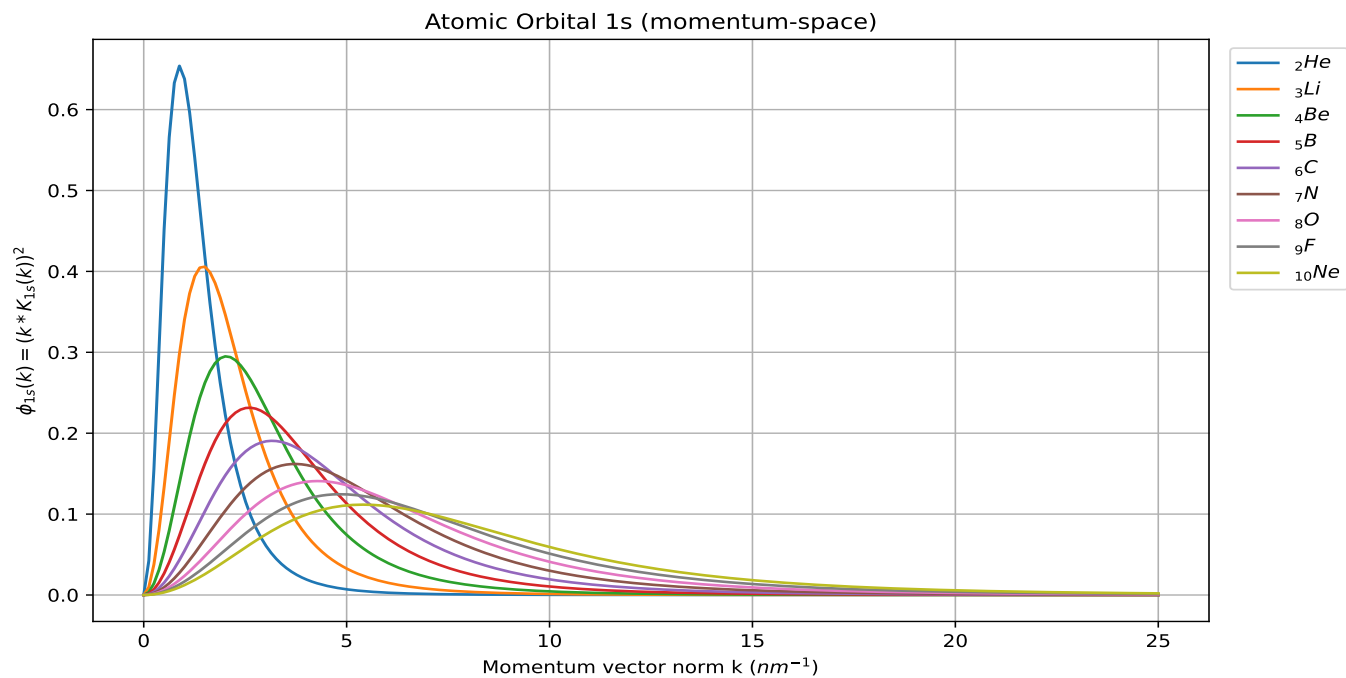Figure 1: Atomic orbital 1s (position space) for **He** to **Ne**

Figure 2: Atomic orbital 1s (momentum space) for **He** to **Ne**

On the other hand, **He** is the element that has the steeper contribution of angular momentum, as shown in Figure 2, with this contribution to become smoother as atomic number increases, meaning heavier atoms have a wider choice of total momentum, confirming *Heisenberg*'s uncertainty principle ($\Delta r \Delta k \geq \frac{1}{2}$).

Moving on, to orbital 2s in Figure 3, we observe a local and a much bigger total maximum, that become steeper in heavier elements. However, this time the total maximum is located further from the nucleus, by at least four times, due to the higher principal quantum number ($n = 2$). Notice also, that **He** does not pop-up in the plot, since it has only 2 electrons and they fully occupy the orbital 1s in ground state. However, the local maximum, indicates, that there is a small chance the electron to be located very close to the nucleus, behaving as if it were on orbital 1s.
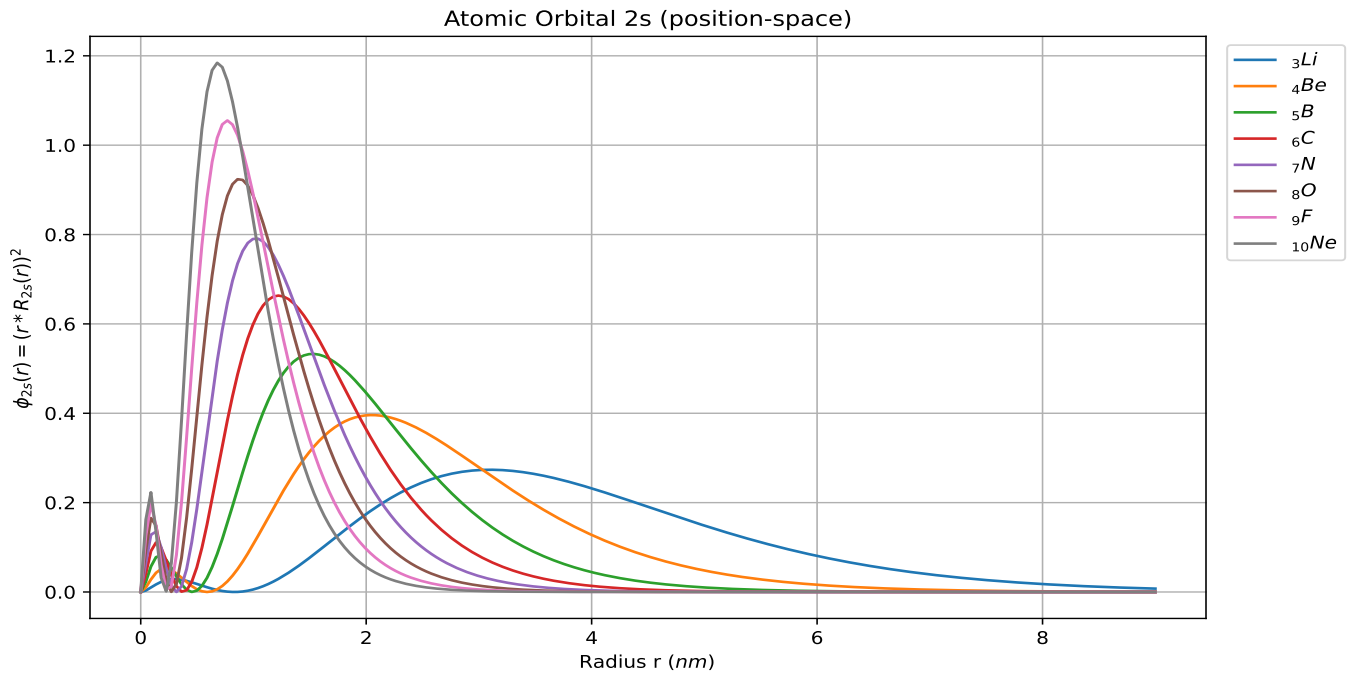

Figure 3: Atomic orbital 2s (position space) for **Li** to **Ne**

On the other hand, the total momentum contribution has the same behavior as in orbital 1s. That is, it becomes smoother as we move from **Li** to **Ne**. Only but now in a much more limited area, as depicted in Figure 4. Thus, the *Heisenberg*'s uncertainty principle is being confirmed once again.
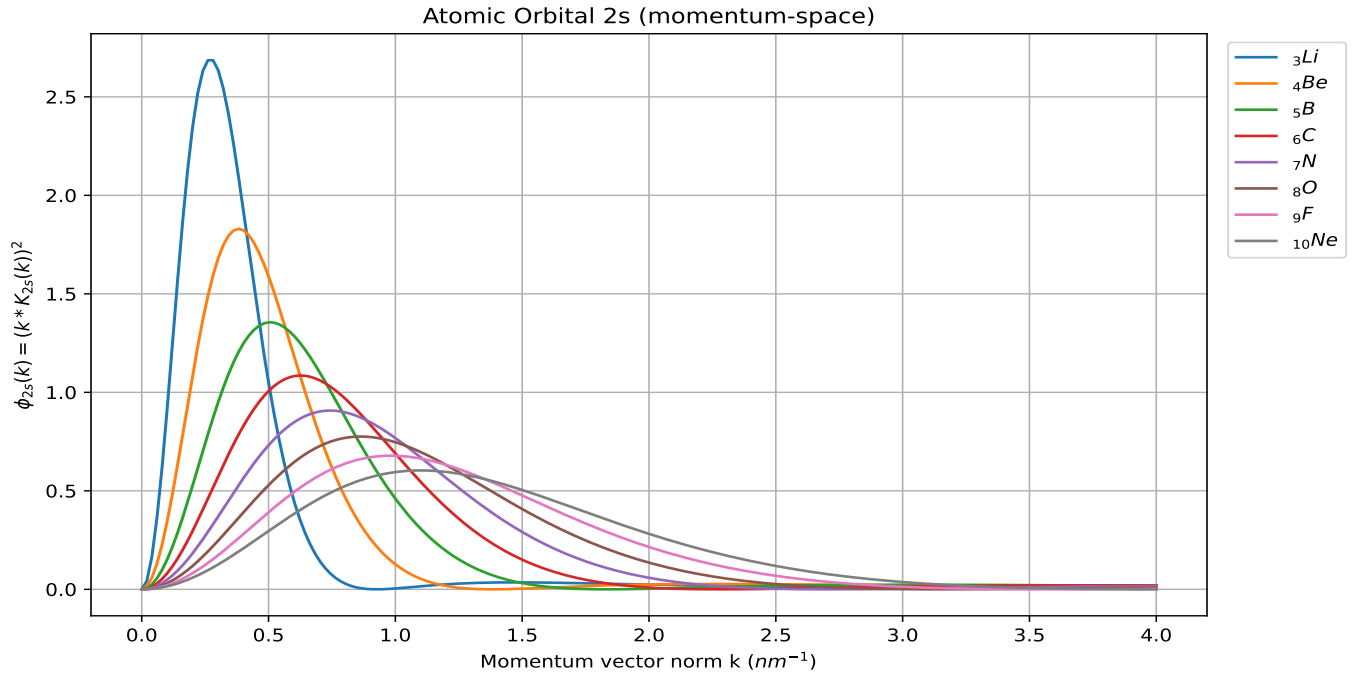
Figure 4: Atomic orbital 2s (momentum space) for **Li** to **Ne**

Finally we have the orbital 2p. The position space graph is shown below
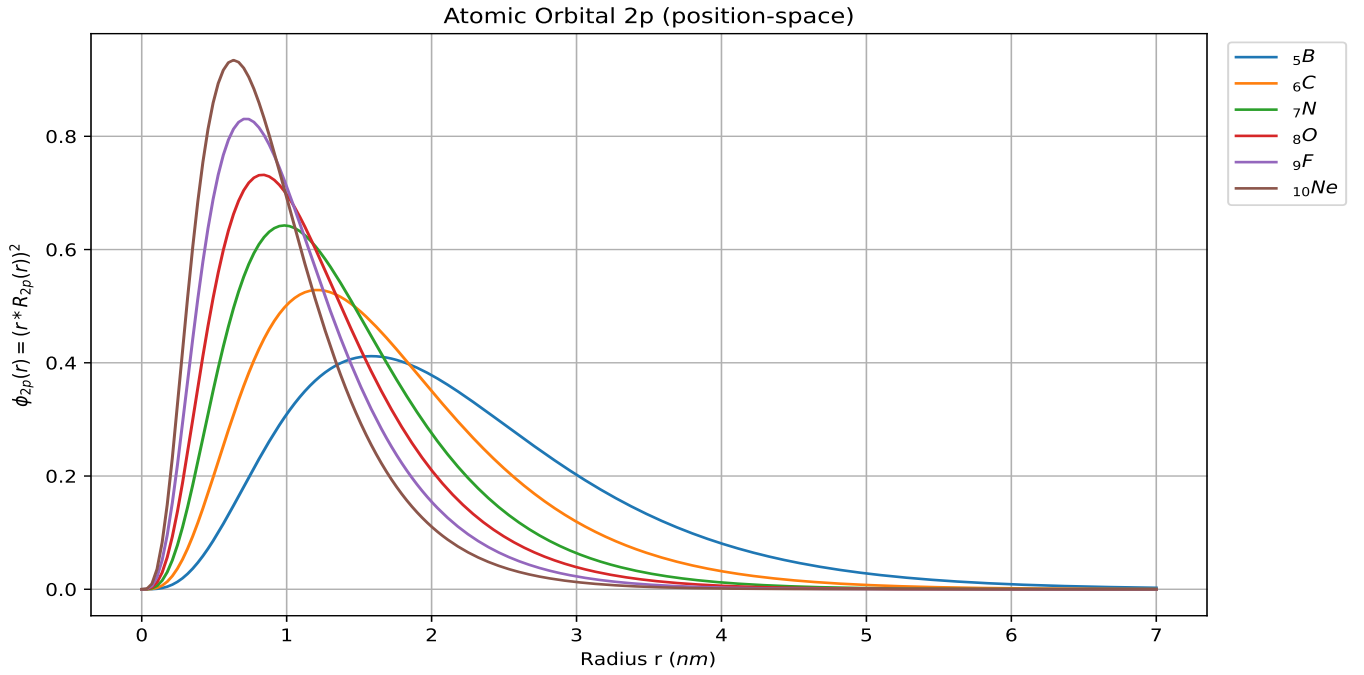

Figure 5: Atomic orbital 2p (position space) for **B** to **Ne**
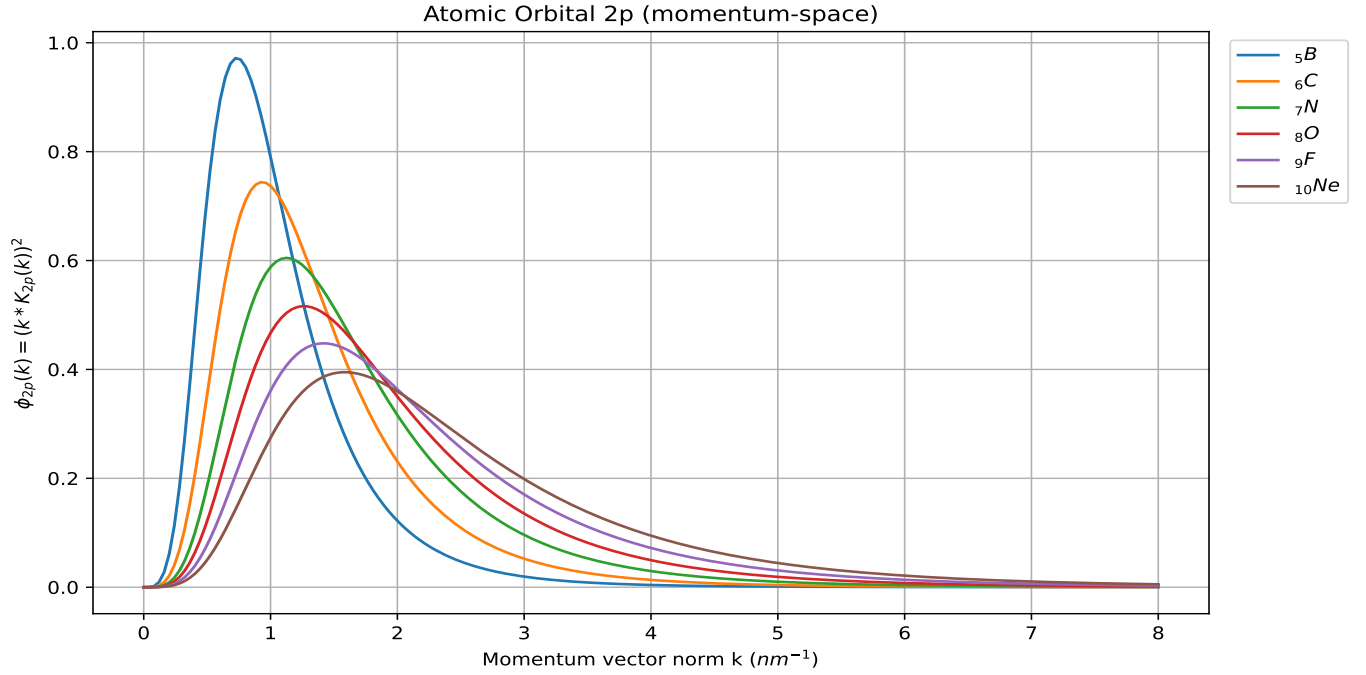
while the momentum space graph is

Figure 6: Atomic orbital 2p (momentum space) for **B** to **Ne**

Notice that we have only 6 elements in these plots, since **B** with $Z = 5$, is the first element whose electrons occupy the orbital 2p in ground state. Here we have only one, total, maximum, as shown in Figure 5 and the probability's distribution is much smoother than on the s-orbitals. Once more, though, it becomes steeper as we move to the heavier **Ne**.

On the other hand, the permissible range of momentum values is larger than the one of orbital 2s. This makes sense, as orbital's angular momentum plays a bigger role now, because the azimuthal quantum number l is now 1 and not 0, like in s-orbitals.

Now, to get an overview of the area occupied by the electron cloud of an element's atom, both in the position space and in the momentum space, we constructed the diagram of the electron density distribution: $4\pi\rho_r r^2$ and the momentum density distribution: $4\pi n_k k^2$. These graphs are presented in the two following pages.

As we can see, in Figures 7 and 8, the lightest elements **He** and **Li** with 2 and 3 electrons respectively, have only one maximum, whereas the heavier elements form a total and a local maximum. The total maximum is closest to the nucleus. Furthermore, the local maximum tends to the value of the total maximum, as we move to **Ne**. This confirms the creation of two shells in these atoms, one for $n = 1$ (**K**-shell) and one for $n = 2$ (**L**-shell). The probability gap the exists between them (between the total and the local maximum), is due to the quantum nature of the electron's trajectories.
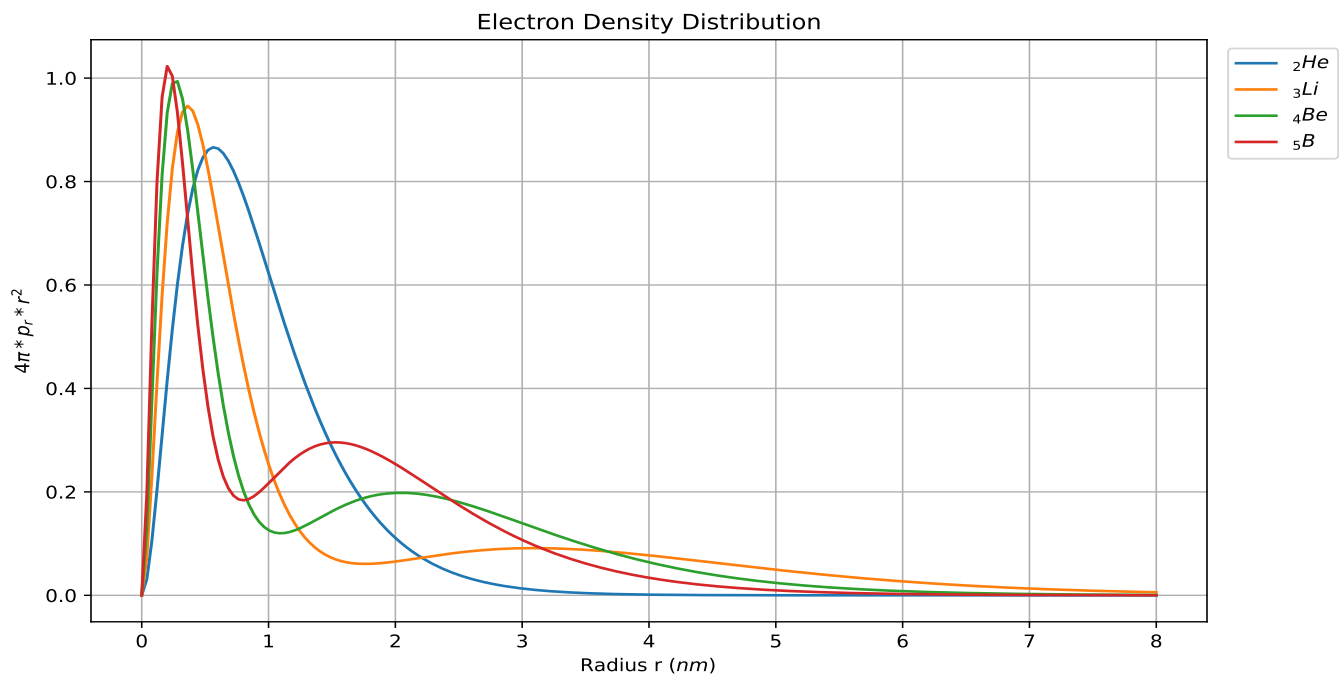
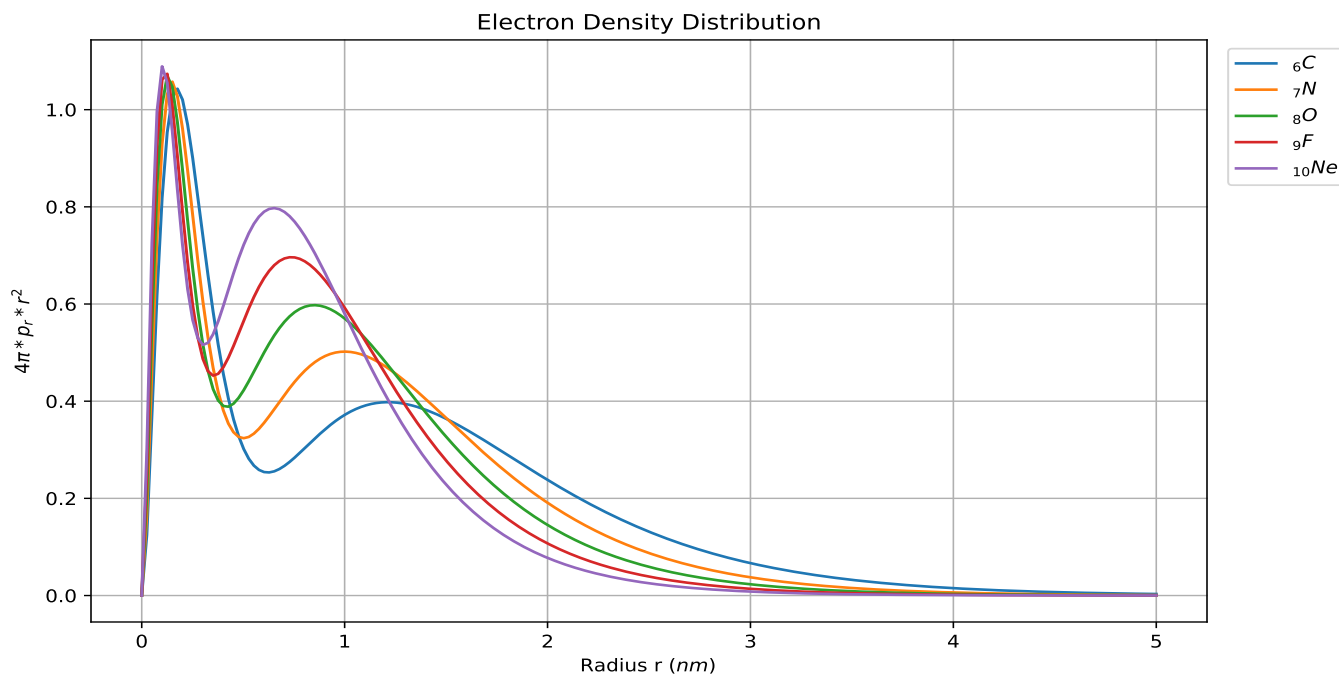Figure 7: Electron density distribution ρ_r for **He** to **B**

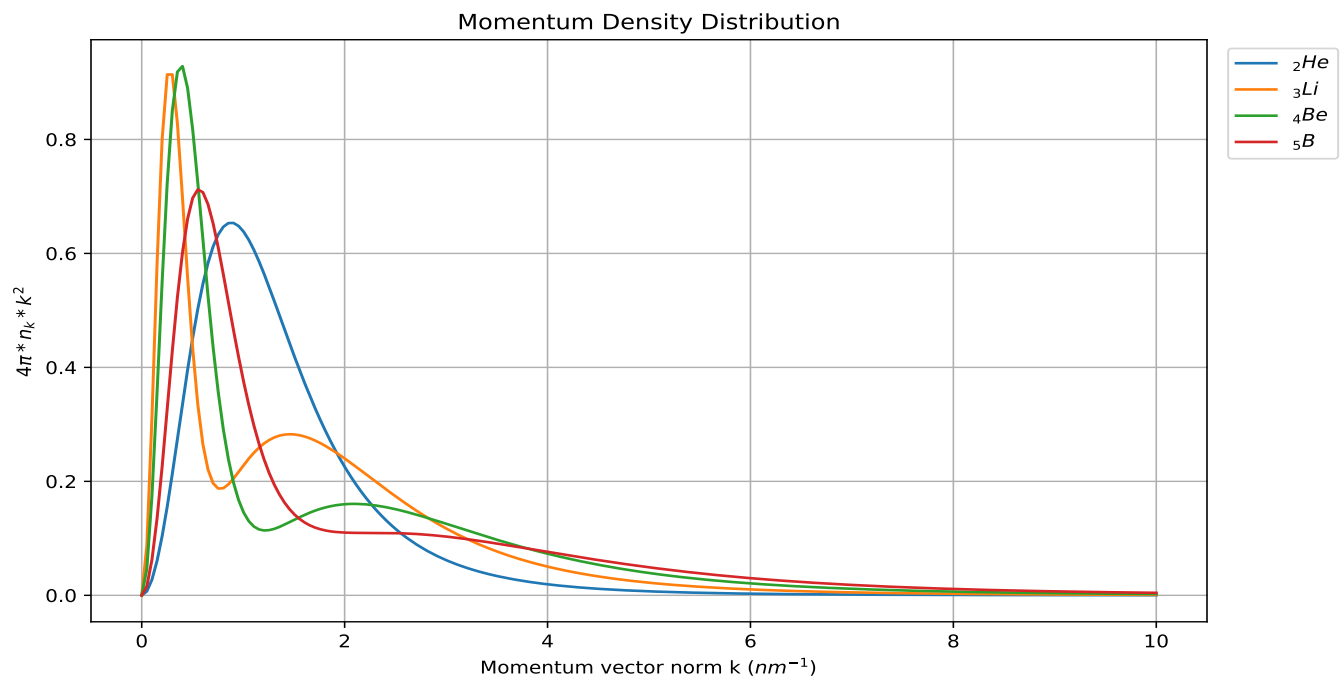Figure 8: Electron density distribution ρ_r for **C** to **Ne**

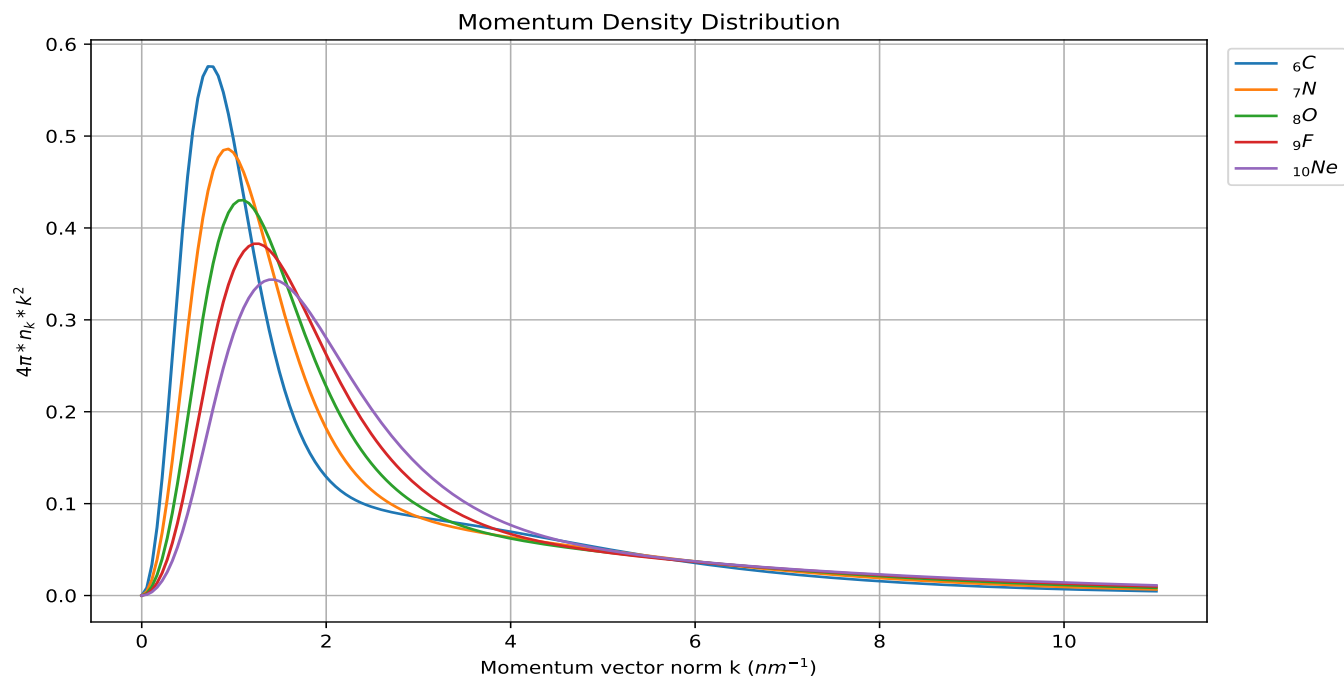Figure 9: Momentum density distribution n_k for **He** to **B**

Figure 10: Momentum density distribution n_k for **C** to **Ne**

We can see, also, that the average range of the atom (i.e the distance from atom's center at which the density ρ_r becomes 0), is around $6nm$ for the elements **Li** up to **B** and around $4nm$ for the elements **C** to **Ne**. This is due to the attraction by the nucleus positive charge, which is being increased for larger . The exception to the aforementioned is He, with a range around $3nm$, since it forms only only one shell, the **K**-shell.

As of the momentum's range, this is similar (more or less), for all elements, as shown in Figures 9 and 10. For **He** we have the range of $0 - 5$ nm^{-1}, for the elements **Li** to **B** the range $0 - 8$ nm^{-1} and for the rest elements the range $0 - 10$ nm^{-1}. However, in all cases the most possible value (i.e the total maximum) is located in the area $0 - 2$ nm^{-1}, with the possibility of taking larger values of k, being significantly decreased beyond this area.
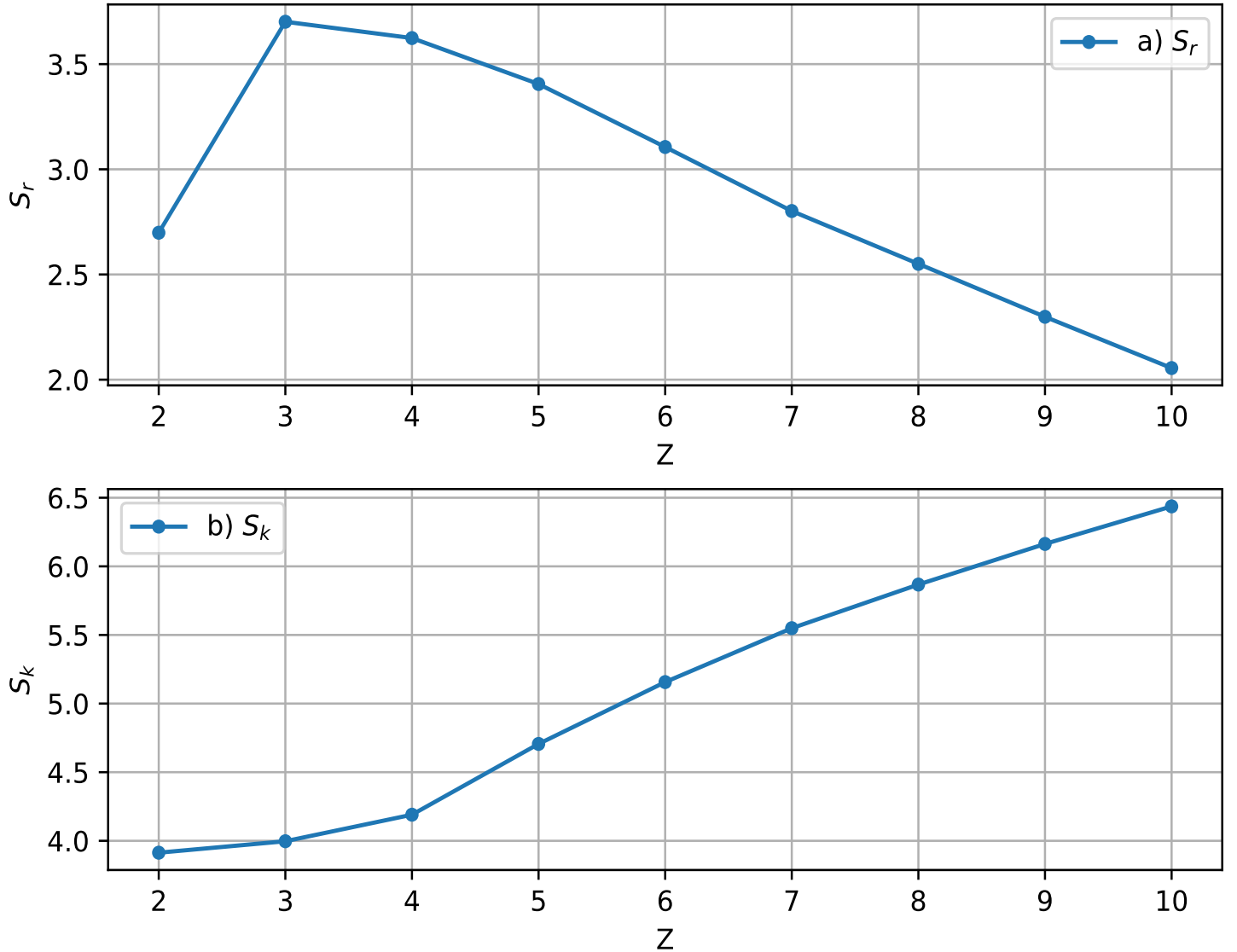

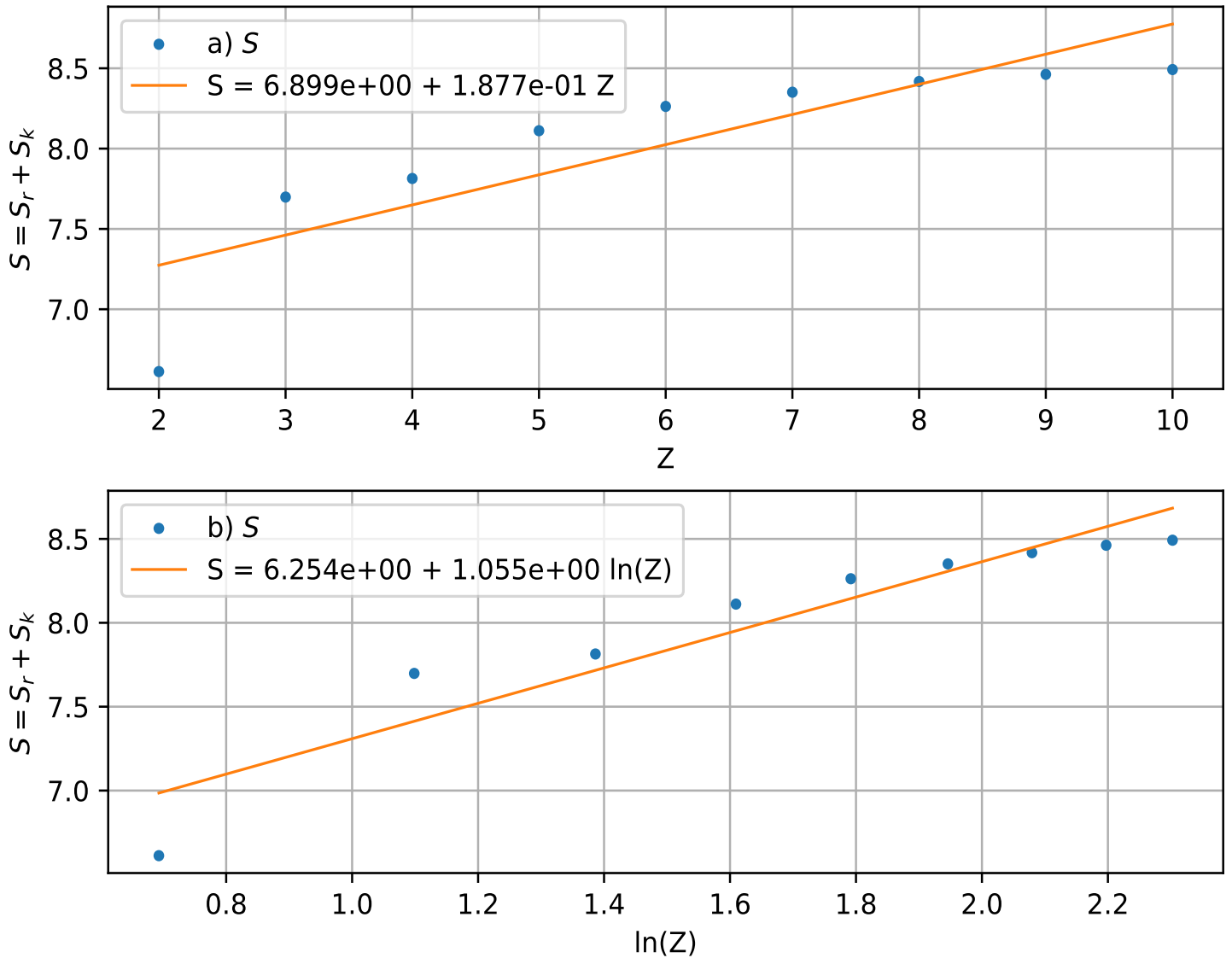Figure 11: *Shannon* information entropy in: a) position space (S_r) and b) momentum space (S_k)

Figure 12: Total *Shannon* information entropy S: a) against Z and b) against $\ln(Z)$

Finally, we present the plots of the *Shannon* information entropy, against the atomic number . As it is shown, in Figure 11, the position space information entropy S_r exhibits a maximum at $Z = 3$, while the momentum space information entropy S_k follows a continuous upward trend. This confirms our results so far. While in **He** the **K**-shell is complete and therefore there is no room space for many changes in the atom's structure in ground-state. On the contrary, when the **L**-shell is first formed with **Li** the electron's are offered lots of choices, as to which orbital can occupy and where to be located, hence the bigger value in S_r. These options are reduced as more electrons need to be distributed and the empty spaces become fewer. As for the S_k, we saw earlier that the range of the atom becomes smaller for larger Z. In this case, *Heisenberg*'s uncertainty principle leads to a wider range of angular momentum values, and therefore more motion choices for electrons and greater entropy S_k.

Last but not least, the total *Shannon* information entropy $(S = S_r + S_k)$ seems to follow

an all way continuous upward trend, as shown in Figure 14. We fitted the data using the *polyfit* command, to examine the possible linear regression between S and Z or $\ln Z$. We resulted in the two orange curves. It seems that the curve in b) graph is a better fit to the data, hinting to an exponential relation between the total entropy and the atomic number. Indeed, the values of 6.254 and 1.055, for incident and slope, are very close to those of [2] (there we have 6.257 and 1.069), validating our results. Working, of course, with more elements, we could perform a better fit of the data and obtain a more complete picture of the entropy S behaviour.

References

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