Probability Distribution and Information entropy in atoms with Z=2-10

Aspasia Pallikaridou [1]

Aristotle University of Thessaloniki
School of Physics
MSc Computational Physics
Professor: K. Chatzisavvas

[1]apallika@physics.auth.gr

Contents

Chapter 1

Introduction

This assignment is about the quantum functions of the atom wave-functions and electron densities for the atoms with $2 \leq Z \leq 10$. Additionally, some extra quantities have been calculated, such as information entropy. The main property that is demonstrated in this report has the form:

$$S = a + b \ln N \tag{1.1}$$

where N is the number of particles in the system and the constants a and b are relevant to the system.

The method that is applied in this report is similar to the methodology that was followed in the paper Information entropy, information distances, and Complexity in atoms. The main calculations were performed with Python code.

Chapter 2

Theoretical Description

The Shannon information entropy S_r is defined both in position space and in momentum space. These representations are respectively:

$$S_r = -\int \rho(r) ln\rho(r) dr \qquad (2.1)$$

$$S_k = -\int n(k) ln n(k) dk \qquad (2.2)$$

where $\rho(r)$ is the electron density distribution normalized to unity, and $n(\mathbf{k})$ is the momentum density distribution normalized to unit.[1]

The S_r increases as the distribution flattens out. Therefore, its determination of S_r is the extent of electron delocalization. On the other hand, S_k a maximum corresponds to a delocalized distribution in momentum space. Furthermore, the total information entropy is defined as:

$$S = S_r + S_k \qquad (2.3)$$

Finally, $\rho(\mathbf{r})$ and $n(\mathbf{k})$ are related to the electrons' distribution in the atoms based on the orbitals to which they belong. To be more specific, they are proportional to the sum of the multiplication of the orbital's wave function and the number of electrons that it contains for every orbital either in position or momentum space.

The orbitals are expressed in Roothaan-Hartree-Fock form, in a Slater-type basis for the ground states of He through Ne. RHF wave-functions can be incorporated into many codes for atomic calculations. These wave-functions are independent-particle-model approximations to the non-relativistic Schrodinger's equation for stationary states. Also, an approximation to the radial atomic orbitals has been done, according to which they are expanded as a finite superposition of primitive radial functions proportional to Slater-type orbitals:[2]

$$R_{nl} = \sum_j S_{gl} C_{jln} \qquad (2.4)$$

Chapter 3

Methodology

The S that exist in 2.4, is taken as a Slater-type orbital normalized set:

$$S_{jl} = N_{jl} r^{(n_{jl}-1)} exp(-Z_{jl}r) \tag{3.1}$$

where:

$$N_{jl} = (2Z_{jl})^{[n_{jl}+1/2]}/[(2n_{jl})!]^{1/2} \tag{3.2}$$

Expect for the mentioned bibliography, a Mathematica notebook by Dr.K. Chatzisavvas was used as a guide for a jupyter notebook. This jupyter notebook contains all the calculations and the plots that were performed in order to present the following results. The main difference between these two notebooks is that on the one hand the mathematica notebook has the calculations only for the Ne but on the other hand, in jupyter notebook there are implementations for the atoms He, Li, Be, B, N, O, F, and Ne ($2 \leq Z \leq 10$).

The numerical data that were used for each atom where taken from Roothaan-Hartree-Fock Ground-State Atomic Wave Functions.[2]

Chapter 4

Results and Discussion

First of all, the graphs 4.1a, 4.1b, and 4.1c present the probability of an electron to exist in orbitals 1s, 2s, and 2p respectively, in position space for each atom with $2 \leq Z \leq 10$. Hence, information about the distance between the electron and the core can be obtained from the horizontal axes. The figure 4.1d depicts the electron distribution probability for the same atoms as a function of their distance from the atom's core. The greater the atomic number, the closer to the core electrons tend to be. Additionally, electrons' position curves are wider for smaller Z.
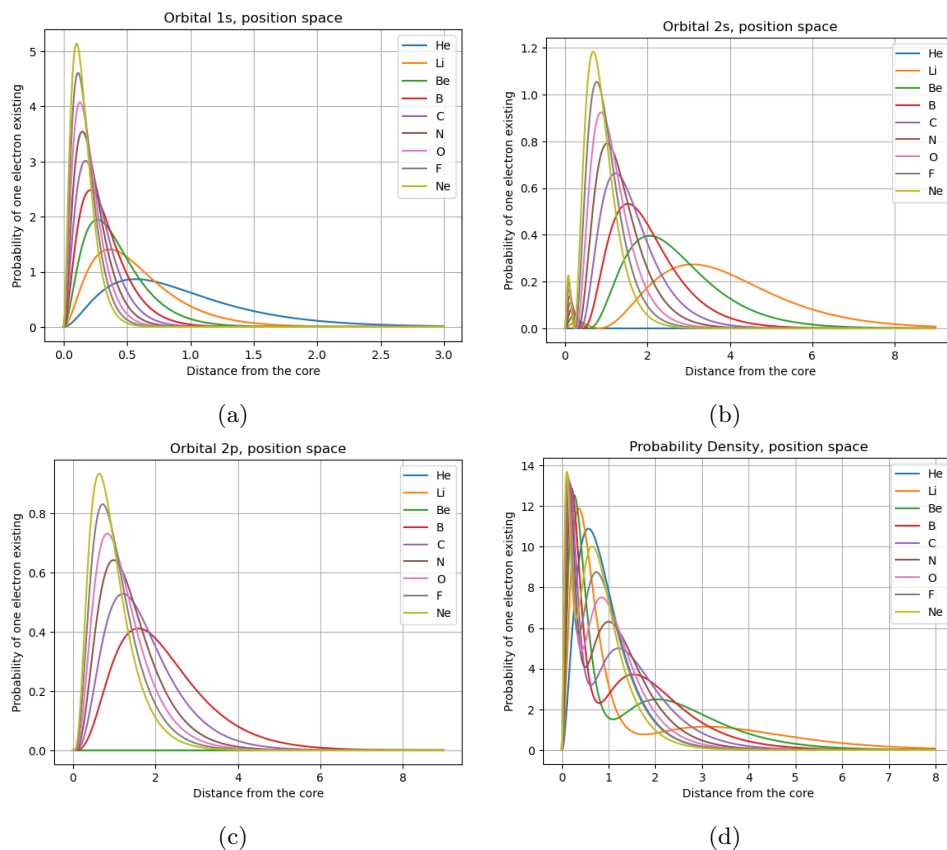

Figure 4.1: Orbitals' plots and probability density figure for atoms with $2 \leq Z \leq 10$ in position space. The greater the atomic number is, the nearer to the core electrons tend to be. Also, electrons' position curves are wider for smaller Z

Secondly, the graphs 4.2a, 4.2b, and 4.2c present the probability of an electron to exist in orbitals 1s, 2s, and 2p respectively, in momentum space for the atoms from Helium to Neon. Hence, information about the distance between the electron and the core can be obtained from the horizontal axes. The figure 4.2d depicts the electrons distribution probability for the same atoms as a function of their momentum.The greater the atomic number is, the greater the electron's momentum possibly is. Also, electrons' position curves are wider for greater Z. This difference between position and momentum space can be explained from the Heisenberg Uncertainty Principle.
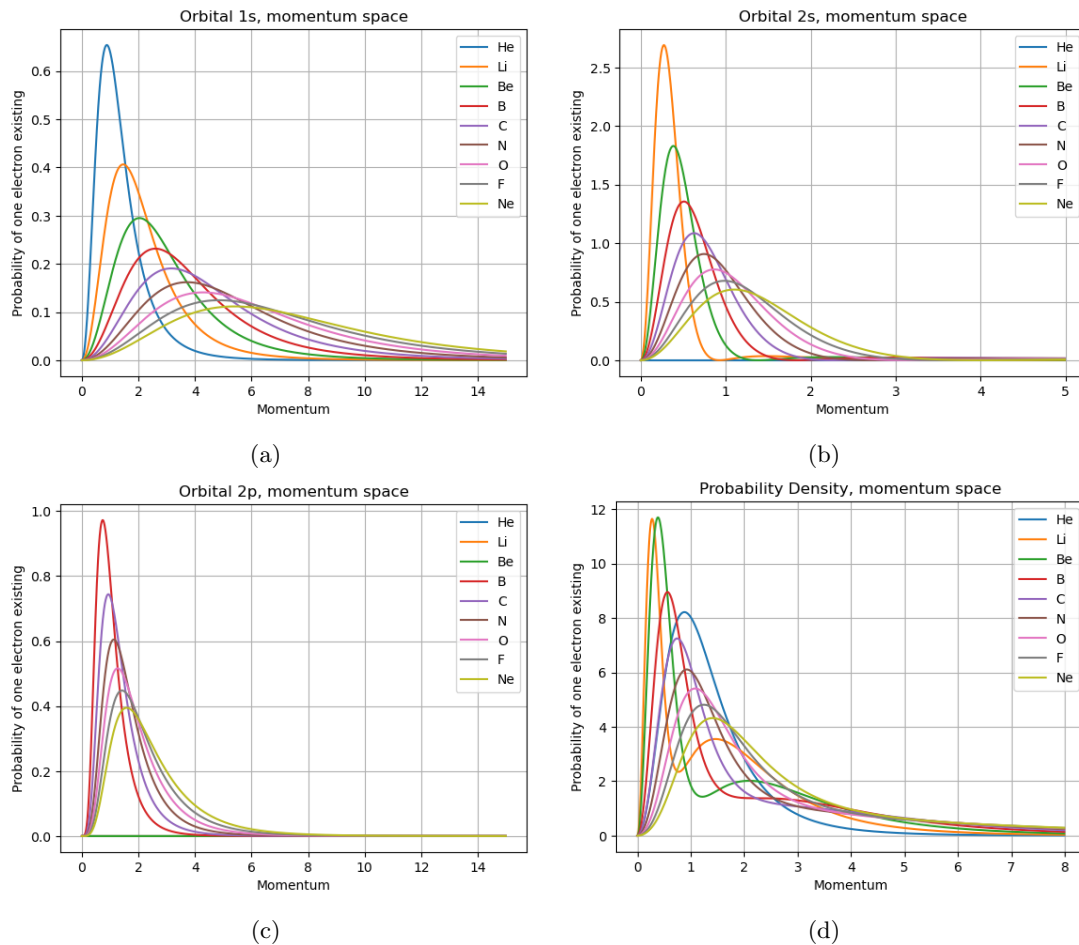

Figure 4.2: Orbitals' plots and probability density figure for atoms with $2 \leq Z \leq 10$ in momentum space. The greater the atomic number is, the greater the electron's momentum possibly is. Also, electrons' position curves are wider for greater Z

Finally, Figure 4.3 depicts the Shannon information entropy defined in position space (up and left), defined in momentum space (up and right), the total information entropy (bottom and left), and the total information entropy in logarithmic scale (bottom and right). It is worth to noticing that Sr decreases after Z=3. That is because He has more compact $\rho(r)$ than its neighboring atoms. while Sk and increase. Furthermore, S increases linearly, following the equation:

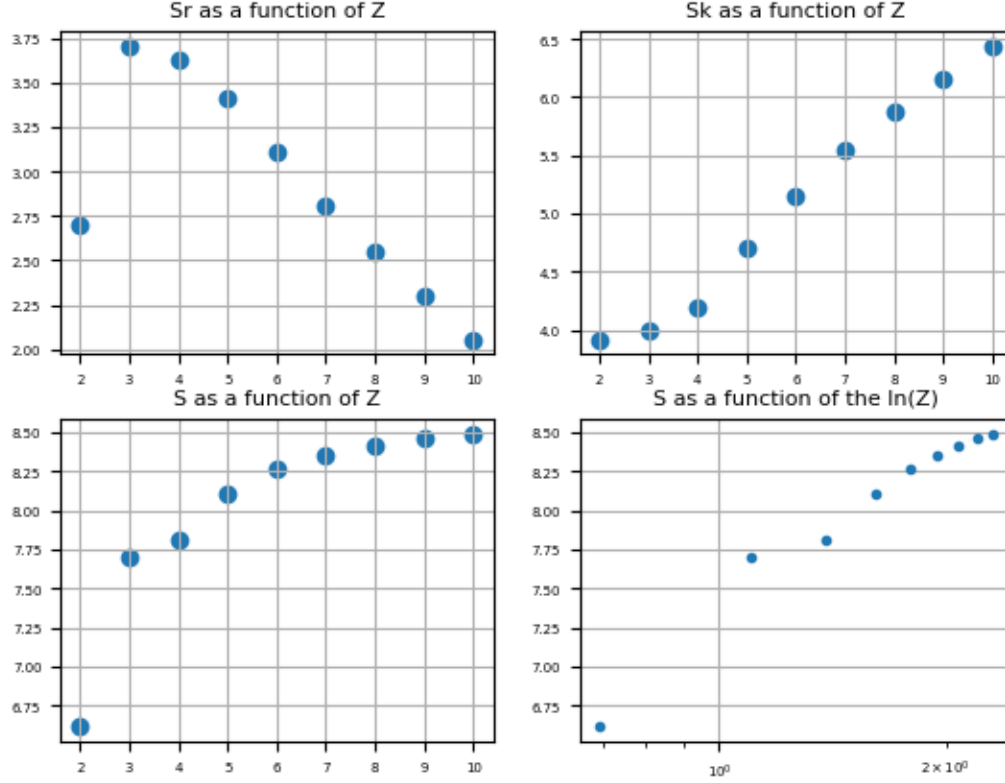$$S = 1.055 lnZ + 6.254 \ \ with \ R^2 = 0.889 \tag{4.1}$$

Figure 4.3: Shannon information entropy defined in position space (up and left), defined in momentum space (up and right), the total information entropy (bottom and left), and the total information entropy in logarithmic scale (bottom and right).

Table 4.1: Information Entropy, atoms with Z=2-10

Atomic number	Atom	Sr	Sk	S
2	He	2.698	3.913	6.612
3	Li	3.701	3.997	7.698
4	Be	3.624	4.19	7.814
5	B	3.405	4.706	8.111
6	C	3.106	5.157	8.263
7	N	2.802	5.549	8.351
8	O	2.551	5.867	8.418
9	F	2.299	6.163	8.462
10	Ne	2.055	6.437	8.492

Chapter 5

Conclusion

In conclusion, this report discusses some quantum mechanical properties of atoms with atomic numbers Z=2-10. Using Python code, the electron distributions in both position and momentum spaces were calculated and the behavior of electrons in different atomic orbitals was explored. The combination of computational tools and quantum theory offers valuable insights into atomic and subatomic phenomena.

Bibliography

[1] Information entropy, information distances, and Complexity in atoms

[2] Roothan-Hartree-Fock Ground-State Atomic Wave Functions: Slater-Type Orbital Expansions and Expectations Values for Z=2-54