

The Locality of Electrons

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ABSTRACT

This short essay briefly explores the behavior of electrons and their placement around atoms. Electron radial wavefunctions and probability densities are calculated and analyzed for various orbitals, quantum numbers, and atomic numbers.

INTRODUCTION

The conventional, classical idea of how far an electron of a certain orbital sits is relatively straightforward, and is taught in chemistry and even introductory physics classes as such. However, once one delves into the quantum mechanics behind this system, it is clear that the picture is a lot fuzzier than first thought. It is thus my interest to explore where the electron may sit according to quantum mechanics. As such, I have developed a script using a combination of equations from [1] and [2] to generally see for any atomic system, where a single electron of any l or n may sit. The script solves the equations numerically, providing a quick look of the systems.

CALCULATION AND RESULTS

To find these characteristics, it is important to first note the normalized radial wavefunction $R_{nl}(r)$:

$$R_{nl}(r) = \left(\frac{\left(\frac{2Z}{n\alpha_0} \right)^3 (n-l-1)!}{2n((n+l)!)^3} \right)^{\frac{1}{2}} e^{-\frac{\rho}{2}} \rho^l L_{n-l-1}^{2l+1}(\rho); \quad \rho = \left(\frac{2Z}{\alpha_0 n} \right) r \quad (1) [1, 2]$$

Where Z is the atomic number, α_0 is the Bohr radius (0.053 nm), and L is the Laguerre polynomial. As an example, Figure 1 shows the $R_{nl}(r)$ of an electron of a hydrogen atom. One would assume by this graph that the electron collapses into the nucleus, since the maximum value of its wavefunction and its probability density $|R_{nl}(r)|^2$ (Figure 2) is at $r = 0$. However, [1] points out that when the wavefunction is at around $r = 0$, that the slope of the momentum increases. Hence, by the uncertainty principle, the location cannot be within that volume.

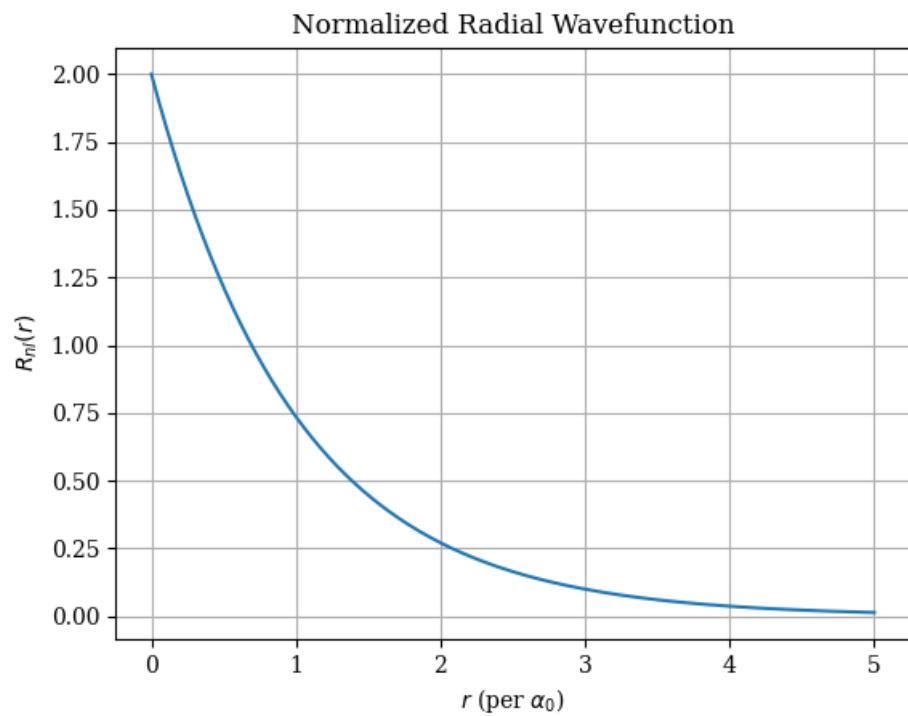


Figure 1: $R_{nl}(r)$ of hydrogen atom's single electron.

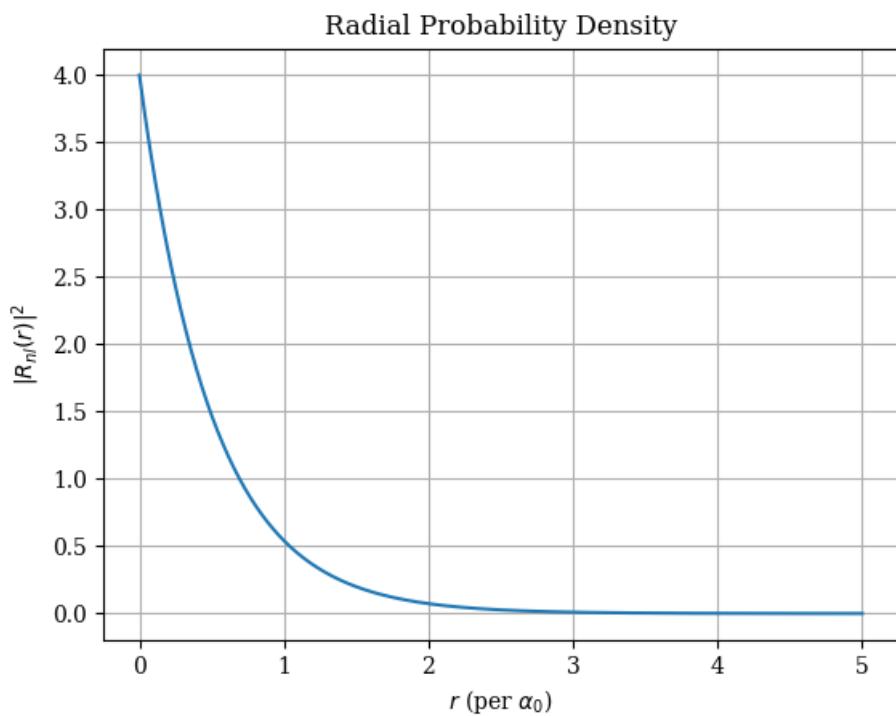


Figure 2: $|R_{nl}(r)|^2$ of hydrogen atom's single electron.

If we calculate the reduced probability density:

$$P(r) = |R_{nl}(r)|^2 r^2 \quad (2)$$

Then we get something more expected (Figure 3), with a maximum at around the Bohr radius. This is clearly due to the r^2 term. Interestingly, the probability that the electron surpasses the “classically forbidden region” is actually relatively high, at about 24%. This is calculated by integrating Equation (2) from $2\alpha_0$ to infinity (as seen in Figure 4).

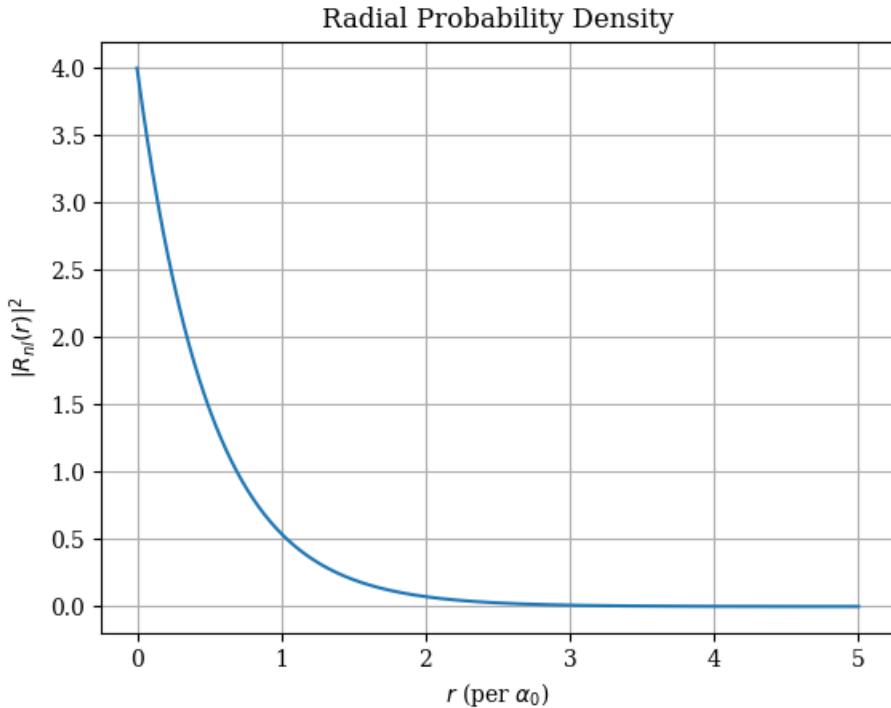


Figure 3: $P(r)$ of hydrogen atom's single electron.

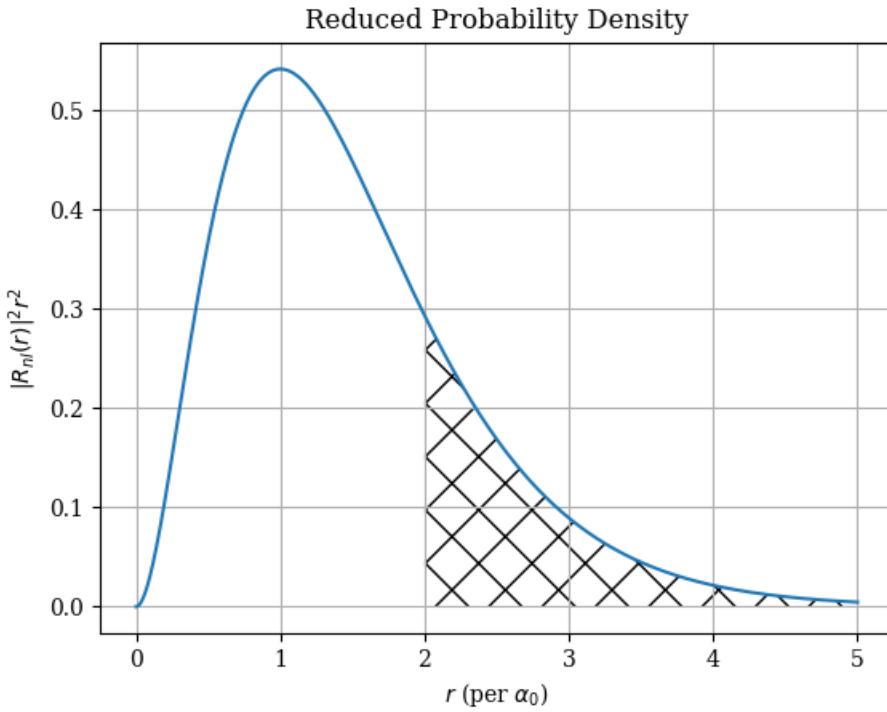


Figure 4: $P(r)$ of hydrogen atom's single electron with the classically forbidden region hatched.

Now, with that basis established, it is of interest to explore other systems. The simplest relationship we can see is for increasing Z . What happens then, with all else still equal ($n = 1, l = 0$), is that the electron is pulled closer to the nucleus, as seen in Figure 5. This is of course due to the attractive Coulomb force. Going back to the hydrogen atom ($Z = 1$), but increasing the quantum number to 2, already produces something interesting. There are two likely spots for this electron to occupy. One is slightly less than the Bohr radius, and one is at about $5\alpha_0$, as seen in Figure 6. This is due to the wavefunction's tendency to change slope direction, as seen in Figure 7. However, there is a discrepancy between my relatively low resolution (1000 points per α_0) program and literature [1]. Actually, the radial probability density should have a δ -function spike, as seen in Figure 8. Meanwhile, the numerical solver does not account for the lack of some infinitesimally small region where the slope = 0.

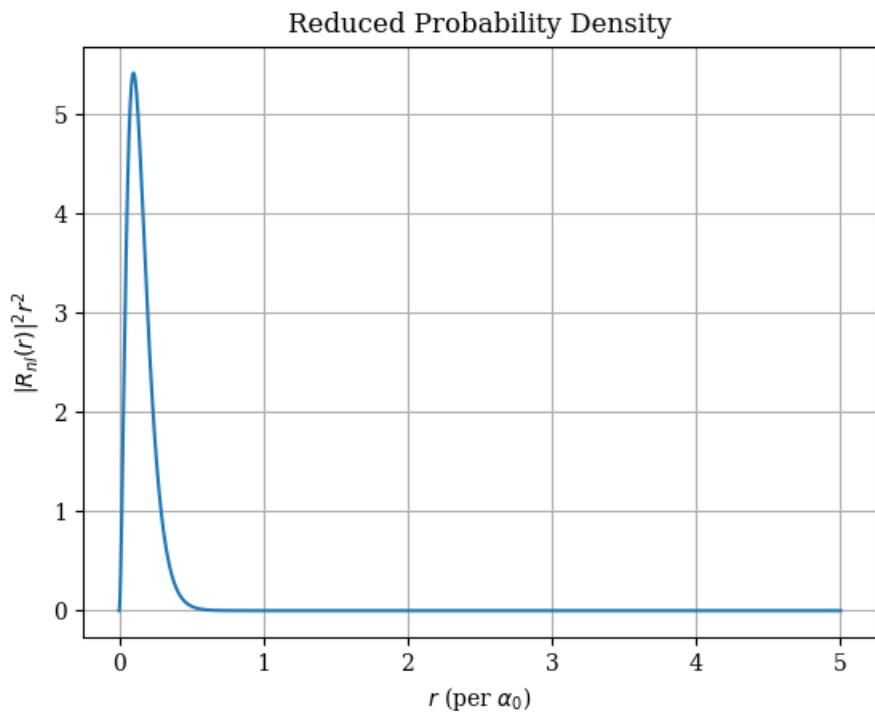


Figure 5: $P(r)$ of neon's 1s electron.

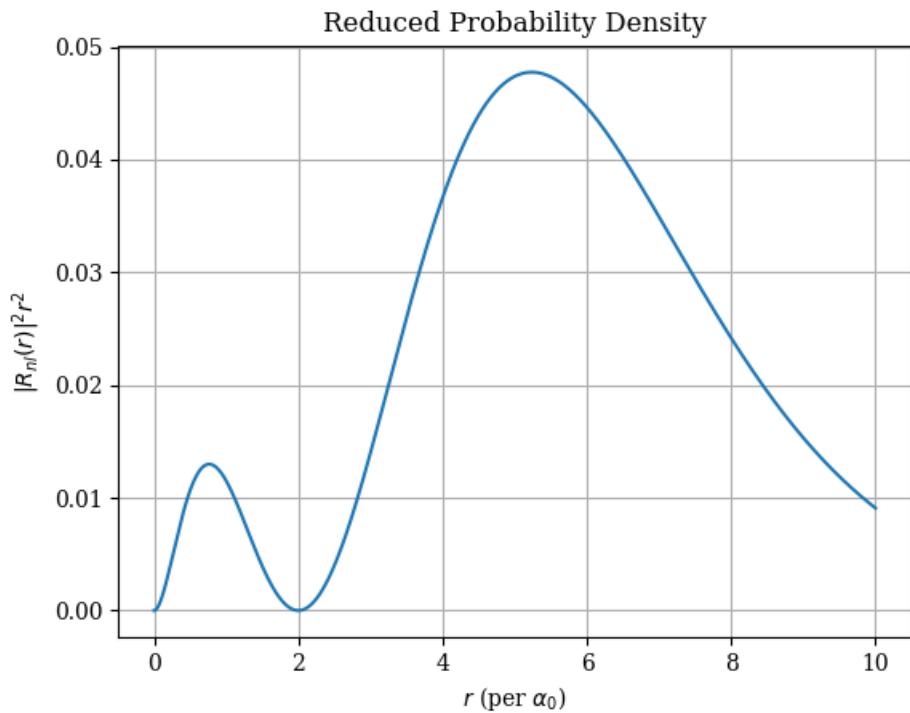


Figure 6: $P(r)$ of a hydrogen 2s electron.

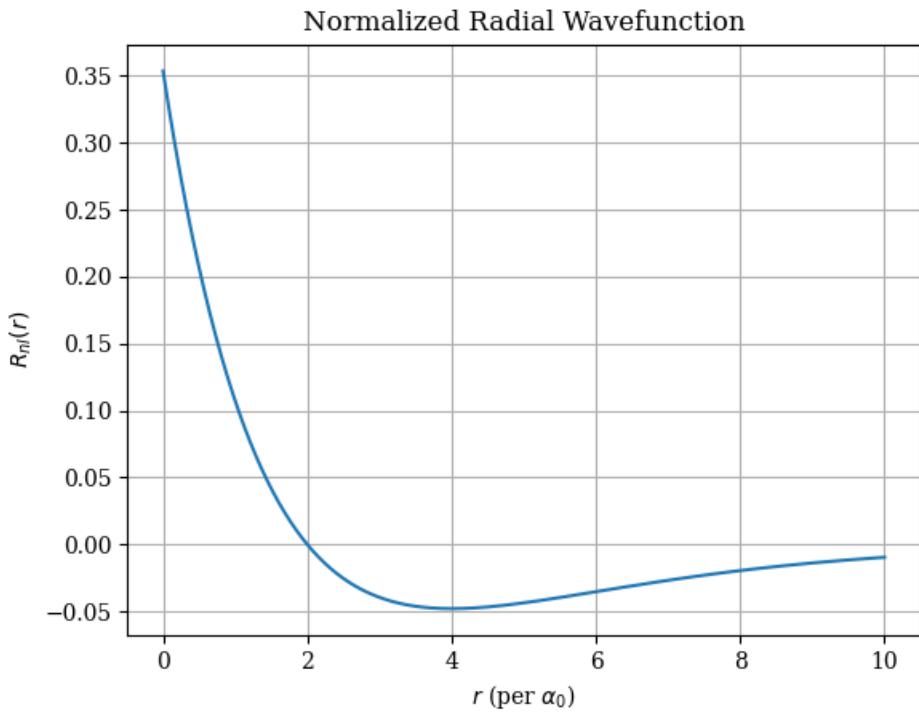


Figure 7: $R_{nl}(r)$ of the hydrogen atom's 2s electron.

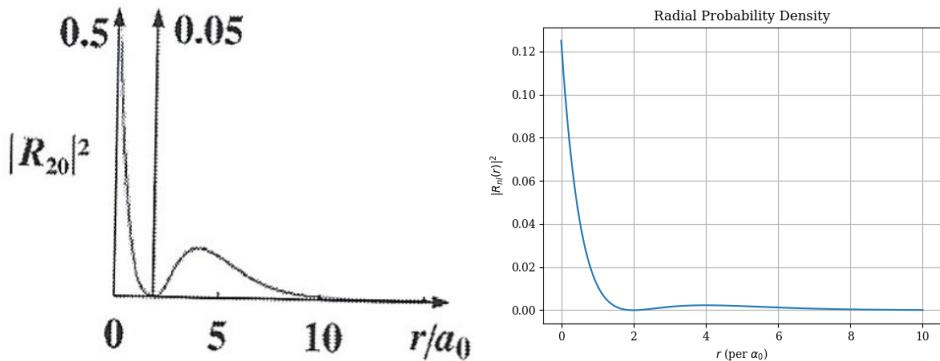


Figure 8: $|R_{nl}(r)|^2$ of the hydrogen atom's 2s electron from literature [1] (right) and by numerical calculation (left).

CONCLUSION

In this essay, we explored some of the dynamics of electron locality. Additionally, we noticed some algorithmic limitations when computing the radial wavefunctions numerically.

REFERENCES

1. Kim, D-M. (2010) *Introductory Quantum Mechanics for Semiconductor Nanotechnology*. Wiley-VCH Verlag GmbH.
2. DeGottardi, W. (2025) Quantum Mechanics I Lectures. Texas Tech University.