

R Programming Challenge: Hydrogenic Orbitals

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1 Introductory Reading

For this R programming challenge, you are asked to do a study of how electrons behave in an atom. In this case, electrons aren't particles, like BB pellets – they behave as a wave. Imagine throwing a rock into the middle of a pond – the waves you see spreading outward demonstrate very clearly how electrons behave as waves.

We can describe the behavior of those waves using mathematics called a "wavefunction". We'll describe that in the Background reading below. Your challenge is to develop an R script that has functions for the 1s, 2s, and 2p wavefunctions. In addition, you'll be asked to write functions for the probability density for each of the 1s, 2s, and 2p wavefunctions, and, finally, plot all three of those probability densities on one graph.

1.1 Vocabulary

Orbitals: the cloud surrounding a nucleus. Orbitals contain electrons moving like a wave about the nucleus. There are different types of orbitals with different shapes. *s* orbitals contain up to two electrons, and are spherical (round) in shape. *p* orbitals can contain up to six electrons, and are shaped roughly like a "figure of eight".

1.2 Background

In quantum chemistry, we use the term **orbitals** to represent the cloud that surrounds a nucleus. In that cloud, the electron or electrons are found. We are unable to pinpoint the exact location of an electron in that cloud. We can only calculate the **probability** of finding that electron at some particular place in the electron cloud. What we can *also* do is show a mathematical equation for the entire electron cloud, from which a probability can be calculated. The mathematical equation (also called a **function**) for any atom with more than one electrons is quite complicated, and cannot be solved by simple tools such

as calculators or spreadsheets. For a single electron atom, such as hydrogen, we can use simple tools to calculate the cloud.

The term used by chemists for the electron cloud is the **wavefunction**, and is represented by the Greek symbol Ψ . Ψ has no meaning in terms of anything we can see. The square of Ψ , the value Ψ^2 , does have physical importance - the probability of finding the electron at a specific place. Probabilities have a range from 0 to 1 (or 100 percent). If the probability is 0, there is no chance that the electron is at that particular place. If the probability is 1, there is a 100 percent chance that the electron is at that particular spot.

While probabilities are important, we are really interested in calculating the **probability density**, $P(r)$, for a given orbital. Since the electron is inside a sphere (imagine a basketball - the electron is inside the ball somewhere), we need to calculate the probability inside that entire sphere. To do that, we simply multiply the wavefunction Ψ times the formula for a volume, $4\pi r^2$, remembering that we also have to square the wavefunction to convert it from a wavefunction to a probability. We now have a number that shows us the probability density of finding the electron somewhere in the sphere.

In the equations below, r is the radius, the distance (in angstroms) that the electron is from the nucleus. We have one constant, a_0 , a value known as the **Bohr radius**, set at a value of 0.529 **angstroms** (\AA). The letter e represents the exponential function, and is programmed in most computer programs with the keyword **exp**. In this model, we want to evaluate the wavefunctions and probabilities from a range of 0 to 4 angstroms, with an interval of 0.1 \AA .

You are reminded that multiplication is implicit in the equations below: in R, however, make sure that you are using the appropriate mathematical symbol!

$$\Psi_{1s}(r) = 2\left(\frac{1}{a_0}\right)^{1.5}e^{-\left(\frac{r}{a_0}\right)} \quad (1)$$

$$\Psi_{2s}(r) = 2\left(\frac{1}{2a_0}\right)^{1.5}\left(1 - \frac{r}{2a_0}\right)e^{-\left(\frac{r}{2a_0}\right)} \quad (2)$$

$$\Psi_{2p}(r) = \frac{1}{\sqrt{3}}\left(\frac{1}{2a_0}\right)^{1.5}\frac{r}{a_0}e^{-\left(\frac{r}{2a_0}\right)} \quad (3)$$

$$P(r) = 4\pi r^2 \Psi^2 \quad (4)$$

2 Computational Approach

We can use any number of computing tools to describe the four mathematical functions shown above in Equations 1 - 4. One possibility is Mathematica (MMA). Another useful tool is a simple spreadsheet, like Microsoft Excel.

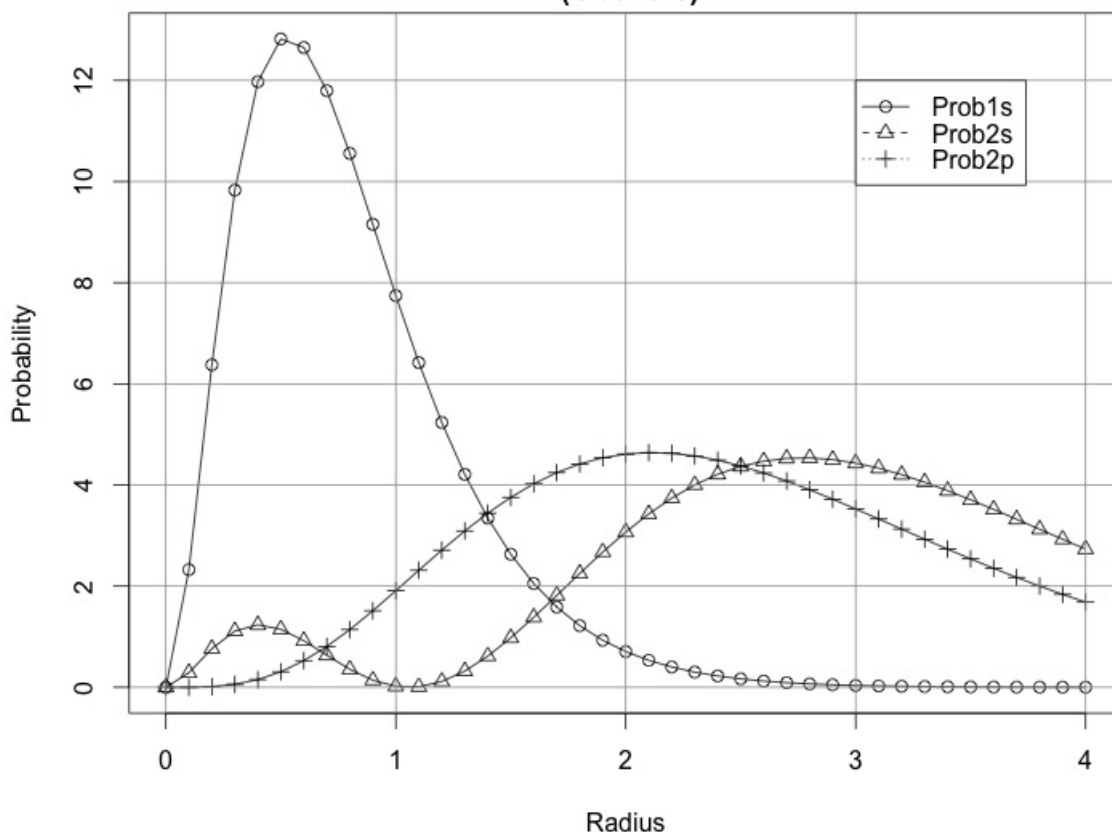
We will, of course, do our work in R.

Regardless of the tool used, the computational results should yield a probability density graph, showing each of the three probability densities, with the distance of the electron (**Radius**) from the nucleus. As an example, with the 1s probability, one sees the highest probability (about 12.5%) right around 0.53 angstroms. This is the **Bohr radius**, named after the great Danish physicist Niels Bohr.

Your graph should look like the figure below. Notice that we are showing the probability density curves, not the wavefunction curves!

Figure 1: All three probabilities

**Plot of Probabilities of
1s, 2s, and 2p orbitals
(Gotwals)**



3 Deliverable

For submission for this activity, you should submit a well-documented copy of your R script. For uploading to Canvas, it's easiest simply to copy the entire script, go to the Submit page on Canvas, and paste it into the text box.

You should ALSO upload a PDF version of a plot showing all three probabilities (1s, 2s, and 2p). Your plot should be nicely labeled. NOTE! My plot has my name on it...why? So you're not tempted to simply copy mine and upload it as yours! Sneaky, huh?

4 Some useful functions

- abs: absolute value
- exp: exponential function
- sqrt: square root