

PHYS-4007/5007: Computational Physics

Problem Set 3 (Due: 14 April 2023)

This problem set is due back to me by 5 p.m. on the date listed above. Note that you will need to supply a short **written analysis** of your work including plots (see below) and you will need to email your codes to me (lutter@etsu.edu). Your written analysis can either be submitted via email or as a hardcopy.

1. (60 pts) Rydberg (1890), Ritz (1908), Planck (1910), and Bohr (1913) were all responsible for developing the theory of the spectrum of the H atom. A transition in an hydrogen-like atom/ion from an upper level m to a lower level n will radiate a photon at frequency

$$\nu_{mn} = c R_A Z^2 \left(\frac{1}{n^2} - \frac{1}{m^2} \right),$$

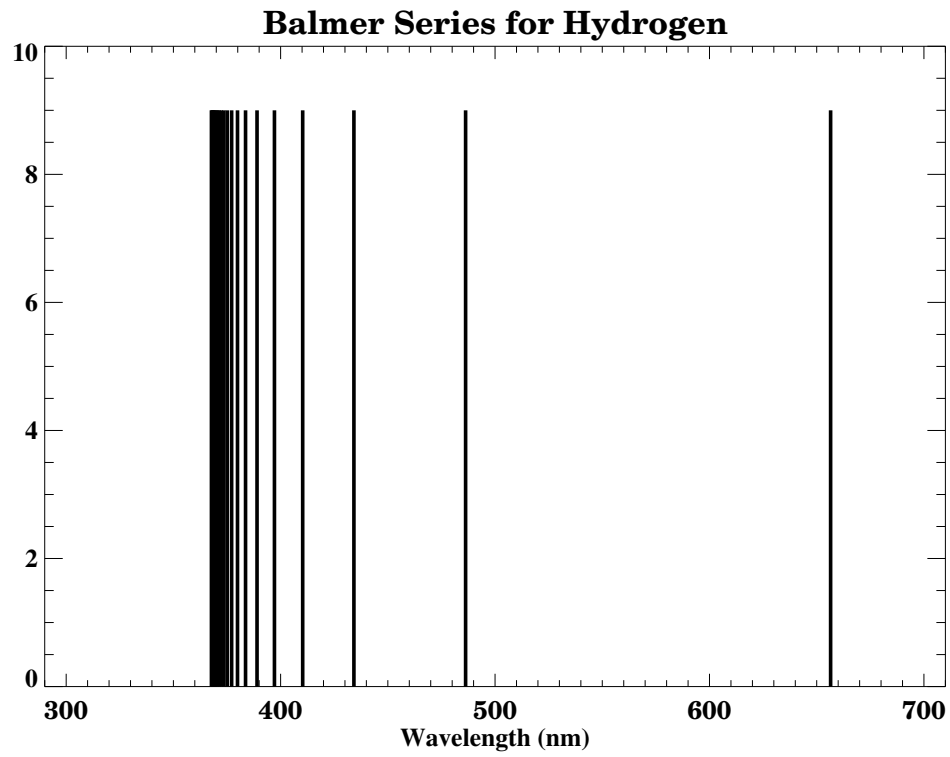
where the velocity of light, $c = 2.997925 \times 10^{10}$ cm/s, Z is the *effective* charge of the nucleus ($Z_H = 1$, $Z_{He} = 2$, etc.), and R_A the Rydberg constant for the hydrogen-like atom/ion. We can also be expressed this equation in terms of wavelengths (vacuum) by

$$\frac{1}{\lambda_{mn}} = R_A Z^2 \left(\frac{1}{n^2} - \frac{1}{m^2} \right).$$

For neutral hydrogen, $R_A = R_H = 109,677.6 \text{ cm}^{-1}$. Write a code in either **Fortran** or **Python 3**, that will calculate the first 20 wavelengths (in nm = nanometers) for any series of hydrogen. Your code should allow the user to specify (via input) which series of hydrogen are to be calculated (*e.g.*, $n = 1$, Lyman series; $n = 2$, Balmer series; $n = 3$, Paschen series, etc.) The code should be able to output the data to an ASCII file in tabular format with the column headings of n (lower-level quantum number), m (upper-level quantum number), and wavelength (in nm) with no more than 3 digits past the decimal point printed.

You are then to calculate the first 20 wavelengths of the Lyman series, ($n = 1$), the Balmer series ($n = 2$), and the Paschen series ($n = 3$). You should present this data in tabular format in your write-up. Your analysis should include a discussion of the physics involved with these calculations, steps you took in the coding, and any issues you encountered when debugging your code. **Use double precision in your value for R_H and note that n and m must be integers with $m > n$.**

2. (20 pt) Now, write a code in Python3 that will plot the output generated in Problem 1 similar to the following plot:



Make plots for the Lyman lines, Balmer lines, and Paschen lines in encapsulated postscript format. Then email these plots to me when you email your code from Problem 1.