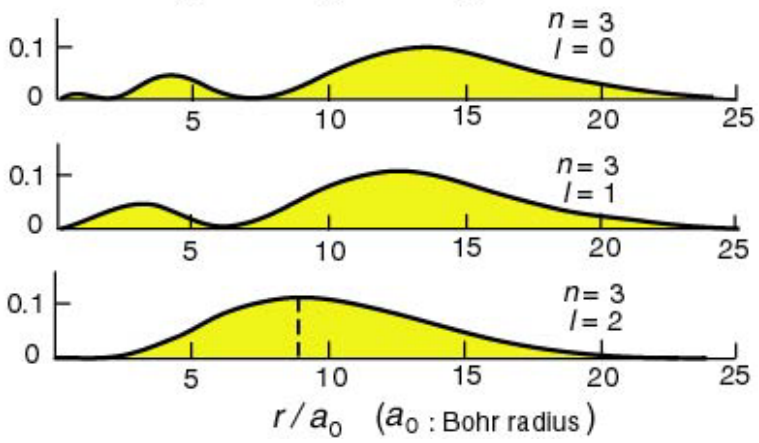
PS 2

1. In a single graph with proper axes labels, draw the radial part of the wavefunction for 1s, 2s, 2p and in another graph draw for 3s, 3p, 3d orbitals for a Hydrogen atom indicating nodes and relative position of the maxima. Repeat the same exercise for the Radial Probability Distribution Function.

2. The radial probability distribution function (RDF), P(r), for the 1s orbital is defined as:
$P_{1s}(r) = 4\pi r^2 [\psi_{1s}(r)]^2$
For an electron in a 1s orbital, how does the RDF vary with distance from the nucleus?
Explain why it is that although the 1s wavefunction is a maximum at the nucleus, the corresponding RDF goes to zero at the nucleus. Also, explain why the RDF shows a maximum, and why the RDF goes to zero for large values of the distance r.

3. The Radial Distribution Function of 3s, 3p, and 3d is shown below.



(i) In which of the orbitals is the highest probability of finding electron [indicated by the maxima of $P_{1s}(r)$] closest to the nucleus
(ii) If you consider distance of $0.1a_0$ from the nucleus, in which of the three orbitals would you have the maximum probability of finding electrons.

4. The RDF for a 1s orbital is $4\pi r^2[\ 1s(r)]^2$.

Given that the 1s wavefunction is $\psi_{1s}(r) = 4N_{1s}^2\ \pi r^2 \exp(-r/a_0)$, show that the RDF is given by
$P_{1s}(r) = 4N_{1s}^2 \pi r^2 \exp(-2r/a_0)$.
(N_{1s} is the pre-exponential constant in the 1s wave function)

We can find the maximum in this RDF by differentiating it with respect to r, and then setting the derivative to zero. Show that the required derivative is
$$\frac{dP_{1s}(r)}{dr} = 8N_{1s}^2 \pi r \exp(-2r/a_0) - 8N_{1s}^2 \pi \frac{r^2}{a_0} \exp(-2r/a_0).$$

Further show that this differential goes to zero at $r = a_0$, and use a graphical argument to explain why this must correspond to a maximum.

For a hydrogen-like atom with nuclear charge Z, the 1s wavefunction is $\psi_{1s}(r) = N_{1s} \exp(-Zr/a_0)$. Show that the corresponding RDF has a maximum at $r = a_0/Z$.

5. The radial part of the 3p AO wave function is:

$$R_{3,1}(r) = N_{3,1}\left[6\left(\frac{r}{a_0}\right) - \left(\frac{r}{a_0}\right)^2\right]\exp\left(-\frac{r}{3a_0}\right).$$

Determine the position of the radial node in the 3p orbital?

6. Show how you will draw contour plots of equal probability iso-surfaces of the 3s orbital from the following plot of the wavefunction (the red has +ve values, while the blue has -ve values):