

## Frequently Asked Questions: Atomic Orbitals

*Q1. At what region does the Radial Probability Distribution Function estimate the probability of finding electron?*

**Answer:** The Radial Probability Distribution Function (also called Radial Distribution Function) for 1s is given by  $P_{1s}(r) = 4\pi r^2 [\psi_{1s}(r)]^2$ . More generally, it is given by:  $P_{nl}(r) = r^2 \times [R_{nl}(r)]^2$ , where  $R_{nl}(r)$  is the radial part of the wavefunction.  $P_{nl}(r)\delta r$  gives the probability of finding the electron at a distance between  $r$  and  $r + \delta r$ , summed over all directions. This is in contrast to  $\psi^2\delta v$  which gives the probability of finding the electron at a small volume  $\delta v$  located at a point.

*Q2. What is the difference between the terms radial node and nodal plane?*

**Answer:** Radial nodes arise from the radial part of the wave function but nodal plane arises from the angular part of the wave function.

A radial node corresponds to a distance from the nucleus (i.e. value of  $r$ ) at which, regardless of direction, the wavefunction is zero. For example, the 2s orbital in hydrogen has a radial node at  $r = 2a_0$ .

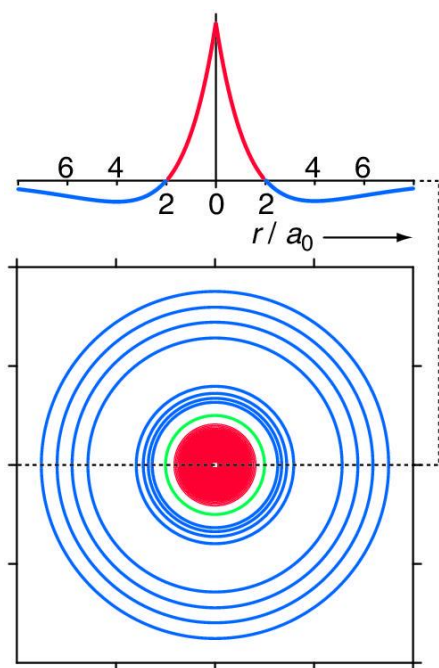
A nodal plane, or angular node, corresponds to a plane in which the wavefunction is zero. For example, the  $2p_x$  orbital has a nodal plane in the  $yz$  plane, the  $2p_y$  in the  $xz$  plane and the  $2p_z$  orbital in the  $xy$  plane.

Recall that the wavefunction can always be written as the product of a radial part, which depends only on  $r$ , and an angular part, which depends only on  $\theta$  and  $\phi$ . Radial nodes occur at values of  $r$  that make the wavefunction zero. Since the radial part of the wavefunction depends on  $r$  while the angular part does not, these values of  $r$  that make the wavefunction zero must exert their effect by making the radial part zero. The product of the zero radial part with the (non-zero) angular part makes the overall wavefunction zero. In other words, radial nodes occur whenever the radial part of the wavefunction is zero.

Similarly, nodal planes occur for particular values of  $\theta$  and/or  $\phi$  that make the wavefunction zero. For example whenever  $\theta = \pi/2$  we are in the  $xy$  plane regardless of the values of  $r$  and  $\phi$ , so  $\theta = \pi/2$  describes the nodal plane in the  $2p_z$  orbital. Since the angular part of the wavefunction depends on  $\theta$  and  $\phi$  while the radial part does not, these values of  $\theta$  and  $\phi$  that make the wavefunction zero must exert their effect by making the angular part zero.

*Q3. In the 2s orbital, if the lobes are separated by nodes, where there is no probability to find an electron. Then how does the electron makes its journey without passing through the node? It looks as if it is breaking the continuity.*

**Answer:** The problem with this query is that you are assuming the electron to be a particle. In that case a journey from one zone to another passing through a node seems incorrect. You need to think of electron as a wave here- an assumption we made while looking at the Schrödinger equation. With that assumption, you can easily consider two regions where the wave has a non-zero amplitude separated by a node where the amplitude is zero (see the plot of wave function below and the corresponding contour plot).



Q4. There are regions in the atom where both the 1s and 2s electron can exist, and yet they have different energies. How is this possible?

**Answer:** This argument arises since you are again considering the electron as a particle and hence if there can be at the same position with respect to the nucleus, they should essentially have the same binding energy. Again, you need to consider for sub-microscopic objects like the electron, it is incorrect to have this assumption. The energy is an “expectation value” obtained by operation of the Hamiltonian operator onto the wavefunction. It has nothing to do with position of the electrons. Additionally, you can argue that two electrons having same position coordinate can have different energy due to their inherent uncertainties in their momentum (re: Uncertainty principle).

Q5. Does the charge distribution plots (below) represents electron cloud? How can the electron charge be distributed over such space?



**Answer:** No, it does not represent an electron cloud or a charge cloud. You can consider this as a thought experiment in which you have taken multiple snapshots of the 2s electron over a large period of time. The overlay of all these snapshots will lead to this diagram. This overlay diagram gives you the relative probability density of finding the electron at a certain distance “r” from the nucleus. This is a scatter plot of the probability density,  $\psi^2$ .