1 Atomic functions

a. Radial Functions

Solution: We know from solving the hydrogen atom that the solutions to the hydrogen atom consist of two parts, the radial and the angular part. For the case when $n = 2$ and $l = 0, 1$ the radial functions are

$$R_{20} = \frac{1}{\sqrt{3}} \left(\frac{Z}{2a_0}\right)^{\frac{3}{2}} \left(1 - \frac{Zr}{2a_0}\right) e^{-Zr/2a_0}, \tag{1}$$

$$R_{21} = 2 \left(\frac{Z}{2a_0}\right)^{\frac{3}{2}} \left(\frac{Zr}{a_0}\right) e^{-Zr/2a_0}, \tag{2}$$

where a_0 is the Bohr radius and Z the nuclear charge. If we assume $Z = 1, a_0 = 1$ we get the following plot.

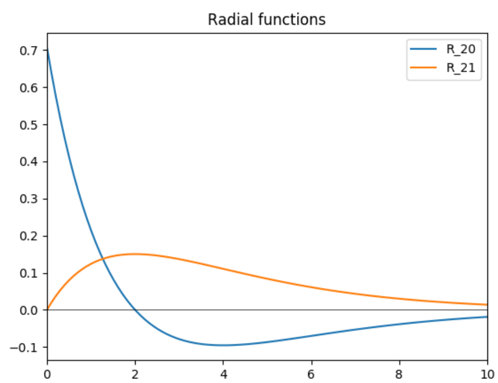


Figure 1: Radial functions R_{20} and R_{21}.

How many radial nodes are present? We don't consider $r = 0$ as a node. So taking that in mind, the number of radial nodes will be $n - l - 1$, therefore R_{20} must have 1 node and R_{21} none, as we can see in fig. 1

b. Qubic Harmonics

Solution:

From previous courses we know how to construct the cubic harmonics with $l = 0, 1$. By definition

$$s = Y_{00}, \tag{3}$$

$$p_z = Y_{10} \tag{4}$$

$$p_x = \sqrt{\frac{1}{2}}(Y_{1-1} - Y_{11}), \tag{5}$$

$$p_y = \sqrt{\frac{1}{2}} i(Y_{1-1} + Y_{11}), \tag{6}$$

The spherical harmonics for $l = 0, 1$ are

$$Y_{00} = \sqrt{\frac{3}{4\pi}}, \tag{7}$$

$$Y_{10} = \sqrt{\frac{3}{4\pi}} \cos\theta, \tag{8}$$

$$Y_{1\pm1} = \mp\sqrt{\frac{3}{8\pi}} \sin\theta e^{\pm i\phi}, \tag{9}$$

Plugging eqs. 7-9 into eqs. 3-4 yields,

$$s = \sqrt{\frac{3}{4\pi}}, \tag{10}$$

$$p_z = \sqrt{\frac{3}{4\pi}} \cos\theta, \tag{11}$$

$$p_x = \sqrt{\frac{3}{4\pi}} \sin\theta\cos\phi, \tag{12}$$

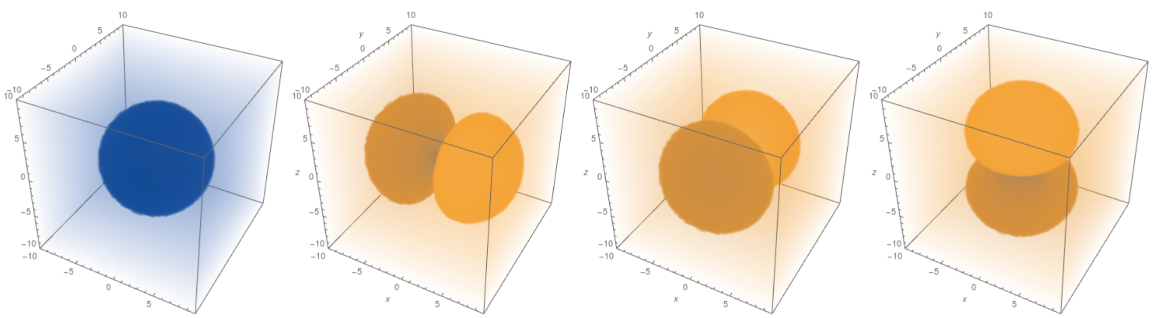
$$p_y = \sqrt{\frac{3}{4\pi}} \sin\theta\sin\phi. \tag{13}$$

Now from this and our knowledge that the wavefunctions are given by

$$\psi_{nlm}(\vec{r}) = AR_{nl}(r)h_{l\alpha}(\theta, \phi), \tag{14}$$

we must be able to complete this exercise.

How do the wavefunctions look like for $n = 2, l = 0$ and $n = 2, l = 1$?

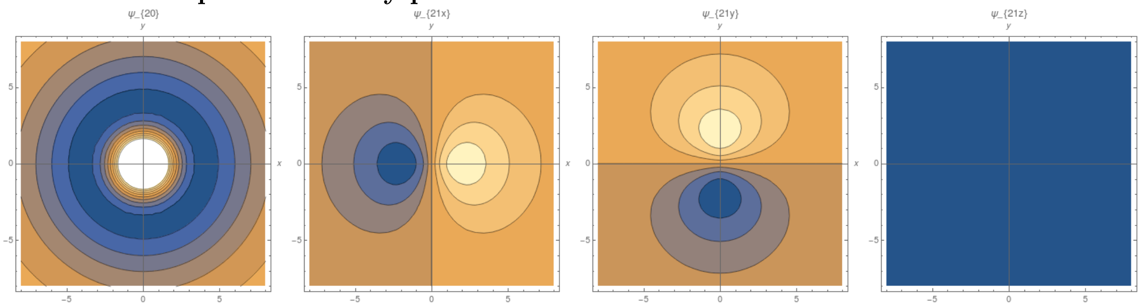


a) b) c) d)

Figure 2: 3D plots for the wavefunctions ψ_{200}, ψ_{21x}, ψ_{21y}, ψ_{21z}, from a) to b) respectively.

Here we can see that the p functions consist of two lobes with different sign each.

Draw contour plots on the xy plane



a) b) c) d)

Figure 3: Contour plots on the xy plane for the wavefunctions ψ_{200}, ψ_{21x}, ψ_{21y}, ψ_{21z}, from a) to b) respectively.

Which functions have inversion symmetry? If we don't consider signs only ψ_{200} has inversion symmetry. But if we are not that rigorous and we allow ourselves to take the absolute value of the functions then all of them have inversion symmetry with respect to the origin.

2 Slater determinants

3 Dirac Delta