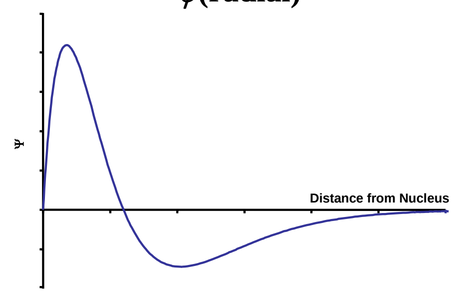
Quiz 8
CHEM 325
Spring 2009

Name: ____

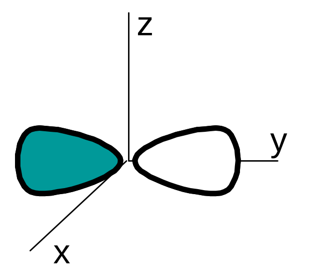
1. (10 Points) From the information given below, fill in the blanks.

a.

ψ(radial)



ψ (angular)

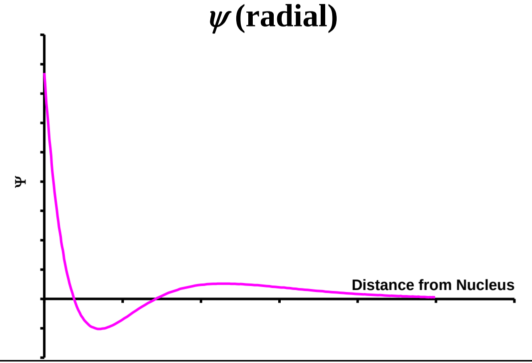


# Radial Nodes	**1**
# Angular Nodes	**1**
ℓ =	**1**
m_ℓ =	**indeterminate**

b. What does the coloration of the lobes of the angular part of this wavefunction show? **phase**

c.

ψ (radial)



# Radial Nodes	**2**
# Angular Nodes	**0**
ℓ =	**0**
Orbital's Full Name	**3s**

2a. (6 Points) Using the radial distribution function, determine the most probable distance for finding an electron in a hydrogen 1s orbital. Given: $\psi_{1s}(r) = 2\left(\frac{Z}{a_0}\right)^{3/2} e^{-\rho/2}$ where $\rho = \frac{2Zr}{na_0}$.

The general form of the radial distribution function is $r^2\Psi(r)^2$, and we may write (because $n = 1$ and $Z = 1$, so $\rho = 2r/a_0$)

$$r^2\psi_{1s}(r) = 4\left(\frac{1}{a_0}\right)^3 r^2 e^{-\rho} = 4\left(\frac{1}{a_0}\right)^3 r^2 e^{-2r/a_0}$$

The most probable distance at which to find this electron is when the derivative of the radial distribution function with respect to r is 0.

$$\frac{\partial r^2\psi_{1s}(r)}{\partial r} = 4\left(\frac{1}{a_0}\right)^3 \left[\left(r^2\right)\left(-\frac{2}{a_0}\right)\left(e^{-2r/a_0}\right) + \left(e^{-2r/a_0}\right)(2r) \right] = 0$$

$$\left(-\frac{2}{a_0}\right)\left(r^2\right) + 2r = 0$$

$$\left(\frac{-2}{a_0}\right) r = -2$$

$$r = a_0$$

3. (3 Points) Is there any place on the z axis where the probability of finding a 3 p_z electron is zero? If so, where?

Yes, there are two places: the nucleus and the radial node (there is one radial node in the 3 p_z wavefunction).

$$\psi_{2s}(r)=\frac{1}{\sqrt{8}}\left(\frac{Z}{a_0}\right)^{3/2}(2-\rho)e^{-\rho/2} \text{ where } \rho=\frac{2Zr}{na_0}$$

4a. (4 Points) From the equation for the hydrogen 2s radial wavefunction, given above, find the location of the radial node in units of a_0.

The only time this wavefunction can equal 0 is if $2-\rho=0$**, which means** $\rho = 2$**.**

Rearranging the given equation for ρ **to solve for** r **gives** $r=\frac{\rho n a_0}{2Z}$ **.**

Substituting in $\rho=2$ **and then using** $Z = 1$ **and** $n = 2$ **gives** $r = 2a_0$**.**

The radial node occurs at $2a_0$**, or** 2 **(in units of** a_0**).**

b. (6 Points) Find the location of the extremes in a hydrogen $\psi_{2s}(r)$, in units of a_0.

The extremes occur when $\frac{d\psi_{2s}(r)}{dr}=\frac{d\psi_{2s}(r)}{d\rho}=0$ **.**

$$\frac{d\psi_{2s}(r)}{d\rho}=\frac{1}{\sqrt{8}}\left(\frac{Z}{a_0}\right)^{3/2}\frac{d}{d\rho}(2-\rho)e^{-\rho/2}$$

$$\frac{d\psi_{2s}(r)}{d\rho}=\frac{1}{\sqrt{8}}\left(\frac{Z}{a_0}\right)^{3/2}\left((2-\rho)\left(\frac{-1}{2}\right)\left(e^{-\rho/2}\right)+\left(e^{-\rho/2}\right)(-1)\right)$$

$$\frac{d\psi_{2s}(r)}{d\rho}=\frac{1}{\sqrt{8}}\left(\frac{Z}{a_0}\right)^{3/2}\left(\frac{-(2-\rho)}{2}-1\right)\left(e^{-\rho/2}\right)=\frac{1}{\sqrt{8}}\left(\frac{Z}{a_0}\right)^{3/2}\left(\frac{\rho-4}{2}\right)\left(e^{-\rho/2}\right)=0$$

$$\rho=4$$

Substituting $\rho = 4$**,** $Z = 1$ **and** $n = 2$ **into the rearranged equation for** ρ **(as in part *a*) leads to**

$$r=\frac{\rho n a_0}{2Z}=\frac{8a_0}{2}=4a_0$$

One extreme occurs at a distance of $4a_0$ **(**4 **in units of** a_0**) from the nucleus and a second extreme occurs at the nucleus,** $r = 0$**. Recall** ψ **for all s orbitals is not zero at the nucleus, and must represent an extreme. Note that this extreme can't be found by differentiation** *(see the Student Solutions Manual for exercise 10.2 for more information)***.**