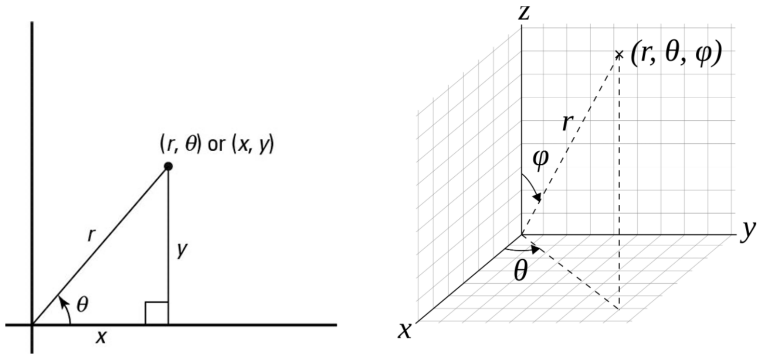
Week 7 Worksheet

Chem 11200-2: Section 33

Feb. 22, 2022



***Problem* 1:** Lets get a little bit more comfortable with polar and spherical coordinates.

a) Using simple trigonometry, show that $x = r\cos(\theta)$ and $y = r\sin(\theta)$. Conclude that any point in the plane (x, y) can be expressed instead as an angle (θ) from the x-axis and distance (r) from the origin (r, θ).

b) From the previous part, show that

$$r = \sqrt{x^2 + y^2} \text{ and } \theta = \arctan\left(\frac{y}{x}\right)$$

c) Recall that the potential generated by a point charge q centered at the origin (in 2D) is of the form

$$V(x, y) = \frac{1}{4\pi\epsilon_0}\frac{q}{\sqrt{x^2 + y^2}}$$

Convert this equation to polar coordinates.

d) Let (x, y) be some vector or point in the $x - y$ plane. We can rotate this by some angle θ around the origin by using the matrix

$$R(\theta) = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix}$$

That is

$$x \to x\cos\theta + y\sin\theta$$
$$y \to -x\sin\theta + y\cos\theta$$

Show that

$$V(x,y) = V(x\cos\theta + y\sin\theta, -x\sin\theta + y\cos\theta)$$

This is what is called a rotationally symmetry and hence the Coulomb force is rotationally symmetric! That is, if we rotate our entire coordinate system, the physics does not change.

e) In 3D, we must include another degree of freedom, ϕ which is the polar angle from the z-axis. Then each point in 3D space can be expressed as (x,y,z) or (ρ,θ,ϕ). Can you find formulas for x,y,z in terms of ρ,θ,ϕ and vice-a-versa?

***Problem* 2:** Draw an example of an s orbital, a p orbital, and a d orbital.

***Problem* 3:** Write out all sets of quantum numbers (n,l,m_l,m_s) possible for an e^- in each of these orbitals.

a) 2s orbital

b) 3p orbital

c) 4d orbital

***Problem* 4:** Suppose some electrons are described by the following (probably unnormalized) wavefunctions.

$$\psi_1(\rho,\theta,\phi) = \frac{1}{\sqrt{2\pi}}\frac{\rho}{a_0}\sin(\theta)e^{-\rho^2/2a_0^2}$$

$$\psi_2(\rho,\theta,\phi) = \frac{1}{\sqrt{2\pi}}\rho\left(12 - 8\frac{\rho}{a_0} + \left(\frac{\rho}{a_0}\right)^2\right)e^{-\rho^2/2a_0^2}$$

For each wavefunction above, answer the following questions:

a) Sketch the radial plot as well as the radial probability density plot.

b) How many radial nodes does ψ have? How many angular nodes?

c) What is a possible n and l value? What orbital would it be most similar to (1s, 2s,2p,3d,4f...)?

The following problems are written by Professor Mcleod or Head TA Miah Turke. They may mimic homework problems closely, but will be highly beneficial for the midterms and final.

***Problem* 5:** Suppose that there is some alternate universe that has the same four quantum numbers to describe an electron, n,l,m_l,m_s, but the rules governing the quantum numbers are somehow different so that

$$m_l = -2l,\ldots,0,\ldots,+2l$$

Describe how this would change the number of electrons in each shell for $n=1$ and $n=3$.

***Problem* 6:** Consider the wavefunction for the $3p_z$ orbital of a hydrogen atom:

$$\psi(\rho,\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos\theta\left[\frac{4}{81\sqrt{6}}\left(\frac{Z}{a_0}\right)^{3/2}\left(6\sigma-\sigma^2\right)e^{-\sigma/3}\right]$$

where $\sigma = \frac{Z}{a_0}\rho$ and $a_0 = \frac{\epsilon_0 h^2}{\pi e^2 m_e} = 0.529\times 10^-10\text{m}$

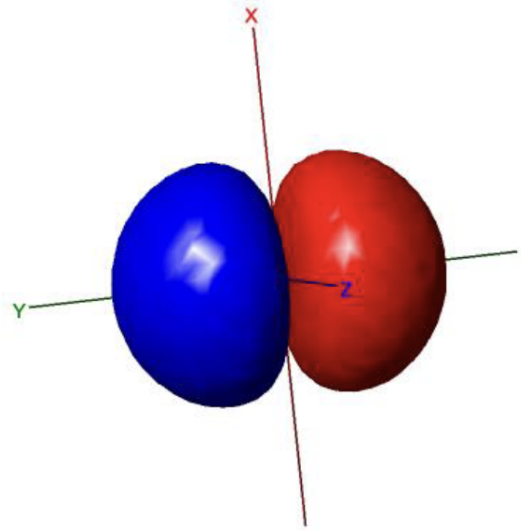
a) Sketch the $3p_z$ radial plot as well as the $3p_z$ radial probability density plot.

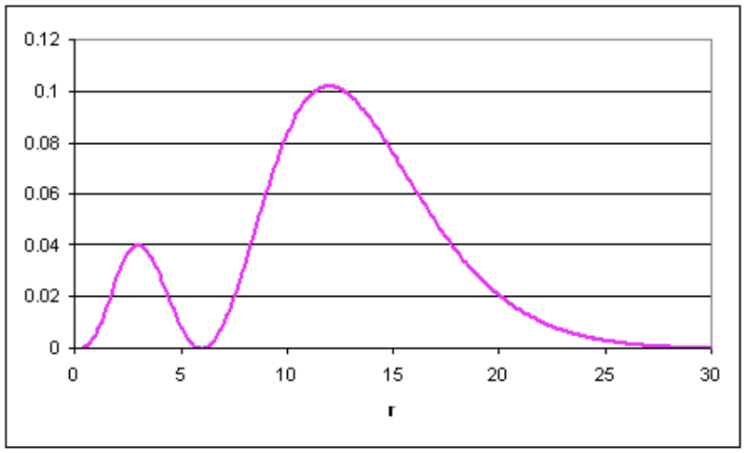
b) What is the average distance of an electron in the $3p_z$ orbital from the nucleus?

c) How many angular and radial nodes does the $3p_z$ orbital have? How can you determine where the nodes are relative to the nucleus of the atom?

d) Sketch the $3p_z$ orbital on an $x, y, z-$coordinate system being sure to include and label the angular and radial node(s).

***Problem* 7:** Identify the following orbital, including orientation (x, y, z). What are its value of n and l? How many radial and angular nodes does this orbital have? Explain your reasoning.





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