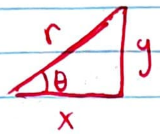
Week 7 Discussion Answers

1) a)



$\cos\theta = \frac{x}{r} = \frac{\text{adjacent}}{\text{hypotenus}}$

$\sin\theta = \frac{y}{r} = \frac{\text{opposite}}{\text{hypotenus}}$

Hence, $\left.\begin{array}{l} x = r\cos\theta \\ y = r\sin\theta \end{array}\right\}$ conversion to polar coordinates

b) $x^2 + y^2 = r^2\cos^2\theta + r^2\sin^2\theta = r^2(\cos^2\theta + \sin^2\theta)$

Note, $\cos^2\theta + \sin^2\theta = 1 \Rightarrow x^2 + y^2 = r^2$

Thus, $\boxed{r = \sqrt{x^2+y^2}}$ (also from Pythagoreas Theorem.

$y = r\sin\theta \qquad x = r\cos\theta$

$\Rightarrow \frac{y}{x} = \frac{\sin\theta}{\cos\theta} = \tan\theta \Rightarrow \boxed{\theta = \arctan\frac{y}{x}}$

c) $V(x,y) = V(r,\theta) = \frac{1}{4\pi\epsilon_0}\frac{q}{r}$

d) Let $x' = x\cos\theta + y\sin\theta$, $y' = -x\sin\theta + y\cos\theta$

$x'^2 = x^2\cos^2\theta + y^2\sin^2\theta + 2xy\cos\theta\sin\theta$

$y'^2 = x^2\sin^2\theta + y^2\cos^2\theta - 2xy\cos\theta\sin\theta$

$x'^2 + y'^2 = x^2\cos^2\theta + y^2\sin^2\theta + 2xy\cos\theta\sin\theta$
$+ x^2\sin^2\theta + y^2\cos^2\theta - 2xy\cos\theta\sin\theta$

$= x^2(\cos^2\theta + \sin^2\theta) + y^2(\cos^2\theta + \sin^2\theta)$

$= x^2 + y^2$. Hence

$x'^2 + y'^2 = x^2 + y^2$.

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

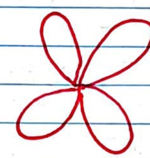
e) In spherical coordinates

$$x = r\sin\varphi\cos\theta \qquad r = \sqrt{x^2+y^2+z^2}$$
$$y = r\sin\varphi\sin\theta \qquad \varphi = \arctan\left(\sqrt{x^2+y^2}/z\right)$$
$$z = r\cos\varphi \qquad \theta = \arctan\left(\frac{y}{x}\right)$$

r : θ are straight forward, φ requires a bit more work.

2) Draw an example of an s orbital, p orbital, and a d orbital.

S-orbital



d-orbital

p orbital

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

n	l	m_l	m_s
2	0	0	-1
2	0	0	+1

b) 3p orbital

n	l	m_l	m_s
3	1	-1	-1
3	1	-1	+1
3	1	0	+1
3	1	0	-1
3	1	+1	-1
3	1	+1	+1

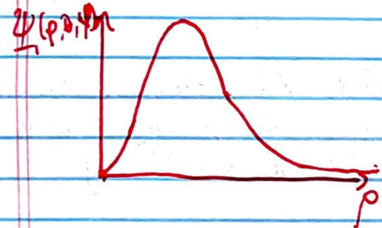
c) 4d orbital

n	l	m_l	m_s
4	2	-2	-1
4	2	-2	+1
4	2	-1	-1
4	2	-1	+1

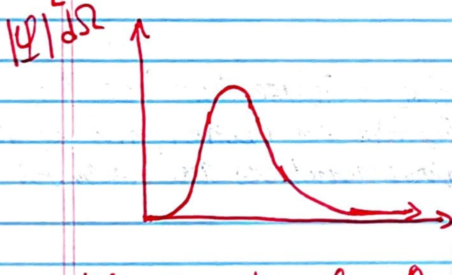
n	l	m_l	m_s
4	2	0	-1
4	2	0	+1
4	2	1	-1
4	2	1	+1
4	2	2	-1
4	2	2	+1

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

$$\Psi_1(\rho,\theta,\varphi) = \frac{1}{\sqrt{2\pi}}\,\frac{\rho}{a_0}\,\sin(\theta)\,e^{-\rho^2/2a_0^2}$$



We see this will only be zero at $\rho=0$

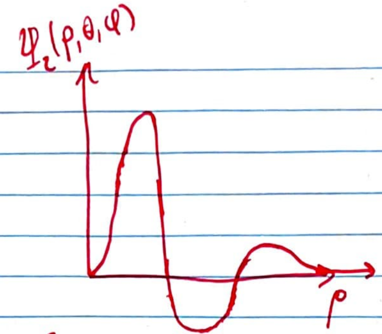


We expect only 0 radial nodes. The $\sin(\theta)$ gives us 1 set of angular nodes.

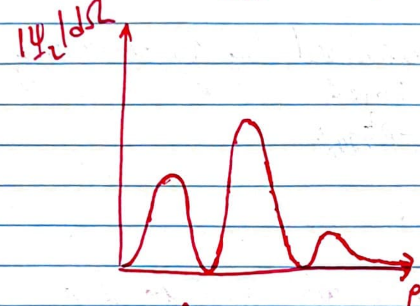
We expect l to be 1 since it has 1 angular node. No radial nodes for a p type orbital implies.

$\boxed{2p}$ - type.

$$\Psi_2(\rho,\theta,\varphi) = \frac{\rho}{\sqrt{2\pi}}\left[12 - 8\frac{\rho}{a_0} + \left(\frac{\rho}{a_0}\right)^2\right] e^{-\rho^2/2a_0^2}$$



We see we have
$\rho^2 - 8\rho + 12 = (\rho-6)(\rho-2)$
so radial nodes at ~ 6 & 2.



we have 2 radial nodes. No angular nodes (since there is no dependence on θ or φ). Hence $\ell=0$ (s-type). 2 radial nodes $\Rightarrow$ $\boxed{3s}$

$\boxed{3s\text{-type}}$

5) Suppose that there is an alternative 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

$$m_\ell = -2\ell, \dots, 0, \dots, +2\ell$$

Describe how this could change the number of e^- in each shell for $n=1$ & $n=3$.

For $n=1$, in our universe we have
$n=1$, $\ell=0$, $m_\ell=0$, $m_s=\pm 1 \Rightarrow 2e^-$.
Alt. universe, $n=1$, $\ell=0$, $m_\ell=0$, $m_s=\pm1 \Rightarrow 2e^-$
So no change.

~~[illegible]~~

For $n=3$, we have
$\ell = 0, 1, 2$ $\quad m_\ell = 0, \pm1, \pm2$, $m_s = \pm 1 \Rightarrow 18e^-$ total.

In alt universe, we increase e^- in $\ell=1$ & $\ell=2$ shells.

So we will have $30e^-$. So $18e^- \rightarrow 30e^-$ in $n=3$

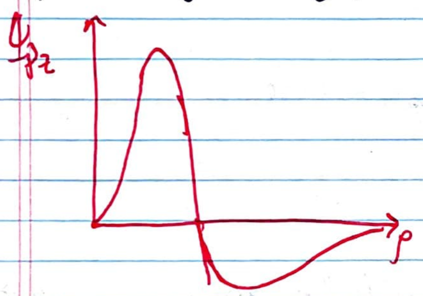
6) Consider the wavefunction of the $3p_z$ orbital of a hydrogen atom:

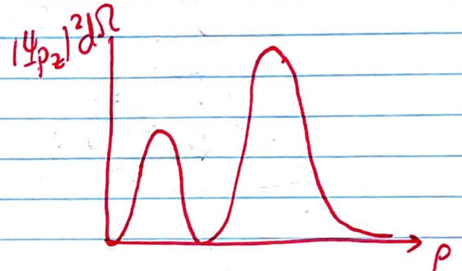
$$\psi(\rho,\theta,\varphi) = \sqrt{\frac{3}{4\pi}}\cos\theta\left[\frac{4}{81\sqrt{6}}\left(\frac{Z}{a_0}\right)^{3/2}(6\sigma-\sigma^2)e^{-\sigma/3}\right]$$

where $\sigma = \frac{Z}{a_0}\rho$

a_0 has units of length.

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





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

$$\bar{r}_{nl} = \frac{n^2 a_0}{Z}\left[1+\frac{1}{2}\left(1-\frac{l(l-1)}{n^2}\right)\right]$$

$n=3,\ l=1 \Rightarrow$

$$= \frac{9(0.529\times10^{-10}\,m)}{1}\left[1+\frac{1}{2}\left[1-\frac{1(1-1)}{9}\right]\right] = \boxed{7.14\times10^{-10}\,m}$$

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?

For orbital with n; l, we have l angular nodes;
$n-l-1$ radial nodes.

In our case, $3-1-1 = 1$ radial node (on graph)
$l=1$ angular node.

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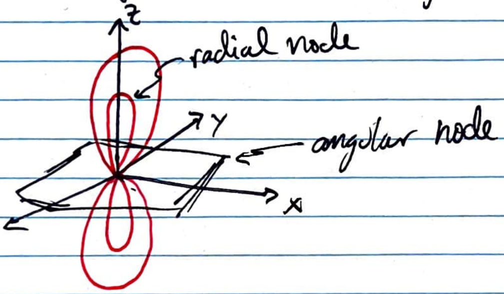
The radial nodes are the zeroes of the radial wavefunction.

$$R(\rho) = \frac{4}{81\sqrt{6}}\left(\frac{Z}{a_0}\right)^{3/2}(6\sigma-\sigma^2)e^{-\sigma/3}$$

$\sigma = 6, 0 \Rightarrow$

$\frac{Zr}{a_0} = 6$ or $r = 0$ or $\frac{6a_0}{Z}$ for the radial node positions.

d) Sketch the $3p_z$ orbital in the x,y,z-coordinate system.



7) Identify the following orbital, including orientation (x,y,z). What are its value of n & l? How many radial & angular nodes does this orbital have?

Has 1 radial node (from graph). 1 angular node.
We also know it's a p_y orbital.

$\Rightarrow$ $3p_y$ since 1 radial node.