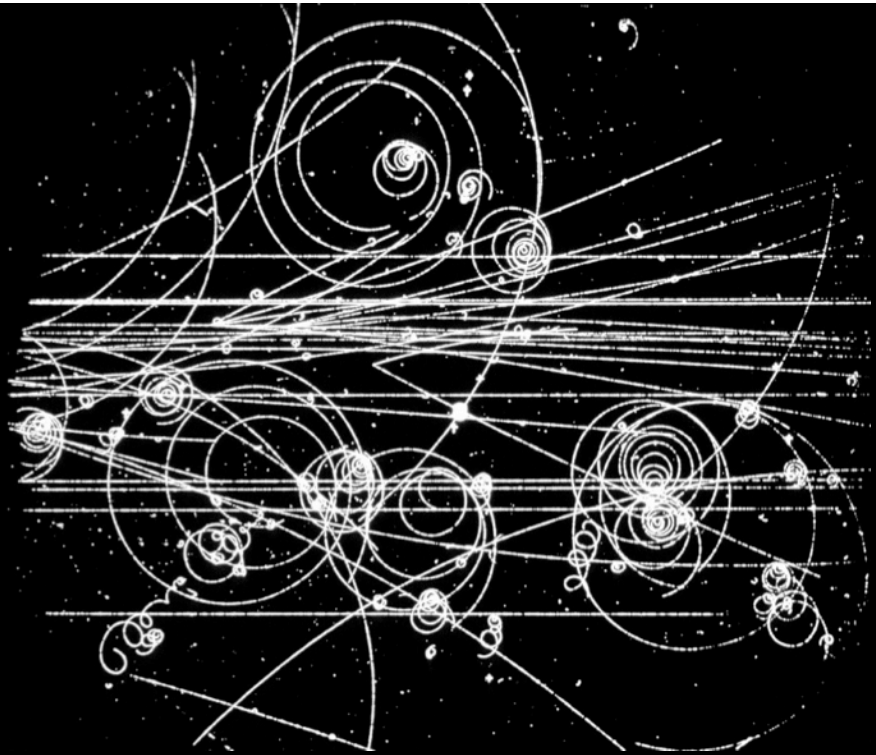
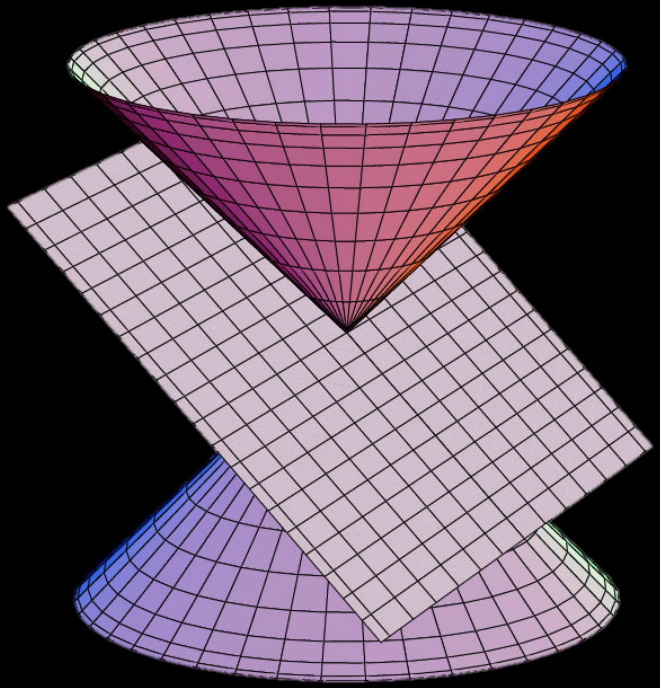




Modern Physics (Phys. IV): 2704

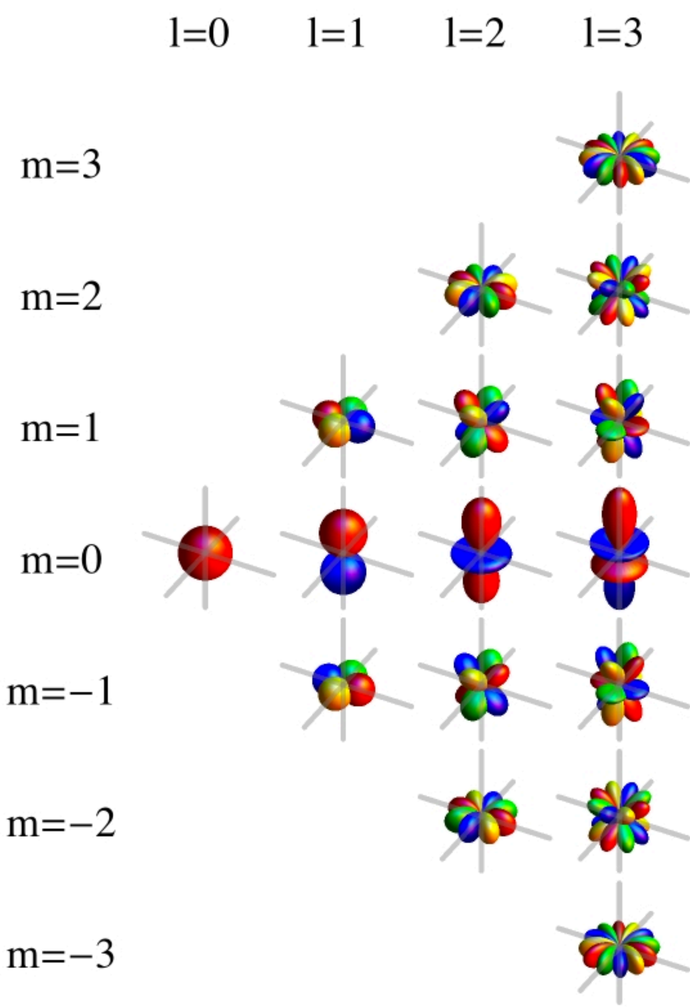
Professor Jasper Halekas
Van Allen 70
MWF 12:30-1:20 Lecture

Announcements

- Midterm #2 Wednesday April 4th
  - Covers Ch. 5-7
  - Same policies as Midterm #1
- Sample midterms posted today
- Monday will be a review day in class
- No labs or homework next week
  - Lab Q9 this week, and HW #8 due Friday

Spherical Harmonics

-real
+real
-imaginary
+imaginary



ℓ	m_ℓ	$Y_{\ell m_l}(\theta,\phi) = \Theta_{\ell m_l}(\theta)\Phi_{m_l}(\phi)$
0	0	$(1/4\pi)^{1/2}$
1	0	$(3/4\pi)^{1/2}\cos\theta$
1	±1	$\mp(3/8\pi)^{1/2}\sin\theta e^{\pm i\phi}$
2	0	$(5/16\pi)^{1/2}(3\cos^2\theta-1)$
2	±1	$\mp(15/8\pi)^{1/2}\sin\theta\cos\theta e^{\pm i\phi}$
2	±2	$(15/32\pi)^{1/2}\sin^2\theta e^{\pm 2i\phi}$

$$\Phi_{m_\ell}(\phi) = \frac{1}{\sqrt{2\pi}} e^{i m_\ell \phi}$$

$$\Theta_{\ell m_\ell}(\theta) = \left[\frac{2\ell+1}{2}\frac{(\ell-m_\ell)!}{(\ell+m_\ell)!}\right]^{1/2} P_\ell^{m_\ell}(\theta)$$

$P_\ell^{m_\ell}(\theta) = associated\ \ Legendre\ \ polynomial$

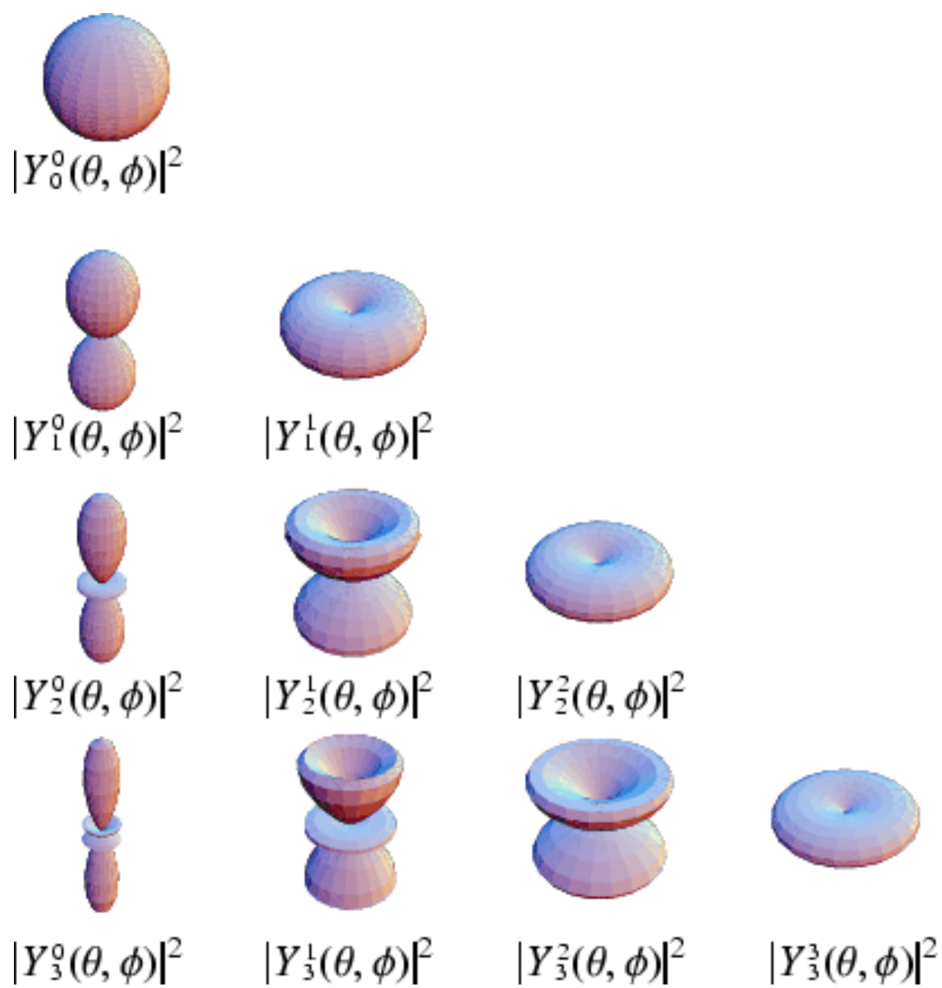
Angular Probability Density

s: l = 0

p: l = 1

d: l = 2

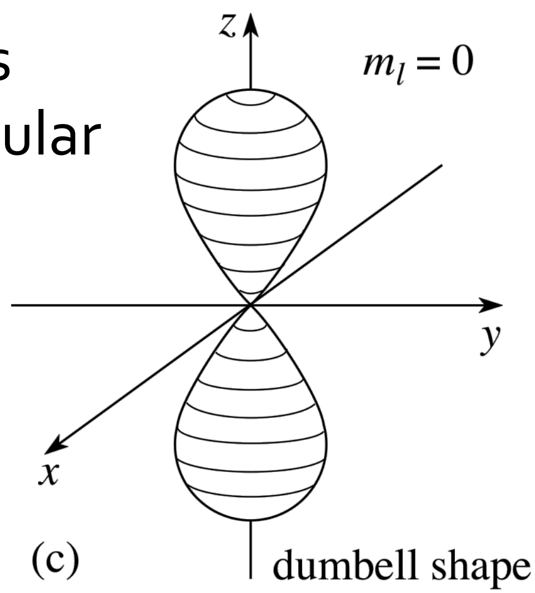
f: l = 3

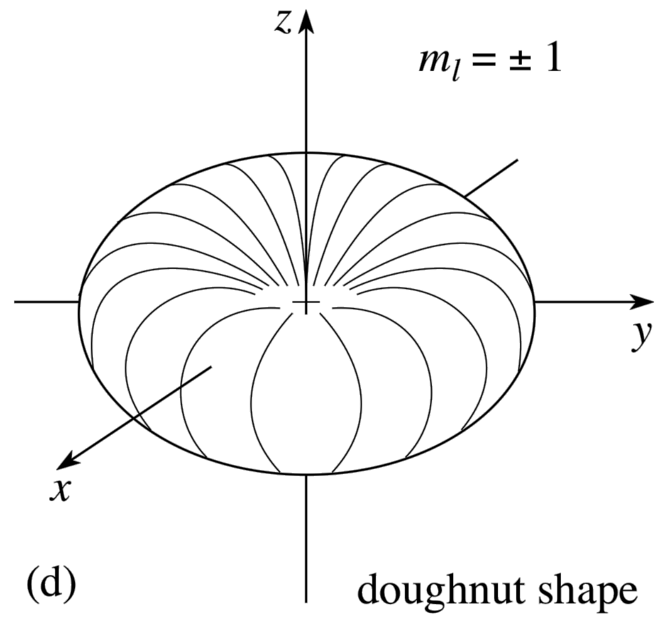


L = 1 Orbitals

Which electron has larger average angular momentum L_z around the Z-axis?

- $m_l = 0$
- $m_l = \pm 1$
- both same
- nothing to do with L

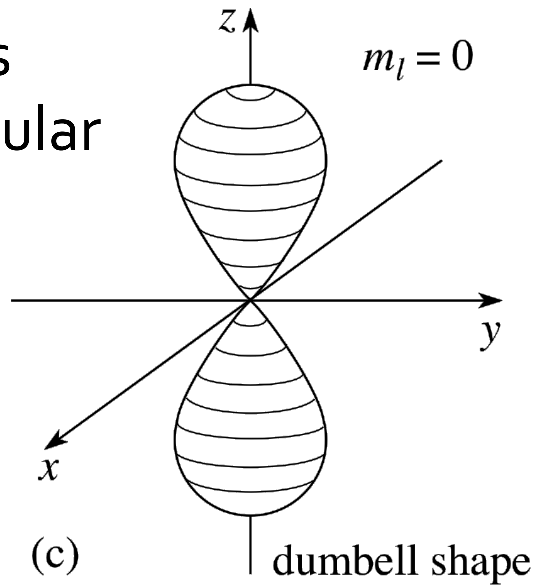




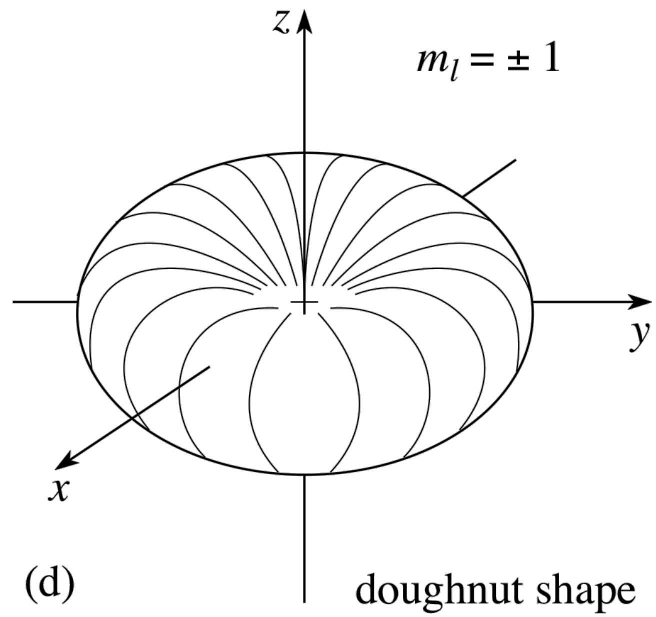
L = 1 Orbitals

Which electron has larger average angular momentum L_z around the Z-axis?

- $m_l = 0$
- $m_l = \pm 1$
- both same
- nothing to do with L



(c)

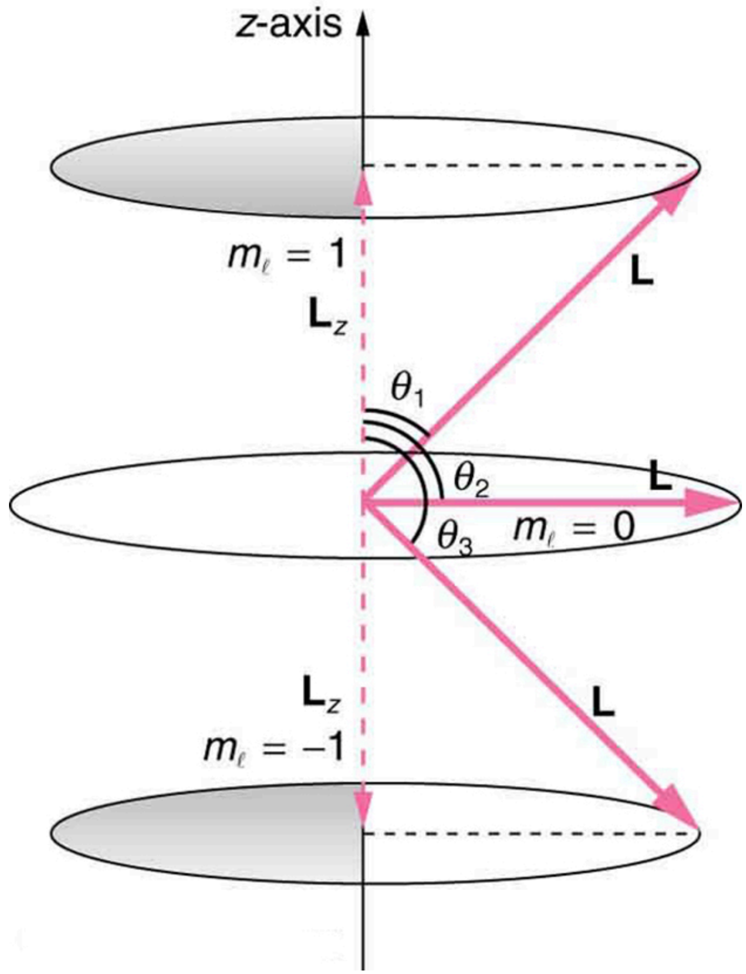


(d)

Energy and Angular Momentum

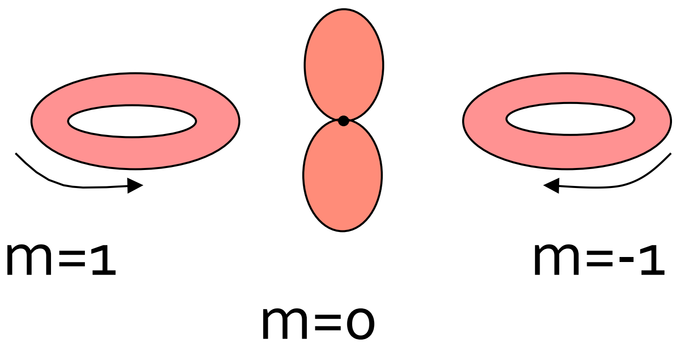
- $L^2 = l(l+1)\hbar^2$
  - $l = 0,1,2,\ldots$
- $L_z = m_l\,\hbar$
  - $m_l = -l,\ -l+1,\ ..,\ l-1,\ l$

L=1 Angular Momentum

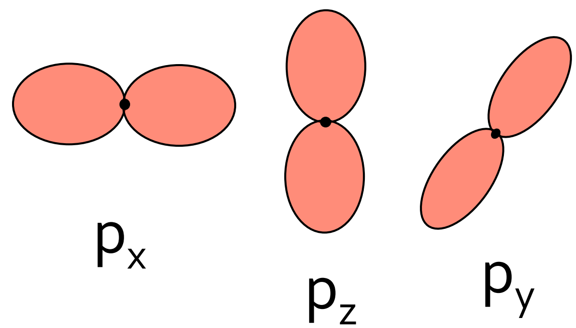


Physics Vs. Chemistry

2p wave functions
(Physics view)
(n=2, l=1)



Dumbbell Orbits
(chemistry)



p_x=superposition
(addition of m=-1 and m=+1)

p_y=superposition
(subtraction of m=-1 and m=+1)

Physics vs. Chemistry

$$Y_1^{\pm 1} = \mp \sqrt{3/8\pi}\, \sin\theta\, e^{\pm i\varphi}$$

$$(Y_1^1 + Y_1^{-1})/\sqrt{2}$$

$$= \sqrt{3/4\pi}\, \sin\theta\, (e^{i\varphi} + e^{-i\varphi})/2$$

$$= \sqrt{3/4\pi}\, \sin\theta \cos\varphi$$

$$= \sqrt{3/4\pi} \cdot \frac{x}{r}$$

Compare to $Y_1^0 = \sqrt{\frac{3}{4\pi}}\, \cos\theta$

$$= \sqrt{3/4\pi} \cdot z/r$$

- So, no preferred direction

chemistry: $|\psi|^2 \propto \frac{|x|}{r}, \frac{|y|}{r}, \frac{|z|}{r}$

physics: $|\psi|^2 \propto \frac{\sqrt{x^2+y^2}}{r}, \frac{\sqrt{x^2+y^2}}{r}, \frac{|z|}{r}$

Back to Radial Equation

$$-\frac{\hbar^2}{2m_e r^2}\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right)+\left[\frac{\hbar^2 l(l+1)}{2m_e r^2}-\frac{e^2}{4\pi\varepsilon_0 r}\right]R(r)=ER(r)$$

Potential Energy

Radial Kinetic Energy

Angular Kinetic Energy

Total Energy

Radial Wave Function

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{me^2 r}{2\pi\varepsilon_0\hbar^2}+\frac{2mE}{\hbar^2 r^2}-\ell(\ell+1)=0$$

- Solutions are Laguerre polynomials

$$R_{n\ell}(r)=A\cdot\frac{1}{r}\rho^{\ell+1}e^{-\rho}L_{n-\ell-1}^{2\ell+1}(2\rho)$$

$$\text{w/ } \rho=\sqrt{\frac{-2mE}{\hbar^2}}\,r$$

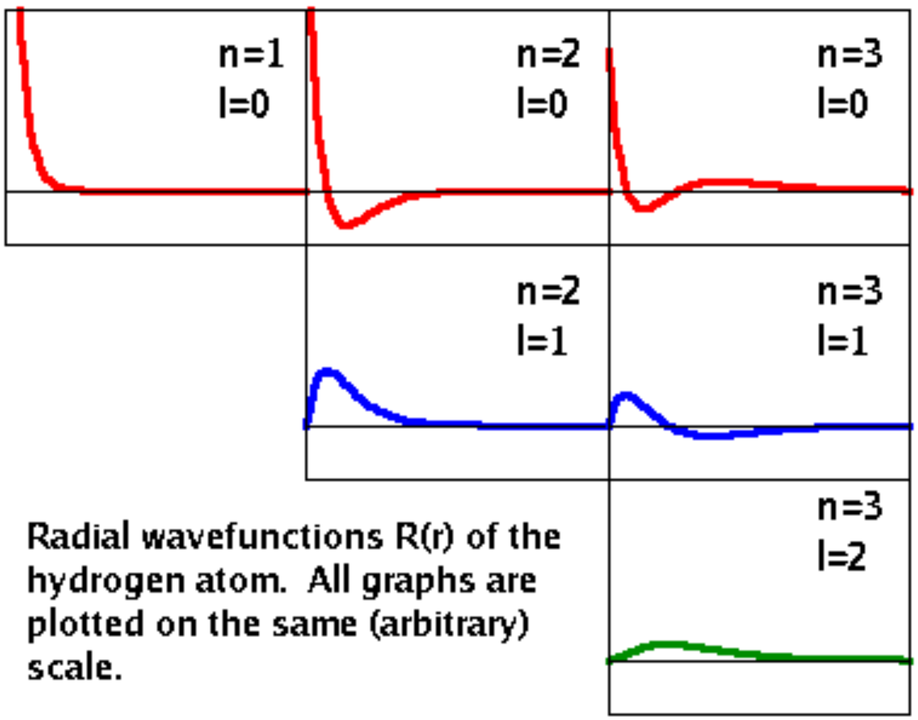
- Valid solution requires

$$E_n=-\frac{me^4}{32\pi^2\varepsilon_0^2\hbar^2}\cdot\frac{1}{n^2}$$

same as Bohr

$$\ell=0,1,\ldots,n-1$$

Radial Wave Functions



Radial wavefunctions R(r) of the hydrogen atom. All graphs are plotted on the same (arbitrary) scale.

$$R_{10} = 2a^{-3/2}\exp(-r/a)$$

$$R_{20} = \frac{1}{\sqrt{2}}a^{-3/2}\left(1-\frac{1}{2}\frac{r}{a}\right)\exp(-r/2a)$$

$$R_{21} = \frac{1}{\sqrt{24}}a^{-3/2}\frac{r}{a}\exp(-r/2a)$$

$$R_{30} = \frac{2}{\sqrt{27}}a^{-3/2}\left(1-\frac{2}{3}\frac{r}{a}+\frac{2}{27}\left(\frac{r}{a}\right)^2\right)\exp(-r/3a)$$

$$R_{31} = \frac{8}{27\sqrt{6}}a^{-3/2}\left(1-\frac{1}{6}\frac{r}{a}\right)\left(\frac{r}{a}\right)\exp(-r/3a)$$

$$R_{32} = \frac{4}{81\sqrt{30}}a^{-3/2}\left(\frac{r}{a}\right)^2\exp(-r/3a)$$

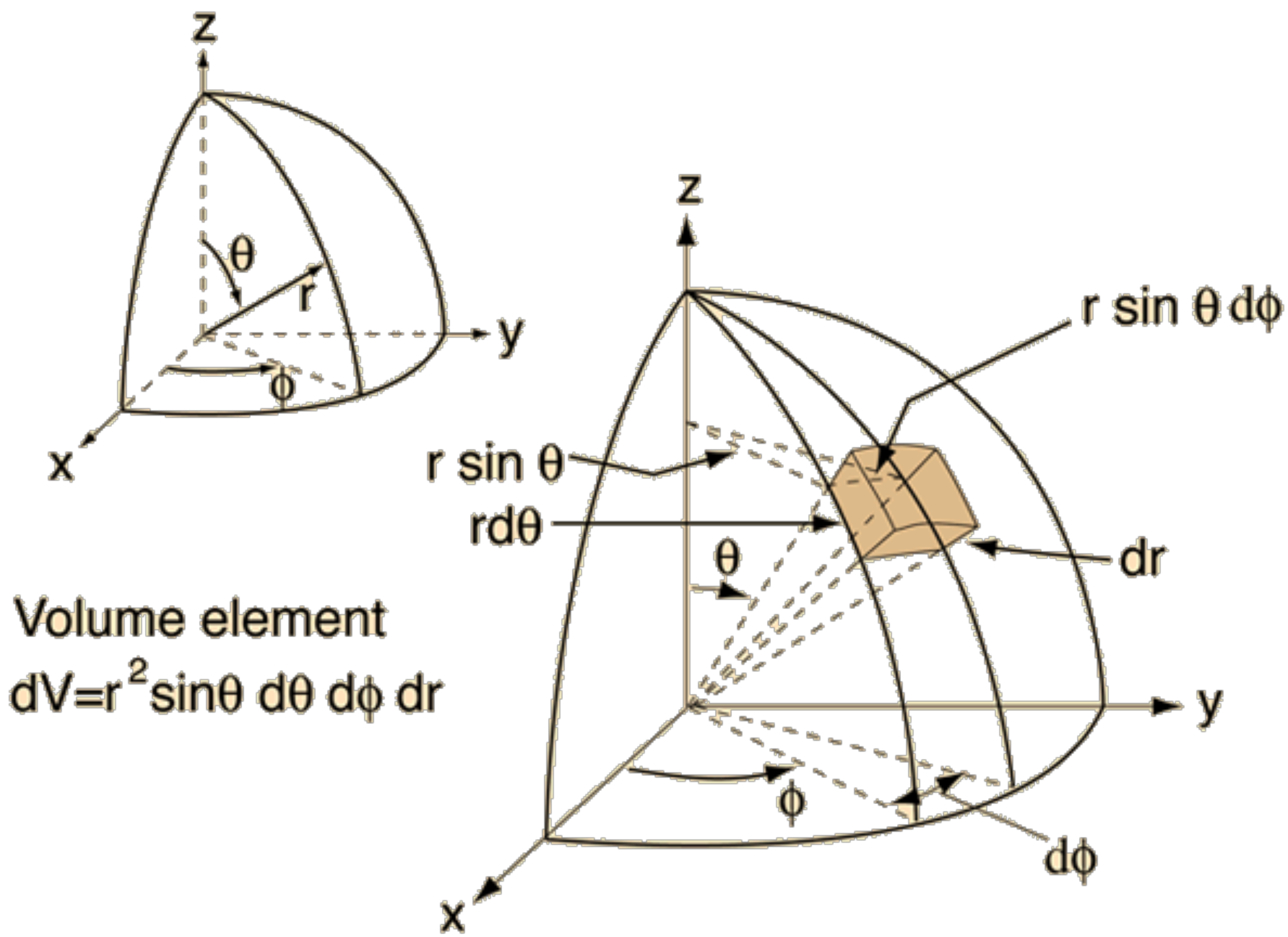
$$R_{40} = \frac{1}{4}a^{-3/2}\left(1-\frac{3}{4}\frac{r}{a}+\frac{1}{8}\left(\frac{r}{a}\right)^2-\frac{1}{192}\left(\frac{r}{a}\right)^3\right)\exp(-r/4a)$$

$$R_{41} = \frac{\sqrt{5}}{16\sqrt{3}}a^{-3/2}\left(1-\frac{1}{4}\frac{r}{a}+\frac{1}{80}\left(\frac{r}{a}\right)^2\right)\frac{r}{a}\exp(-r/4a)$$

$$R_{42} = \frac{1}{64\sqrt{5}}a^{-3/2}\left(1-\frac{1}{12}\frac{r}{a}\right)\left(\frac{r}{a}\right)^2\exp(-r/4a)$$

$$R_{43} = \frac{1}{768\sqrt{35}}a^{-3/2}\left(\frac{r}{a}\right)^3\exp(-r/4a)$$

Volume Integrals in Spherical Coordinates



Normalization

$$\psi_{100} = \frac{1}{\sqrt{4\pi}} \cdot \frac{2}{a_0^{3/2}} e^{-r/a_0}$$

$$|\psi_{100}|^2 = \frac{1}{\pi a_0^3} e^{-2r/a_0}$$

$$\iiint |\psi_{100}|^2 \, dV$$

$$= \int_0^\infty \int_0^{2\pi} \int_0^\pi \cdot \frac{1}{\pi a_0^3} e^{-2r/a_0} r^2 \sin\theta \, d\theta \, d\varphi \, dr$$

$$\int_0^\pi \sin\theta \, d\theta = -\cos\theta \Big|_0^\pi = 2$$

$$\Rightarrow \int_0^\infty \int_0^{2\pi} \frac{2}{\pi a_0^3} e^{-2r/a_0} r^2 \, dr \, d\varphi$$

$$\int_0^{2\pi} d\varphi = 2\pi$$

$$\Rightarrow \int_0^\infty \frac{4}{a_0^3} r^2 e^{-2r/a_0} \, dr$$

$$\int_0^\infty x^2 e^{-bx} = 2/b^3$$

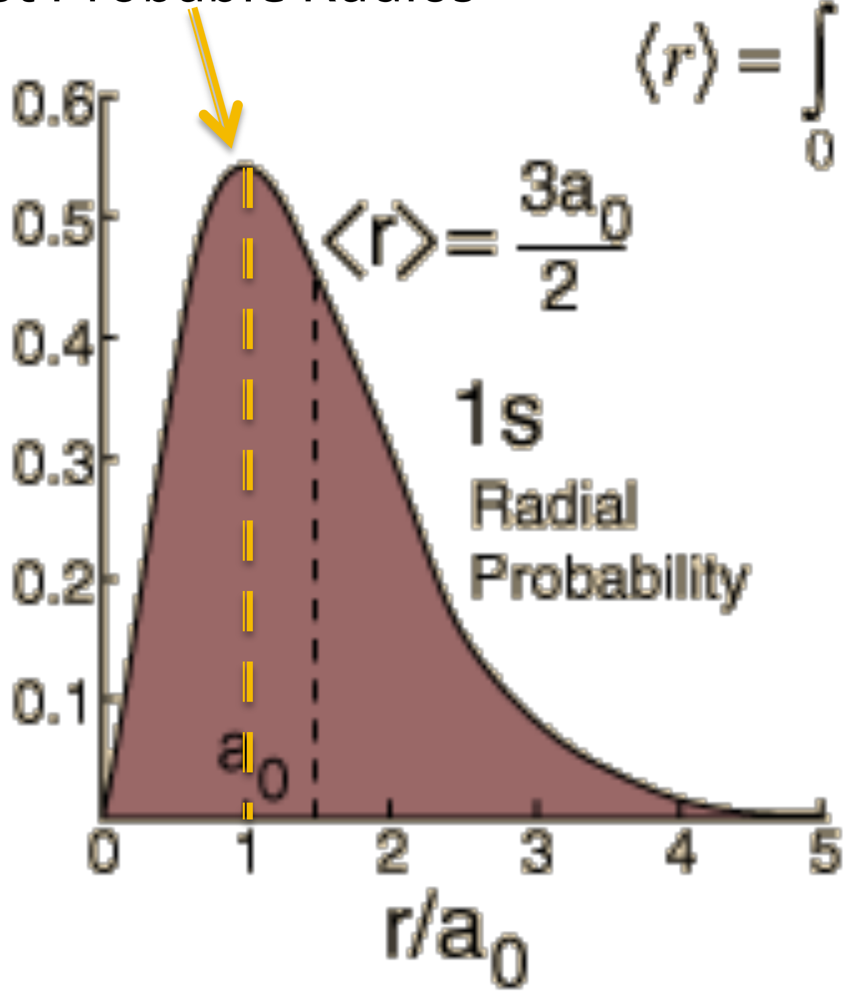
$$\Rightarrow 4/a_0^3 \cdot 2/(2/a_0)^3 = 1 \quad //$$

Most Probable & Average Radius

Most Probable Radius

$$\langle r \rangle = \int_0^\infty rP(r)\ dr = \frac{4}{a_0^3}\int_0^\infty r^3 e^{-2r/a_0} dr$$

$a_o P(r)$



Radial Probability Density

$P(r) = r^2 \, |R(r)|^2$

Radial Probability Density

$$P(r) = r^2 R^2(r)$$

For $n=1$, $l=0$

$$R_{10}(r) = \frac{2}{a_0^{3/2}} e^{-r/a_0}$$

$$\Rightarrow P(r) = \frac{4r^2}{a_0^3} e^{-2r/a_0}$$

Maximum when

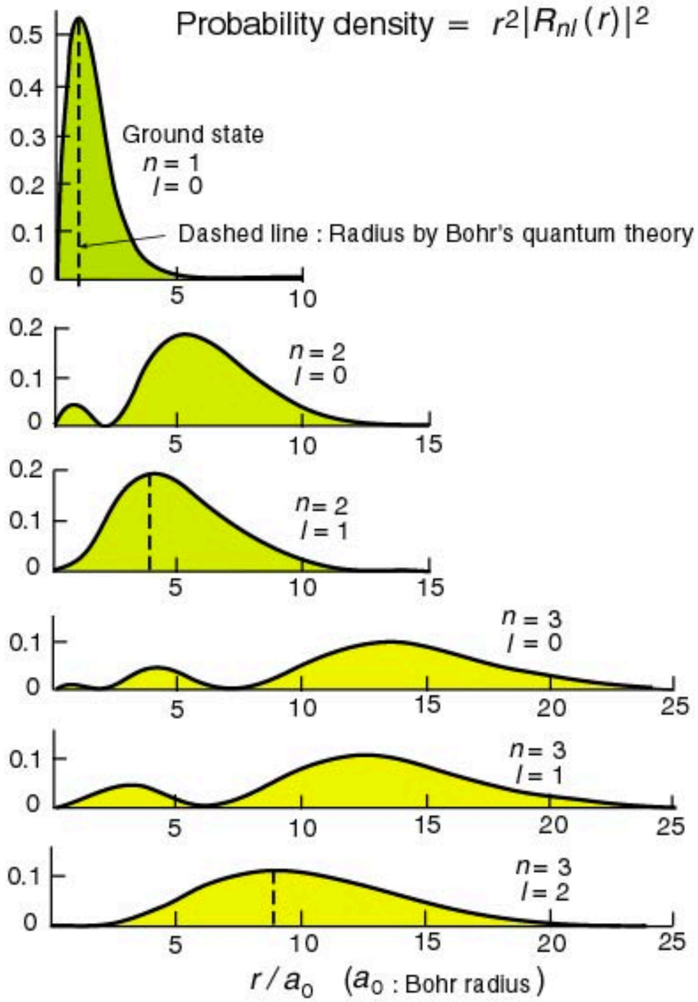
$$\frac{d}{dr}\left(P(r) \right) = 0$$

TBD in HW 7.12

Average

$$\langle r \rangle = \int_0^\infty r\, P(r)\, dr$$

Radial Probability Distribution



***s*: *l* = 0**
***p*: *l* = 1**
***d*: *l* = 2**