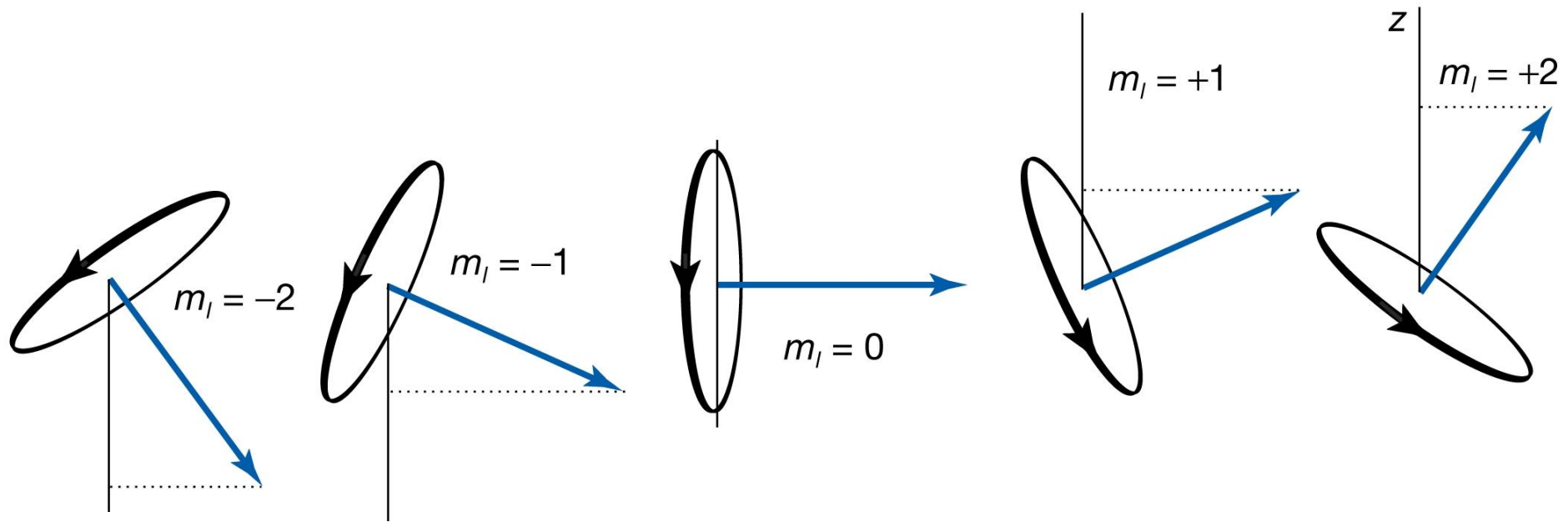
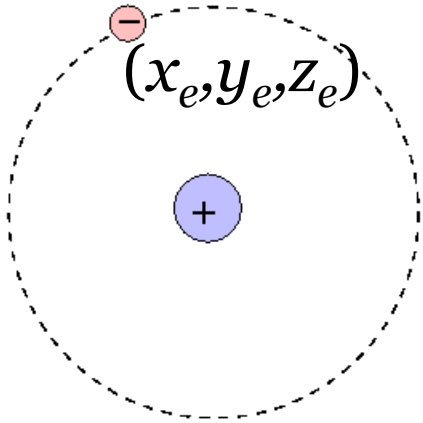


Hydrogen Atom: Magnetic and Azimuthal quantum numbers



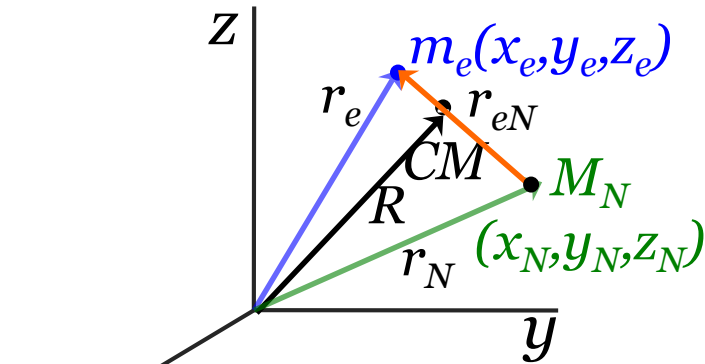
Atkins' Physical Chemistry

Hydrogen Atom: Relative Frame of Reference



$$\left(-\frac{\hbar^2}{2m_N} \nabla_N^2 - \frac{\hbar^2}{2m_e} \nabla_e^2 - \frac{QZe^2}{r_{eN}} \right) \Psi_{Total} = E_{Total} \cdot \Psi_{Total}$$

Separation of \hat{H} into Center of Mass and Internal co-ordinates



$$r_N = \sqrt{(x_N^2 + y_N^2 + z_N^2)}$$

$$r_e = \sqrt{(x_e^2 + y_e^2 + z_e^2)}$$

$$x = x_e - x_N$$

$$y = y_e - y_N$$

$$z = z_e - z_N$$

$$\begin{aligned} r = r_{eN} &= r_e - r_N \\ &= \sqrt{(x^2 + y^2 + z^2)} \end{aligned}$$

$$X = \frac{m_e x_e + m_N x_N}{m_e + m_N}$$

$$Y = \frac{m_e y_e + m_N y_N}{m_e + m_N}$$

$$Z = \frac{m_e z_e + m_N z_N}{m_e + m_N}$$

$$R = \frac{m_e r_e + m_N r_N}{m_e + m_N}$$

Hydrogen Atom: Separation of CM motion

$$\left(-\frac{\hbar^2}{2M} \nabla_R^2 - \frac{\hbar^2}{2\mu} \nabla_r^2 - \frac{QZe^2}{r} \right) \Psi_{Total} = E_{Total} \cdot \Psi_{Total}$$

$$\hat{H} = \hat{H}_N + \hat{H}_e$$

$$\Psi_{Total} = \chi_N \times \psi_e$$

$$E_{Total} = E_N + E_e$$

$$\hat{H}_N \chi_N = \left(-\frac{\hbar^2}{2M} \nabla_R^2 \right) \chi_N = E_N \chi_N$$

Free particle!
Kinetic energy of the atom

$$E_N = \frac{\hbar^2 k^2}{2M}$$

Hydrogen Atom: Electronic Hamiltonian

$$\hat{H}_e \cdot \psi_e = \left(-\frac{\hbar^2}{2\mu} \nabla_r^2 - \frac{QZe^2}{r} \right) \psi_e = E_e \cdot \psi_e$$

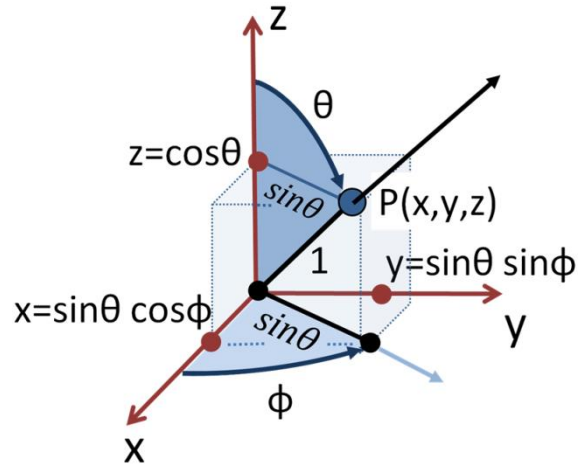
$$\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$\frac{QZe^2}{\sqrt{(x^2 + y^2 + z^2)}} \psi_e(x, y, z)$$

$$y_e \models y_e(x, y, z)$$

Not possible to separate out into three different co-ordinates.
Need a new co-ordinate system

Spherical Polar Co-ordinates



$$z = r \cos \theta$$

$$x = r \sin \theta \cos \phi$$

$$y = r \sin \theta \sin \phi$$

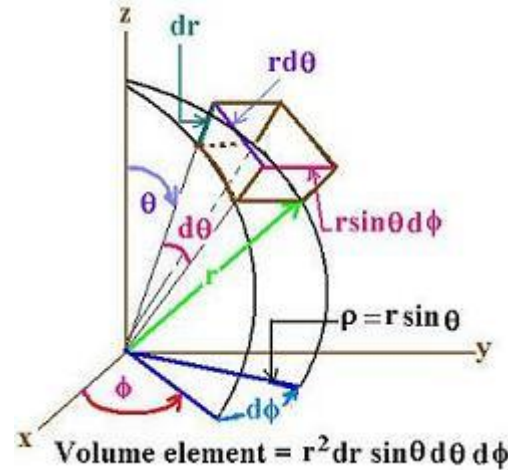


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$$r: 0 \text{ to } \infty$$

$$\theta: 0 \text{ to } \pi$$

$$\phi: 0 \text{ to } 2\pi$$



$$r = \sqrt{(x^2 + y^2 + z^2)}$$

$$\theta = \cos^{-1} \left(\frac{z}{r} \right)$$

$$\phi = \tan^{-1} \left(\frac{y}{x} \right)$$

$$dt = r^2 \times dr \times \sin \theta \times d\theta \times d\phi$$

Separation of variables

$$\frac{1}{R} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) + \frac{2\mu r Q Z e^2}{\hbar^2} + \frac{2\mu r^2}{\hbar^2} E_e = \beta$$

Radial equation

$$\frac{\sin q}{Q} \frac{\partial}{\partial q} \left(\frac{\partial Q}{\partial q} \right) + b \sin^2 q = m^2$$

Angular equation

Separation of variables

$$\frac{1}{R} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) + \frac{2\mu r Q Z e^2}{\hbar^2} + \frac{2\mu r^2}{\hbar^2} E_e = \beta$$

$$\frac{\sin q}{Q} \frac{\partial}{\partial q} \left(\frac{\partial}{\partial q} \right) \sin q + b \sin^2 q = m^2$$

$$\frac{1}{F} \frac{\partial^2 F}{\partial f^2} = -m^2$$

The three variables r , θ and ϕ are separated

Solution to ϕ part

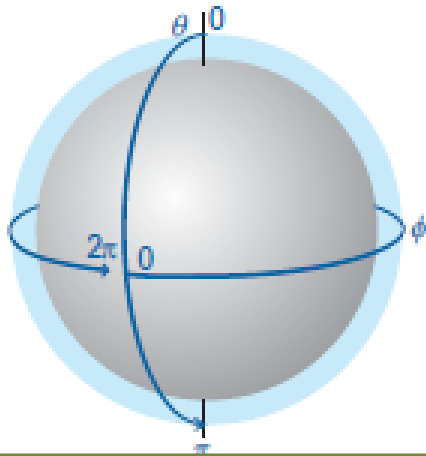
$$\frac{1}{F(f)} \frac{\nabla^2 F(f)}{\nabla f^2} + m^2 = 0$$



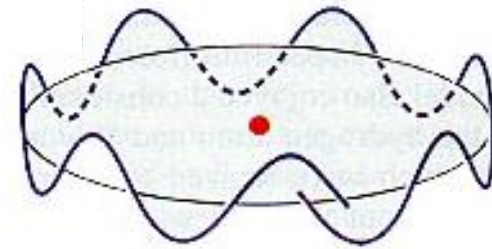
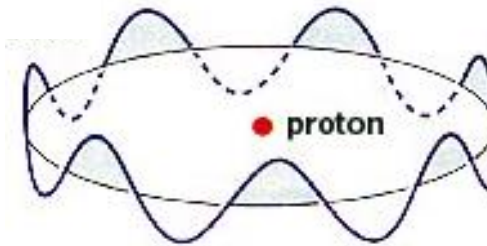
$$\frac{\nabla^2 F(f)}{\nabla f^2} = -m^2 F(f)$$

Trial solution: $\Phi(\phi) = Ae^{\pm im\phi}$

$$\frac{\nabla F}{\nabla f} = \pm imF$$



' ϕ ' ranges from 0 to 2π



Wavefunction has to be single-valued

$$\Rightarrow \Phi(\phi + 2\pi) = \Phi(\phi)$$

Periodic Boundary Condition

z-component of angular momentum

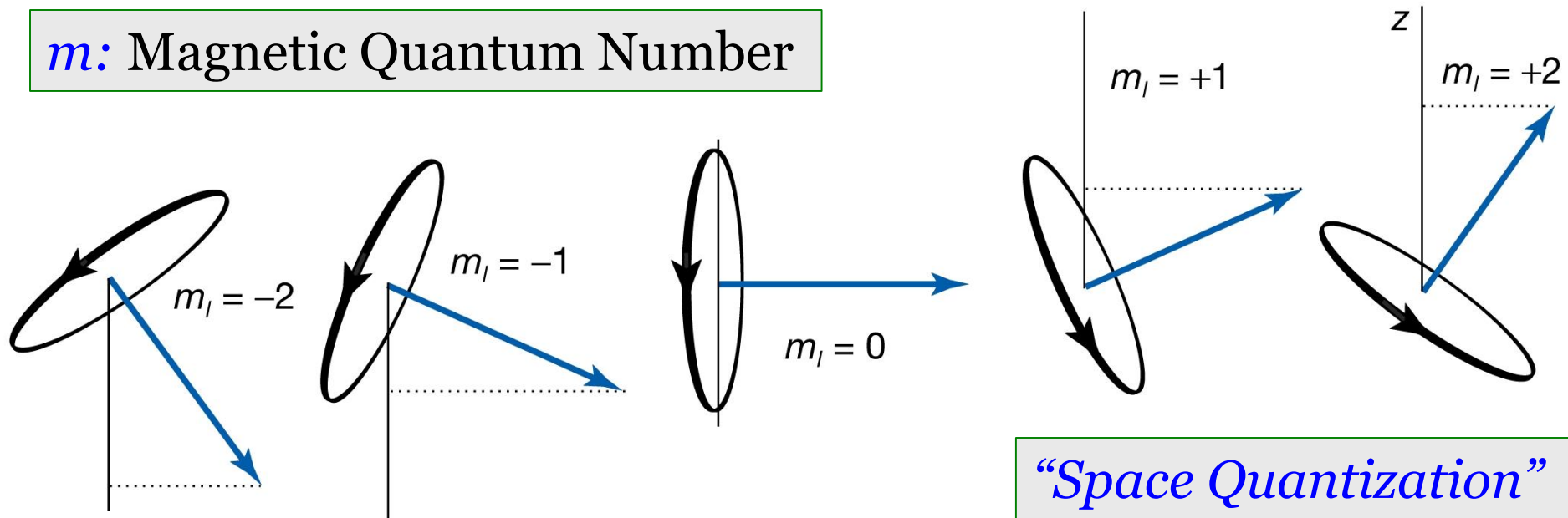
$$\hat{L}_z = \frac{\hbar}{i} \frac{\partial}{\partial \phi}$$

$$\Phi(\phi) = Ae^{\pm im\phi}$$

$$\hat{L}_z \Phi = \frac{\hbar}{i} \frac{\partial}{\partial \phi} \Phi = \frac{\hbar}{i} im \Phi = m\hbar \Phi$$

z-component of angular momentum

m : Magnetic Quantum Number



Solution to ϕ part: Magnetic quantum number

- $m=0, \pm 1, \pm 2, \pm 3, \pm 4, \dots$
- m is the **magnetic quantum number**
- m is restricted by another quantum number (orbital Angular momentum), l , such that $|m| < l$

$$\frac{\sin \theta}{r} \frac{\partial}{\partial \theta} \left(\frac{1}{\sin \theta} \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} + \frac{2m\mu_B B}{\hbar^2} \psi = 0$$

$$\frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} = -m^2 \psi$$

The Θ part

$$\frac{1}{\sin q} \frac{d}{dq} \left(\sin q \frac{dQ(q)}{dq} \right) + \frac{m^2}{\sin^2 q} Q(q) + bQ(q) = 0$$

$$P_l^m(\cos q) = \frac{(-1)^m}{2^l l!} (1 - \cos^2 q)^{m/2} \frac{d^{l+m}}{dx^{l+m}} (\cos^2 q - 1)^l$$

$$\Theta(\theta) =$$

$$P_l^{-m}(\cos q) = (-1)^m \frac{(l-m)!}{(l+m)!} P_l^m(\cos q)$$

$$b = l(l+1)$$

$P_l^m(\cos \theta)$: Associated Legendre Polynomials

Azimuthal quantum number $l = 0, 1, 2, 3, \dots$,

$$m \leq l$$

The angular ($\Theta \cdot \Phi$) part

The angular part of the solution

$Y_l^m(\theta, \phi) \Rightarrow \Theta(\theta) \cdot \Phi(\phi)$ are called spherical harmonics

$$Y_l^m(q, f) = \sqrt{\frac{(2l+1)}{4\rho} \frac{(l-m)!}{(l+m)!}} P_l^m(\cos q) e^{imf}$$

$$l=0,1,2,3\dots$$

$$m=0, \pm 1, \pm 2, \pm 3\dots \text{ and } |m| \leq l$$

The angular ($\Theta \cdot \Phi$) part:

$$\vec{L} = (yp_z - zp_y)\vec{i} + (xp_z - zp_{yx})\vec{j} + (xp_y - yp_x)\vec{k}$$

$$\hat{L}^2 = \hat{L}_x \cdot \hat{L}_x + \hat{L}_y \cdot \hat{L}_y + \hat{L}_z \cdot \hat{L}_z$$

$$= -\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \quad \text{in spherical polar co-ords.}$$

Angular equation:

$$-\frac{\hbar^2}{2m} \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{\hbar^2}{2m} \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} = E$$

Multiply by

$$Y(\theta, \phi) = \Theta \Phi$$

The angular ($\Theta \cdot \Phi$) part:

$$\vec{L} = (yp_z - zp_y)\vec{i} + (xp_z - zp_{yx})\vec{j} + (xp_y - yp_x)\vec{k}$$

$$\hat{L}^2 = \hat{L}_x \cdot \hat{L}_x + \hat{L}_y \cdot \hat{L}_y + \hat{L}_z \cdot \hat{L}_z$$

$$= -\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \quad \text{in spherical polar co-ords.}$$

Angular equation:

$$-\frac{\hbar^2}{2m} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \Theta \Phi = E \Theta \Phi$$

Multiply by

$$Y(\theta, \phi) = \Theta \Phi$$

$$-\left[\frac{\Phi}{\sin \theta} \frac{\partial \Theta}{\partial \theta} \sin \theta \frac{\partial \Theta}{\partial \theta} + \frac{\Theta}{\sin^2 \theta} \frac{\partial^2 \Phi}{\partial \phi^2} \right] = \beta \Phi \Theta$$

The angular ($\Theta \cdot \Phi$) part:

$$\vec{L} = (yp_z - zp_y)\vec{i} + (xp_z - zp_{yx})\vec{j} + (xp_y - yp_x)\vec{k}$$

$$\hat{L}^2 = \hat{L}_x \cdot \hat{L}_x + \hat{L}_y \cdot \hat{L}_y + \hat{L}_z \cdot \hat{L}_z$$

$$= -\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \quad \text{in spherical polar co-ords.}$$

Angular equation:

$$-\frac{\hbar^2}{2m} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \Theta \Phi = E \Theta \Phi$$

Multiply by

$$Y(\theta, \phi) = \Theta \Phi$$

$$-\hbar^2 \left[\frac{\Phi}{\sin \theta} \frac{\partial \Theta}{\partial \theta} \sin \theta \frac{\partial \Theta}{\partial \theta} + \frac{\Theta}{\sin^2 \theta} \frac{\partial^2 \Phi}{\partial \phi^2} \right] = E \Theta \Phi$$

The angular ($\Theta \cdot \Phi$) part:

$$\vec{L} = (yp_z - zp_y)\vec{i} + (xp_z - zp_{yx})\vec{j} + (xp_y - yp_x)\vec{k}$$

$$\hat{L}^2 = \hat{L}_x \cdot \hat{L}_x + \hat{L}_y \cdot \hat{L}_y + \hat{L}_z \cdot \hat{L}_z$$

$$= -\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \quad \text{in spherical polar co-ords.}$$

Angular equation:

$$-\frac{\hbar^2}{2m} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \Phi \Theta = E \Phi \Theta$$

Multiply by

$$Y(\theta, \phi) = \Theta \Phi$$

$$-\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \Phi \Theta = E \Phi \Theta$$

The angular ($\Theta \cdot \Phi$) part: Total angular momentum

$$\vec{L} = (yp_z - zp_y)\vec{i} + (xp_z - zp_{yx})\vec{j} + (xp_y - yp_x)\vec{k}$$

$$\hat{L}^2 = \hat{L}_x \cdot \hat{L}_x + \hat{L}_y \cdot \hat{L}_y + \hat{L}_z \cdot \hat{L}_z$$

$$= -\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \quad \text{in spherical polar co-ords.}$$

Angular equation:

$$-\frac{\hbar^2}{2m} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] Y(\theta, \phi) = E Y(\theta, \phi)$$

Multiply by

$$Y(\theta, \phi) = \Theta \Phi$$

$$-\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] Y(\theta, \phi) = \hbar^2 \beta Y(\theta, \phi)$$

$$\hat{L}^2 Y(\theta, \phi) = \hbar^2 l(l+1) Y(\theta, \phi)$$

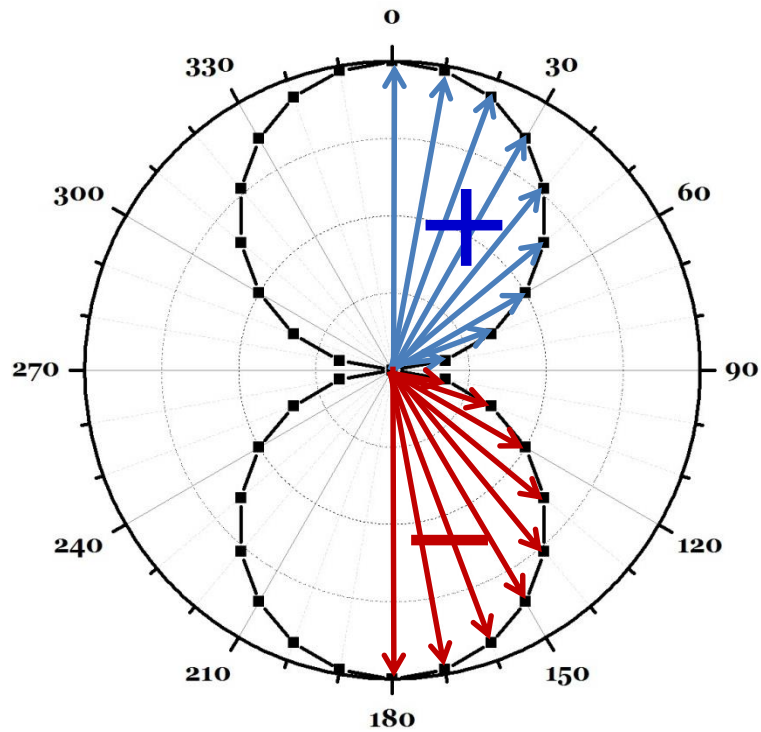
Angular Distribution Functions

p -Orbitals

$$\psi_{210} = \psi_{2p_z} = N\rho e^{-\rho/2} \cos\theta$$

$$Y_{210} = Y_{2p_z} = C \cos\theta \quad (m=0)$$

Angular part: Polar plot of $2p_z$ --- $\cos\theta$



θ	$\cos\theta$
0	1.000
10	0.985
20	0.940
30	0.866
40	0.766
50	0.643
60	0.500
70	0.342
80	0.174
90	0.000
120	-0.500
150	-0.866
180	-1.000

Hydrogen Atom: Principal quantum number

$n = 4$  $l = 0, 1, 2, 3$

$n = 3$  $l = 0, 1, 2$

$m = 0, \pm 1, \pm 2, \dots$

$n = 2$  $l = 0, 1$

$n = 1$  $l = 0$

Separation of variables for Schrodinger equation

$$\frac{1}{R} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) + \frac{2\mu r Q Z e^2}{\hbar^2} + \frac{2\mu r^2}{\hbar^2} E_e = \beta$$

$$\frac{\sin q}{Q} \frac{\partial^2 \chi}{\partial q^2} \sin q \frac{\partial^2 Q}{\partial q^2} + b \sin^2 q = m^2$$

$$\frac{1}{F} \frac{\partial^2 F}{\partial f^2} = -m^2$$

ϕ -part: Magnetic quantum number

$$\frac{1}{R} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) + \frac{2\mu r Q Z e^2}{\hbar^2} + \frac{2\mu r^2}{\hbar^2} E_e = \beta$$

$$\frac{\sin \theta}{r} \frac{\partial}{\partial \theta} \left(r \sin \theta \frac{\partial \Psi}{\partial \theta} \right) + \frac{\partial^2 \Psi}{\partial \phi^2} + b \sin^2 \theta = m^2$$

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \Psi}{\partial r} \right) = -m^2$$

$$\Phi(\phi) = A e^{\pm i m \phi}$$

$$\widehat{L}_z \Phi = \frac{\hbar}{i} \frac{\partial}{\partial \phi} \Phi = \frac{\hbar}{i} i m \Phi = m \hbar \Phi$$

z-component of angular momentum

m : Magnetic Quantum Number

θ -part: Azimuthal quantum number

$$\frac{1}{R} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) + \frac{2\mu r Q Z e^2}{\hbar^2} + \frac{2\mu r^2}{\hbar^2} E_e = \beta$$

$$\frac{\sin q}{Q} \frac{\partial}{\partial q} \left(\frac{\partial Q}{\partial q} \right) + b \sin^2 q = m^2$$

$$\frac{1}{F} \frac{\partial^2 F}{\partial f^2} = -m^2$$

Azimuthal quantum number
 $l = 0, 1, 2, 3, \dots,$
 $m \leq l$

$$b = l(l+1)$$

$$\hat{L}^2 Y(\theta, \phi) = \hbar^2 l(l+1) Y(\theta, \phi)$$

$$\Theta(\theta) =$$

$$P_l^m(\cos q) = \frac{(-1)^m}{2^l l!} (1 - \cos^2 q)^{m/2} \frac{d^{l+m}}{dx^{l+m}} (\cos^2 q - 1)^l$$

$$P_l^{-m}(\cos q) = (-1)^m \frac{(l-m)!}{(l+m)!} P_l^m(\cos q)$$

Associated Legendre Polynomials

r- part

$$\frac{1}{R} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) + \frac{2\mu r Q Z e^2}{\hbar^2} + \frac{2\mu r^2}{\hbar^2} E_e = \beta$$

$$\frac{\partial}{\partial r} \left(r^2 \frac{\partial R(r)}{\partial r} \right) + \frac{2\mu r^2}{\hbar^2} \left(\frac{Q Z e^2}{r} + E_e \right) R(r) - \beta R(r) = 0$$

Solution to R(r) are

$$a = \frac{\hbar^2}{Q\mu e^2} = \frac{4\pi\epsilon_0 \hbar^2}{\mu e^2}$$

$$R_{nl}(r) = -\frac{(n-l-1)!}{2n(n+l)!} \left(\frac{2Zr}{na_0} \right)^{l+3/2} r^l e^{-Zr/na_0} L_{n+l}^{2l+1} \left(\frac{2Zr}{na_0} \right)$$

Restriction on $l < n$

Where $L_{n+l}^{2l+1} \left(\frac{2Zr}{na_0} \right)$ are called associated *Laguerre* functions

The new quantum number is 'n' called principal quantum number

Energy of the Hydrogen Atom

$$E_n = -\frac{2Q^2 Z^2 \mu e^4}{\hbar^2 n^2} = -\frac{Z^2 \mu e^4}{8\epsilon_0^2 h^2 n^2} = -\frac{Z^2 e^4}{8\pi\epsilon_0 a_0 n^2} (\mu \approx m_e)$$

$$E_n = \frac{-13.6\text{eV}}{n^2}$$

Energy is dependent only on 'n'

Energy obtained by full quantum mechanical treatment is equal to Bohr energy

Potential energy term is only dependent on the **Radial** part and has no contribution from the **Angular** parts

Quantum Numbers of Hydrogen Atom

n	Principal Quantum number Specifies the energy of the electron
l	Orbital Angular Momentum Quantum number Specifies the magnitude of the electron's orbital angular momentum
m	Z-component of Angular Momentum Quantum number Specifies the orientation of the electron's orbital angular momentum
s	Spin Angular Momentum Quantum number Specifies the orientation of the electron's spin angular momentum

Radial Functions of Hydrogen Atom

$$R_{nl}(r) = - \left[\frac{(n-l-1)!}{2n[(n+l)!]^3} \right]^{1/2} \left(\frac{2}{na_0} \right)^{l+3/2} r^l e^{-r/na_0} L_{n+l}^{2l+1} \left(\frac{2r}{na_0} \right)$$

$$n=1; l=0 \quad 2 \left(\frac{1}{a_0} \right)^{3/2} e^{-r/a_0}$$

$$\rho = \frac{2Zr}{na}$$

$$n=2; l=0 \quad \frac{1}{8^{1/2}} \left(\frac{1}{a_0} \right)^{3/2} \left(2 - \frac{r}{a_0} \right) e^{-r/2a_0}$$

$$a = \frac{4\pi\epsilon_0\hbar^2}{\mu e^2}$$

$$n=2; l=1 \quad \frac{1}{24^{1/2}} \left(\frac{1}{a_0} \right)^{3/2} \left(\frac{r}{a_0} \right) e^{-r/2a_0}$$

$$a = a_0 \quad (\text{for } \mu = m_e)$$

$$n=3; l=0 \quad 2 \left(\frac{1}{3a_0} \right)^{3/2} \left(1 - \frac{2}{3} \left[\frac{r}{a_0} \right] - \frac{2}{27} \left[\frac{r}{a_0} \right]^2 \right) e^{-r/3a_0}$$

$$n=3; l=1 \quad \frac{1}{486^{1/2}} \left(\frac{1}{a_0} \right)^{3/2} \left(4 - \frac{2r}{3a_0} \right) e^{-r/3a_0}$$

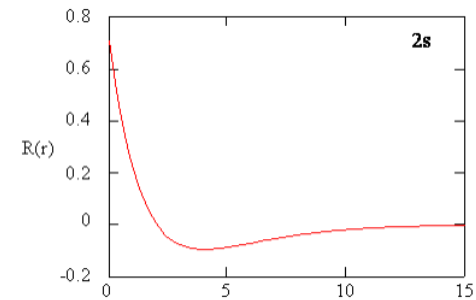
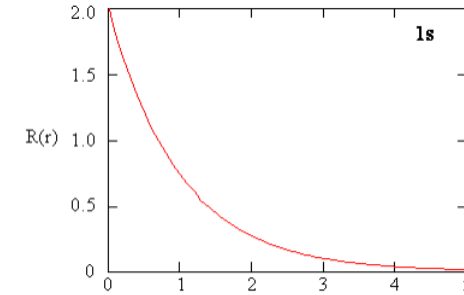
$$n=3; l=2 \quad \frac{1}{2430^{1/2}} \left(\frac{1}{a_0} \right)^{3/2} \left(\frac{2r}{3a_0} \right)^2 e^{-r/3a_0}$$

Number of radial nodes =
 $n-l-1$

1s and 2s Orbitals

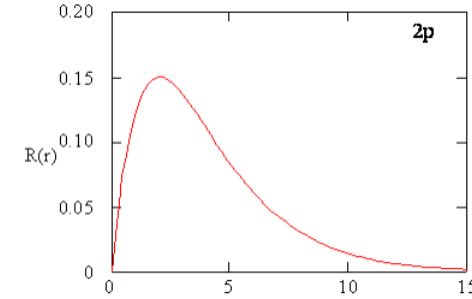
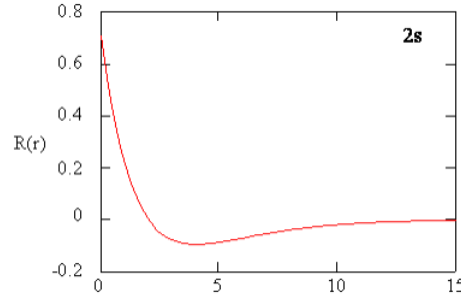
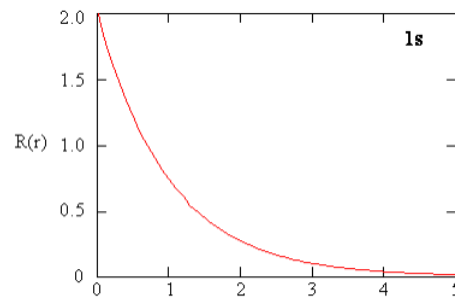
$$\psi_{1,0,0} = \psi_{1s} = \frac{1}{\sqrt{\pi}} \left(\frac{1}{a_o} \right)^{3/2} e^{-r/a_o}$$

$$\psi_{2,0,0} = \psi_{2s} = \frac{1}{4\sqrt{2\pi}} \left(\frac{1}{a_o} \right)^{3/2} \left(2 - \frac{r}{a_o} \right) e^{-r/2a_o}$$



Functions of only ' r '

Radial functions

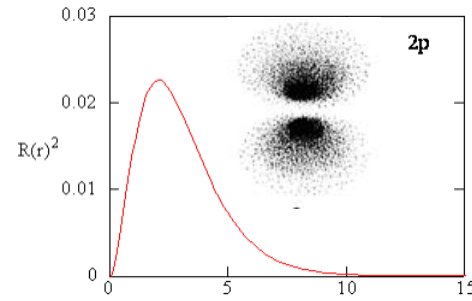
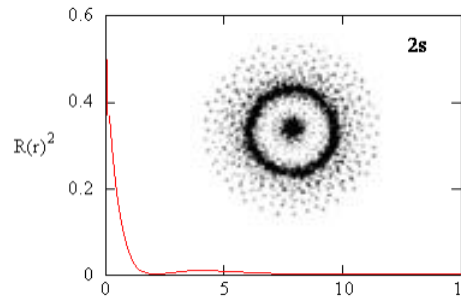
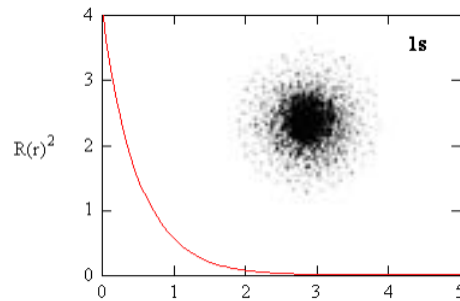


$$\rho = \frac{r}{a_0}$$

$$\psi_{1s}^{100} = N'e^{-\rho}$$

$$\psi_{2s}^{200} = N''(2-\rho)e^{-\rho/2}$$

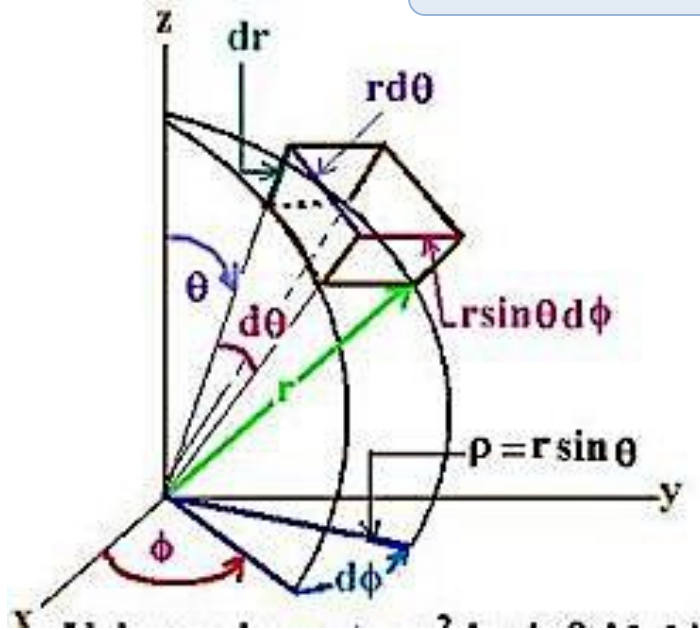
$$\psi_{2p_z}^{210} = N'''\rho e^{-\rho/2}$$



For s-Orbitals the maximum probability density of finding the electron is on the nucleus

Probability: Volume element in spherical polar coordinates

$$\text{Volume element} = r^2 dr \sin\theta d\theta d\phi$$



For a s orbital

$$P = \int \psi^* \psi d\tau$$

$$= \int_0^\infty R^2 r^2 dr \int_0^\pi \Theta^2 \sin \theta d\theta \int_0^{2\pi} \Phi^* \Phi d\phi$$

The equation is annotated with callouts: a yellow callout points to $R^2 r^2 dr$, a light green callout points to $\int_0^\pi \Theta^2 \sin \theta d\theta$ with a '2' above it, and a light orange callout points to $\int_0^{2\pi} \Phi^* \Phi d\phi$ with a 2π above it.

Radial Probability distribution function

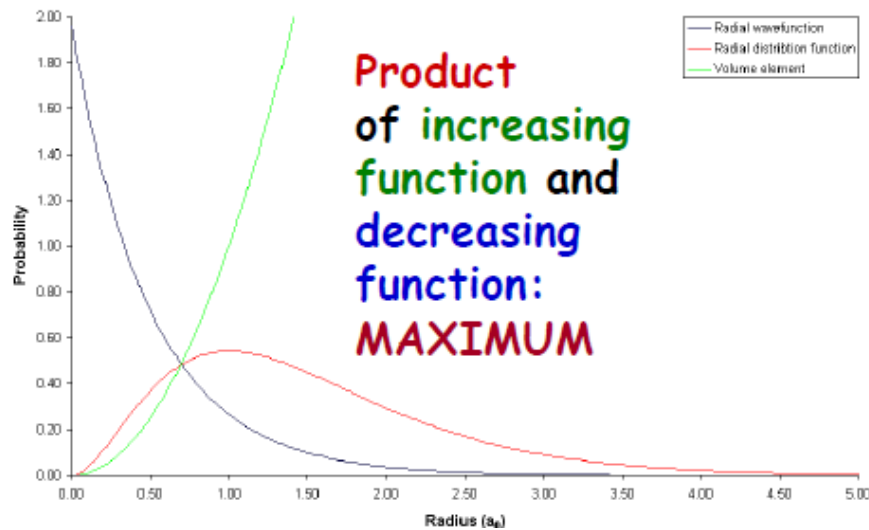
Radial Distribution Functions

Probability of finding the electron in a shell of thickness dr at radius $r =$

$$4\pi r^2 R_{nl}^2(r) dr \text{ (for s)}$$

$r^2 \rightarrow$ increasing function

$$4\pi r^2 R_{nl}^2(r) dr \rightarrow 0 \text{ as } 4\pi r^2 dr \rightarrow 0$$



For s-Orbitals :

- Maximum probability density of finding the electron is on the nucleus
- Probability of finding the electron on the nucleus zero

Radial Distribution Functions

$$4\pi r^2 R_{nl}^2(r)$$

$$n=1; l=0 \quad 2\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$$

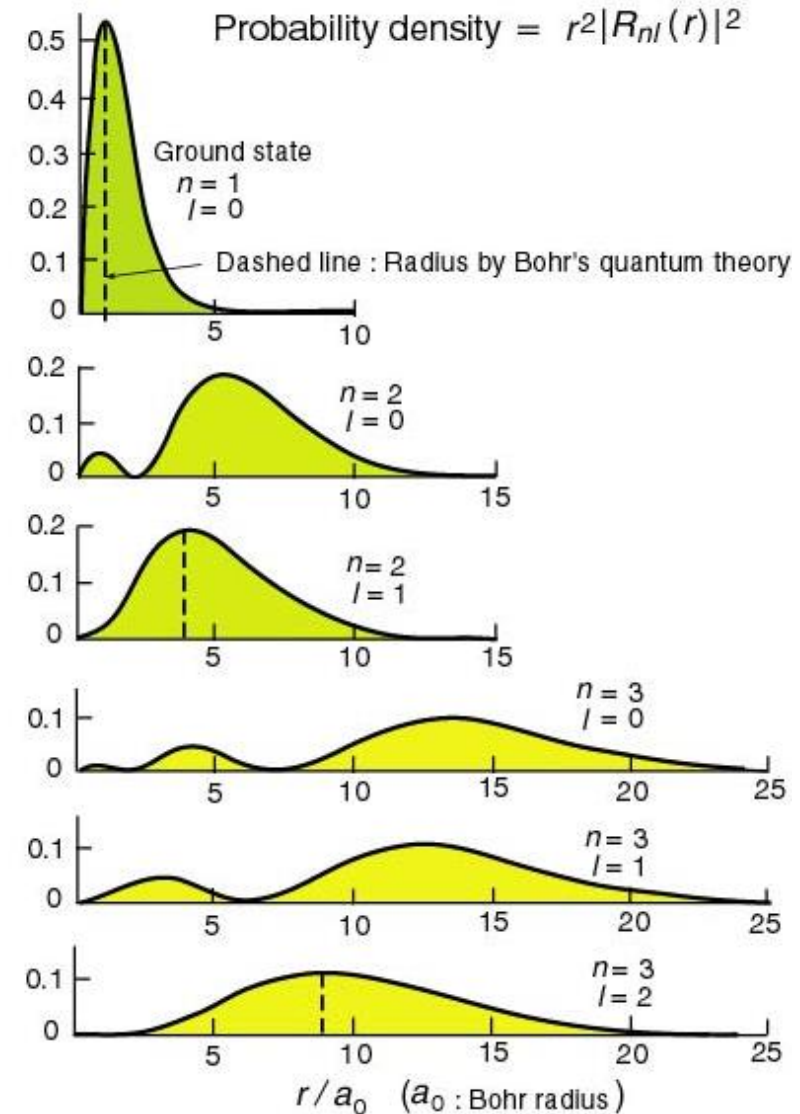
$$n=2; l=0 \quad \frac{1}{8^{1/2}}\left(\frac{1}{a_0}\right)^{3/2} \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0}$$

$$n=2; l=1 \quad \frac{1}{24^{1/2}}\left(\frac{1}{a_0}\right)^{3/2} \left(\frac{r}{a_0}\right) e^{-r/2a_0}$$

$$n=3; l=0 \quad 2\left(\frac{1}{3a_0}\right)^{3/2} \left(1 - \frac{2}{3}\left[\frac{r}{a_0}\right] - \frac{2}{27}\left[\frac{r}{a_0}\right]^2\right) e^{-r/3a_0}$$

$$n=3; l=1 \quad \frac{1}{486^{1/2}}\left(\frac{1}{a_0}\right)^{3/2} \left(4 - \frac{2r}{3a_0}\right) e^{-r/3a_0}$$

$$n=3; l=2 \quad \frac{1}{2430^{1/2}}\left(\frac{1}{a_0}\right)^{3/2} \left(\frac{2r}{3a_0}\right)^2 e^{-r/3a_0}$$



Radial Distribution Functions

$$n=1; l=0 \quad 2\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$$

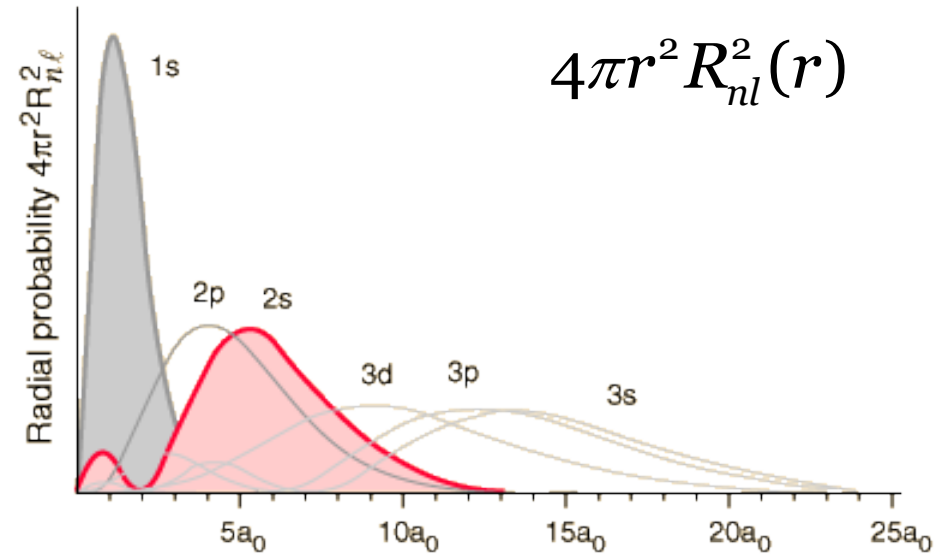
$$n=2; l=0 \quad \frac{1}{8^{1/2}}\left(\frac{1}{a_0}\right)^{3/2} \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0}$$

$$n=2; l=1 \quad \frac{1}{24^{1/2}}\left(\frac{1}{a_0}\right)^{3/2} \left(\frac{r}{a_0}\right) e^{-r/2a_0}$$

$$n=3; l=0 \quad 2\left(\frac{1}{3a_0}\right)^{3/2} \left(1 - \frac{2}{3}\left[\frac{r}{a_0}\right] - \frac{2}{27}\left[\frac{r}{a_0}\right]^2\right) e^{-r/3a_0} \quad \langle r \rangle = \langle \Psi_{ns} | r | \Psi_{ns} \rangle$$

$$n=3; l=1 \quad \frac{1}{486^{1/2}}\left(\frac{1}{a_0}\right)^{3/2} \left(4 - \frac{2r}{3a_0}\right) e^{-r/3a_0}$$

$$n=3; l=2 \quad \frac{1}{2430^{1/2}}\left(\frac{1}{a_0}\right)^{3/2} \left(\frac{2r}{3a_0}\right)^2 e^{-r/3a_0}$$



Average value of radius:

Most probable value of radius:

$$\frac{dP_r}{dr} = 0$$

Coming next: Put them all together

