Announcements

- Homework #2 will be handed out on Tuesday (21st) and due Monday noon (27th)
- Schedule a review time before the first exam on 28th

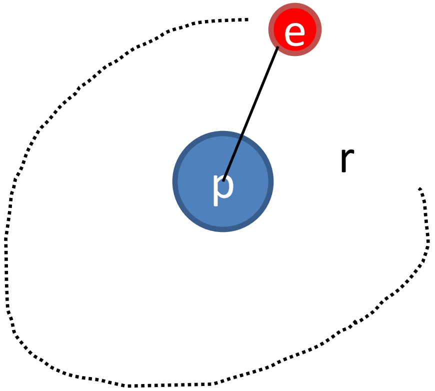
PH102: Interactive Lecture 4

- Topics
  - Quantization of angular momentum (L)
  - Normalization
  - Electron whereabouts

Hydrogen atom

- Potential created by Coulomb interactions between electron (-*e*) and proton (+*e*)

$$U(r) = \frac{1}{4\pi\varepsilon_0}\frac{-e^2}{r}$$



Schrodinger Equation: Hydrogen Atom

$$\frac{-\hbar^2}{2m} \nabla^2 \psi(\vec{x}) + U(\vec{x})\psi(\vec{x}) = E\,\psi(\vec{x})$$

$$U(r) = -\frac{1}{4\pi\varepsilon_0}\frac{e^2}{r}$$

$$\left[\frac{-\hbar^2}{2m} \nabla^2 + U(\vec{x})\right] \psi(\vec{x}) = E\,\psi(\vec{x})$$

Hamiltonian (H) = T (kinetic) + U (Potential)

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$$\mathbf{H}\psi_{n,l,m_l} = E_n\psi_{n,l,m_l}$$

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Kinetic energy w.r.t. r + Kinetic energy w.r.t. rotation

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Kinetic energy w.r.t. r + Kinetic energy w.r.t. rotation

$$\begin{cases} -\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) - \frac{2mr^2}{\hbar^2}\left(E - U(r)\right) = C = -l(l+1) \\ \frac{1}{\Theta}\csc\theta\,\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right) + \frac{1}{\Phi}\csc^2\theta\,\frac{\partial^2\Phi}{\partial\phi^2} = C = -l(l+1) \end{cases}$$

$$\frac{\partial^2\Phi}{\partial\phi^2} = -m_l^2\Phi$$

Schrodinger Equation: Hydrogen Atom

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$$\left[\frac{-\hbar^2}{2m}\nabla^2 + U(\vec{x})\right]\psi(\vec{x}) = E\,\psi(\vec{x}) \qquad \mathbf{H}\psi_{n,l,m_l} = E_n\psi_{n,l,m_l}$$

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$$\mathbf{L}^2\psi_{n,l,m_l} = l(l+1)\hbar^2\psi_{n,l,m_l}$$

$$\frac{\partial^2\Phi}{\partial\phi^2} = -m_l^2\Phi \qquad \mathbf{L}_z\psi_{n,l,m_l} = m_l\hbar\psi_{n,l,m_l}$$

Schrodinger Equation

$$\begin{cases} \dfrac{\partial^2 \Phi}{\partial \phi^2} = -m_l^2 \Phi \\ \sin\theta \dfrac{\partial}{\partial \theta}\left(\sin\theta \dfrac{\partial \Theta}{\partial \theta}\right) + [l(l+1)\sin^2\theta - m_l^2]\Theta = 0 \\ \dfrac{\partial}{\partial r}\left(r^2 \dfrac{\partial R}{\partial r}\right) + \dfrac{2mr^2}{\hbar^2}\left(E - U(r)\right)R - l(l+1)R = 0 \end{cases}$$

Azimuthal Equation

Polar Equation

Radial Equation

Hydrogen atom Solutions

- Principal quantum number, $n = 1, 2, 3, \ldots$
- Orbital quantum number, $l = 0, 1, 2, \ldots (n - 1)$ where l =1*(s)*, =2*(p)*, =3*(d)*, =4*(f)*, *etc.*
- Magnetic quantum number, $m_l = 0, \pm 1, \pm 2, \ldots \pm l$

Wave function = $\psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi) = R_{n,l}\Theta_{l,m_l}\Phi_{m_l}$

where $\Theta_{l,m_l}\Phi_{m_l} = \mathbf{Y}_l^{m_l}$ (Spherical harmonics)

Wave functions

n	l	m_l	$\Phi(\phi)$	$\Theta(\theta)$	$R(r)$	$\psi(r,\theta,\phi)$
1	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{2}{a_0^{3/2}} e^{-r/a_0}$	$\frac{1}{\sqrt{\pi}\, a_0^{3/2}} e^{-r/a_0}$
2	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{2\sqrt{2}\, a_0^{3/2}} \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0}$	$\frac{1}{4\sqrt{2\pi}\, a_0^{3/2}} \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0}$
2	1	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{6}}{2} \cos\theta$	$\frac{1}{2\sqrt{6}\, a_0^{3/2}} \frac{r}{a_0} e^{-r/2a_0}$	$\frac{1}{4\sqrt{2\pi}\, a_0^{3/2}} \frac{r}{a_0} e^{-r/2a_0} \cos\theta$
2	1	±1	$\frac{1}{\sqrt{2\pi}} e^{\pm i\phi}$	$\frac{\sqrt{3}}{2} \sin\theta$	$\frac{1}{2\sqrt{6}\, a_0^{3/2}} \frac{r}{a_0} e^{-r/2a_0}$	$\frac{1}{8\sqrt{\pi}\, a_0^{3/2}} \frac{r}{a_0} e^{-r/2a_0} \sin\theta\, e^{\pm i\phi}$
3	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{2}{81\sqrt{3}\, a_0^{3/2}} \left(27 - 18\frac{r}{a_0} + 2\frac{r^2}{a_0^2}\right) e^{-r/3a_0}$	$\frac{1}{81\sqrt{3\pi}\, a_0^{3/2}} \left(27 - 18\frac{r}{a_0} + 2\frac{r^2}{a_0^2}\right) e^{-r/3a_0}$
3	1	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{6}}{2} \cos\theta$	$\frac{4}{81\sqrt{6}\, a_0^{3/2}} \left(6 - \frac{r}{a_0}\right) \frac{r}{a_0} e^{-r/3a_0}$	$\frac{\sqrt{2}}{81\sqrt{\pi}\, a_0^{3/2}} \left(6 - \frac{r}{a_0}\right) \frac{r}{a_0} e^{-r/3a_0} \cos\theta$
3	1	±1	$\frac{1}{\sqrt{2\pi}} e^{\pm i\phi}$	$\frac{\sqrt{3}}{2} \sin\theta$	$\frac{4}{81\sqrt{6}\, a_0^{3/2}} \left(6 - \frac{r}{a_0}\right) \frac{r}{a_0} e^{-r/3a_0}$	$\frac{1}{81\sqrt{\pi}\, a_0^{3/2}} \left(6 - \frac{r}{a_0}\right) \frac{r}{a_0} e^{-r/3a_0} \sin\theta\, e^{\pm i\phi}$
3	2	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{10}}{4} (3\cos^2\theta - 1)$	$\frac{4}{81\sqrt{30}\, a_0^{3/2}} \frac{r^2}{a_0^2} e^{-r/3a_0}$	$\frac{1}{81\sqrt{6\pi}\, a_0^{3/2}} \frac{r^2}{a_0^2} e^{-r/3a_0} (3\cos^2\theta - 1)$
3	2	±1	$\frac{1}{\sqrt{2\pi}} e^{\pm i\phi}$	$\frac{\sqrt{15}}{2} \sin\theta\cos\theta$	$\frac{4}{81\sqrt{30}\, a_0^{3/2}} \frac{r^2}{a_0^2} e^{-r/3a_0}$	$\frac{1}{81\sqrt{\pi}\, a_0^{3/2}} \frac{r^2}{a_0^2} e^{-r/3a_0} \sin\theta\cos\theta\, e^{\pm i\phi}$
3	2	±2	$\frac{1}{\sqrt{2\pi}} e^{\pm 2i\phi}$	$\frac{\sqrt{15}}{4} \sin^2\theta$	$\frac{4}{81\sqrt{30}\, a_0^{3/2}} \frac{r^2}{a_0^2} e^{-r/3a_0}$	$\frac{1}{162\sqrt{\pi}\, a_0^{3/2}} \frac{r^2}{a_0^2} e^{-r/3a_0} \sin^2\theta\, e^{\pm 2i\phi}$

n	l	m_l	E_n(eV)	$\lvert L\rvert$	L_z	ψ_{n,l,m_l} =	$R_{n,l}\mathbf{Y}_l^{m_l}$	degeneracies	Orbital name
1	0	0	-13.6	0	0	ψ_{100}	$R_{10}\mathbf{Y}_0^0$	Non-degenerate	1s
2	0	0	-3.40	0	0	ψ_{200}	$R_{20}\mathbf{Y}_0^0$	4 (=2[2])	2s
	1	-1		$\sqrt{2}\hbar$	$-\hbar$	ψ_{21-1}	$R_{21}\mathbf{Y}_1^{-1}$		2p
		0			0	ψ_{210}	$R_{21}\mathbf{Y}_1^0$		
		1			$+\hbar$	ψ_{211}	$R_{21}\mathbf{Y}_1^{+1}$		
3	0	0	-1.51	0	0	ψ_{300}	$R_{30}\mathbf{Y}_0^0$	9 (=3[2])	3s
	1	-1		$\sqrt{2}\hbar$	$-\hbar$	ψ_{31-1}	$R_{31}\mathbf{Y}_1^{-1}$		3p
		0			0	ψ_{310}	$R_{31}\mathbf{Y}_1^0$		
		1			$+\hbar$	ψ_{311}	$R_{31}\mathbf{Y}_1^1$		
	2	-2		$\sqrt{6}\hbar$	$-2\hbar$	ψ_{32-2}	$R_{32}\mathbf{Y}_2^{-2}$		3d
		--1			$-\hbar$	ψ_{32-1}	$R_{32}\mathbf{Y}_2^{-1}$		
		0			0	ψ_{320}	$R_{32}\mathbf{Y}_2^0$		
		1			$+\hbar$	ψ_{321}	$R_{32}\mathbf{Y}_2^1$		
		2			$+2\hbar$	ψ_{322}	$R_{32}\mathbf{Y}_2^2$		

Symbolic designation of atomic states

	s $l = 0$	*p* $l = 1$	*d* $l = 2$	*f* $l = 3$	*g* $l = 4$	*h* $l = 5$
$n = 1$	*1s*					
$n = 2$	*2s*	*2p*				
$n = 3$	*3s*	*3p*	*3d*			
$n = 4$	*4s*	*4p*	*4d*	*4f*		
$n = 5$	*5s*	*5p*	*5d*	*5f*	*5g*	
$n = 6$	*6s*	*6p*	*6d*	*6f*	*6g*	*6h*

Origin of angular momentum quantization

$$\begin{cases} \dfrac{\partial^2 \Phi}{\partial \phi^2} = -m_l^2 \Phi \\ sin\theta \dfrac{\partial}{\partial \theta}\left(sin\theta \dfrac{\partial \Theta}{\partial \theta}\right) + [l(l+1)sin^2\theta - m_l^2]\Theta = 0 \\ \dfrac{\partial}{\partial r}\left(r^2 \dfrac{\partial R}{\partial r}\right) + \dfrac{2mr^2}{\hbar^2}(E - U(r))R - l(l+1)R = 0 \end{cases}$$

$$\frac{\partial}{\partial r}\left(r^2 \frac{\partial R}{\partial r}\right) + \frac{2mr^2}{\hbar^2}[E - U(r) - \frac{l(l+1)\hbar^2}{2mr^2}]R = 0$$

Origin of angular momentum quantization

$$\frac{\partial}{\partial r}\left(r^2 \frac{\partial R}{\partial r}\right) + \frac{2mr^2}{\hbar^2}\,(E - U(r))R\; - l(l+1)R = 0$$

$$\frac{\partial}{\partial r}\left(r^2 \frac{\partial R}{\partial r}\right) + \frac{2mr^2}{\hbar^2}\,[E - U(r)\; - \frac{l(l+1)\hbar^2}{2mr^2}]R = 0$$

$$\mathrm{E} = \text{Kinetic E (radial)} + \text{Kinetic E (orbital)} + U(r)$$

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$$\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)+\frac{2mr^2}{\hbar^2}\left(E-U(r)\right)R-l(l+1)R=0$$

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$$\mathrm{E}=\text{Kinetic E (radial)}+\text{Kinetic E (orbital)}+U(r)$$

$$\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)+\frac{2mr^2}{\hbar^2}\left[Kineric\ E\ (radial)+\ Kinetic\ E\ (orbital)-\frac{l(l+1)\hbar^2}{2mr^2}\right]R=0$$

$$Kinetic\ E\ (orbital)=\frac{l(l+1)\hbar^2}{2mr^2}$$

Origin of angular momentum quantization

$$\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)+\frac{2mr^2}{\hbar^2}(E-U(r))R-l(l+1)R=0$$

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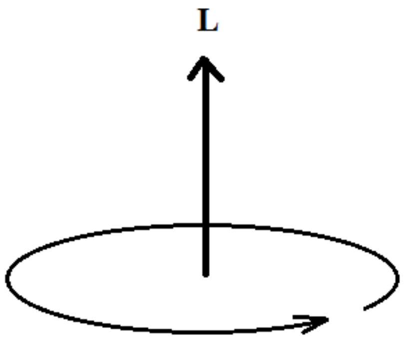
$$Kinetic\ E\ (orbital)=\frac{l(l+1)\hbar^2}{2mr^2}$$



$$\frac{1}{2}m\,v_{orbital}^2=\frac{L^2}{2mr^2}$$

$$L=mv_{orbital}r \rightarrow v_{orbital}=\frac{L}{mr}$$

Origin of angular momentum quantization

$$\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)+\frac{2mr^2}{\hbar^2}\left(E-U(r)\right)R\ -l(l+1)R=0$$

$$\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)+\frac{2mr^2}{\hbar^2}\ [E-U(r)\ -\frac{l(l+1)\hbar^2}{2mr^2}]R=0$$

$$\mathrm{E} = \text{Kinetic E (radial)} + \text{Kinetic E (orbital)} + U(r)$$

$$\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)+\frac{2mr^2}{\hbar^2}\ [Kineric\ E\ (radial) +\ Kinetic\ E\ (orbital)\ -\frac{l(l+1)\hbar^2}{2mr^2}]R=0$$

$$Kinetic\ E\ (orbital)=\frac{l(l+1)\hbar^2}{2mr^2}$$

$$\frac{1}{2}m\ v_{orbital}^2=\frac{L^2}{2mr^2}$$

$$L=mv_{orbital}r \rightarrow v_{orbital}=\frac{L}{mr}$$

$$\frac{L^2}{2mr^2}=\frac{l(l+1)\hbar^2}{2mr^2}$$

$$L^2=\ l(l+1)\hbar^2$$

Origin of angular momentum quantization

$$\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)+\frac{2mr^2}{\hbar^2}(E-U(r))R\ -l(l+1)R=0$$

$$\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)+\frac{2mr^2}{\hbar^2}[E-U(r)\ -\frac{l(l+1)\hbar^2}{2mr^2}]R=0$$

$$\text{E} = \text{Kinetic E (radial)} + \text{Kinetic E (orbital)} + U(r)$$

$$\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)+\frac{2mr^2}{\hbar^2}[Kineric\ E\ (radial)+\ Kinetic\ E\ (orbital)\ -\frac{l(l+1)\hbar^2}{2mr^2}]R=0$$

$$Kinetic\ E\ (orbital)=\frac{l(l+1)\hbar^2}{2mr^2}$$

$$\frac{1}{2}m\ v_{orbital}^2=\frac{L^2}{2mr^2}$$

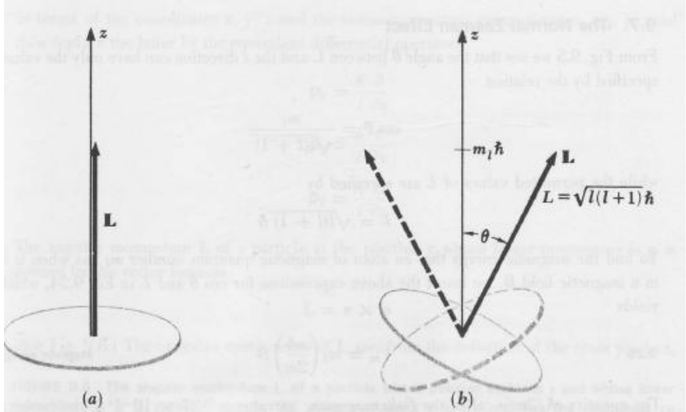
$$L=mv_{orbital}r \rightarrow v_{orbital}=\frac{L}{mr}$$

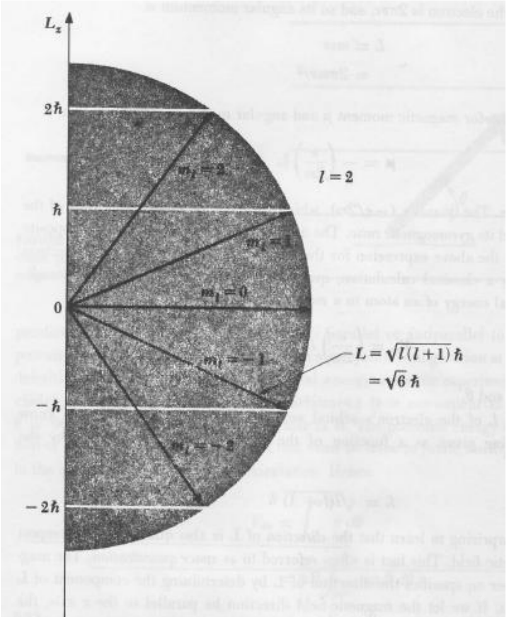
$$\frac{L^2}{2mr^2}=\frac{l(l+1)\hbar^2}{2mr^2}$$

$$L^2=\ l(l+1)\hbar^2$$

Angular momentum is quantized

Angular Momentum (L)

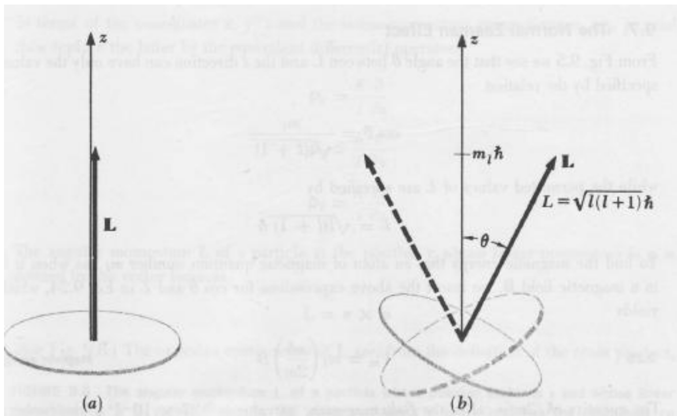


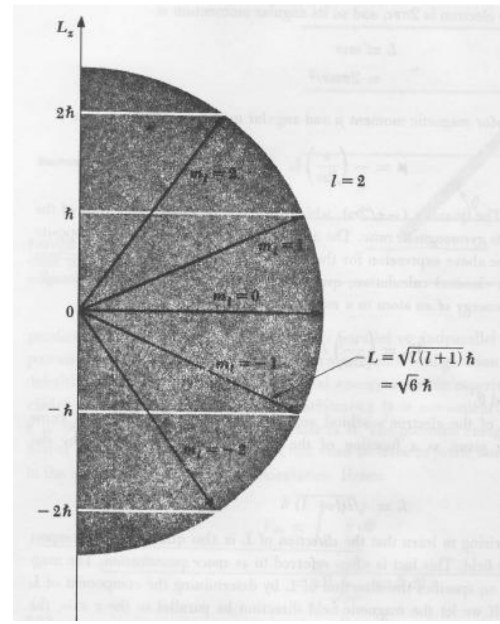


Amount =

Direction =

Angular Momentum (L)

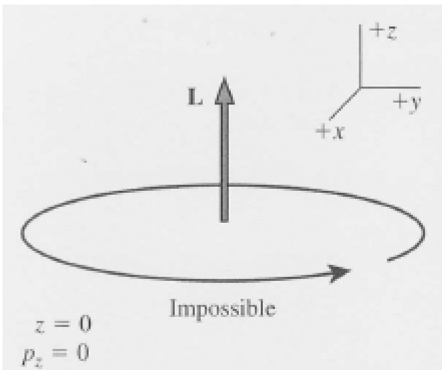




Amount = $L = \sqrt{l(l+1)}\hbar$

Direction = the m_l *value* determines the direction of L

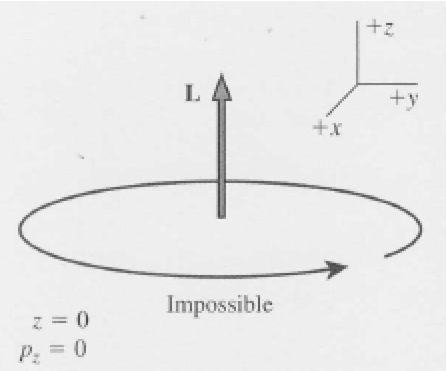
Lz and Uncertainty principle

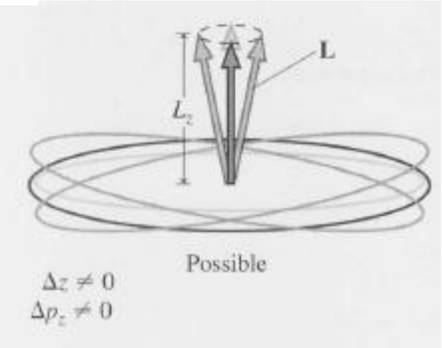


$$\Delta z \Delta p_z > \frac{\hbar}{2}$$

Lz and Uncertainty principle

$$\Delta z \Delta p_z > \frac{\hbar}{2}$$

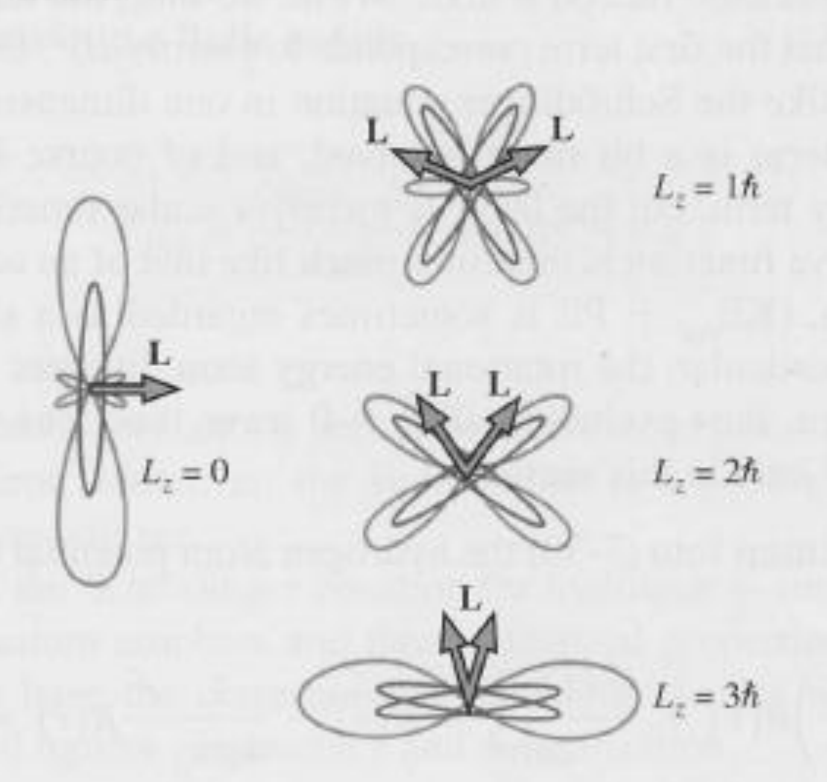


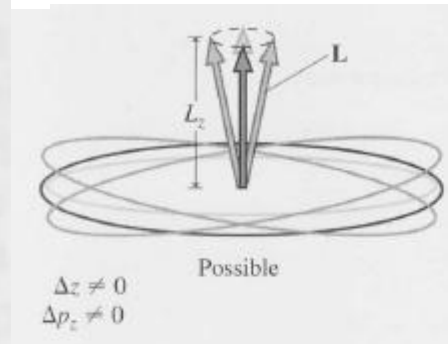


Lz and Uncertainty principle

$$\Delta z \Delta p_z > \frac{\hbar}{2}$$

Figure 7.14 A crude correspondence to orbital motion.





Normalization

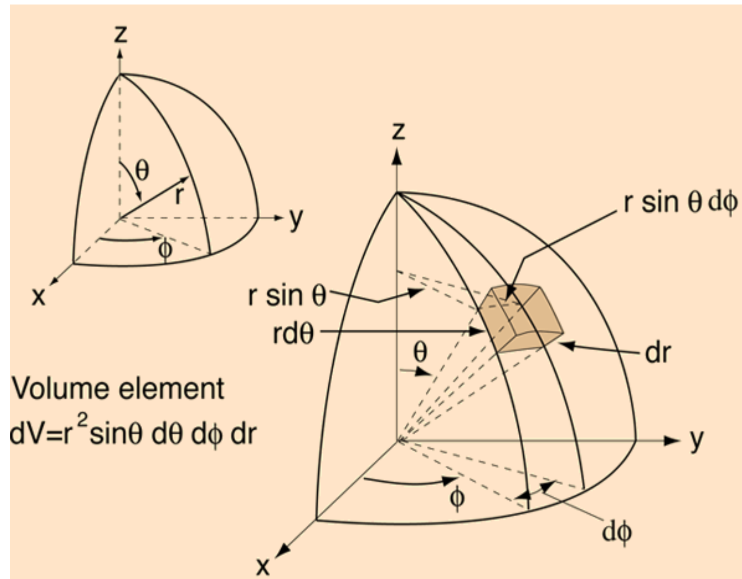
$$|\psi_{n,l,m_l}|^2 = R(r)^2\Theta(\theta)^2\Phi(\phi)^2$$

$$\int |\psi_{n,l,m_l}|^2 \, dV = \int |\psi_{n,l,m_l}|^2 \, r^2 sin\theta \; dr d\theta d\phi$$

$$= \int_0^\infty R(r)^2 r^2 \, dr \int_0^\pi \Theta(\theta)^2 sin\theta \; d\theta \int_0^{2\pi} \Phi(\phi)^2 d\phi$$

$$(x, y, z) \quad \leftrightarrow \quad (r, \theta, \phi)$$

$$\begin{cases} r = \sqrt{x^2 + y^2 + z^2} \\ \phi = \tan^{-1}\dfrac{y}{x} \\ \theta = \cos^{-1}\dfrac{z}{r} \end{cases}$$



$$\begin{cases} x = r\sin\theta\cos\phi \\ y = r\sin\theta\sin\phi \\ z = r\cos\theta \end{cases}$$

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

$$\nabla^2 = \frac{1}{r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \csc\theta\,\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial}{\partial\theta}\right) + \csc^2\theta\,\frac{\partial}{\partial\phi^2}\right]$$

$$= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial}{\partial\phi^2}$$

Normalization

$$|\psi_{n,l,m_l}|^2 = R(r)^2\Theta(\theta)^2\Phi(\phi)^2$$

$$\int |\psi_{n,l,m_l}|^2\, dV = \int |\psi_{n,l,m_l}|^2\, r^2 sin\theta\ dr d\theta d\phi$$
$$= \int_0^\infty R(r)^2 r^2\, dr \int_0^\pi \Theta(\theta)^2 sin\theta\ d\theta \int_0^{2\pi} \Phi(\phi)^2 d\phi$$

$$\begin{cases} \int_0^\infty R(r)^2 r^2\, dr = 1 \\ \int_0^\pi \Theta(\theta)^2 sin\theta\ d\theta \int_0^{2\pi} \Phi(\phi)^2 d\phi = 2\pi \int_0^\pi \Theta(\theta)^2 sin\theta\ d\theta = 1 \end{cases}$$

Angular Probability Density

$$\Theta(\theta)^2\Phi(\phi)^2 \equiv \mathbf{Y}_l^{m_l *}\mathbf{Y}_l^{m_l}$$

n	l	m_l	$\Phi(\phi)$	$\Theta(\theta)$	$R(r)$	$\psi(r,\theta,\phi)$
1	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{2}{a_0^{3/2}} e^{-r/a_0}$	$\frac{1}{\sqrt{\pi}\, a_0^{3/2}} e^{-r/a_0}$
2	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{2\sqrt{2}\, a_0^{3/2}}\left(2-\frac{r}{a_0}\right) e^{-r/2a_0}$	$\frac{1}{4\sqrt{2\pi}\, a_0^{3/2}}\left(2-\frac{r}{a_0}\right) e^{-r/2a_0}$
2	1	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{6}}{2}\cos\theta$	$\frac{1}{2\sqrt{6}\, a_0^{3/2}}\frac{r}{a_0} e^{-r/2a_0}$	$\frac{1}{4\sqrt{2\pi}\, a_0^{3/2}}\frac{r}{a_0} e^{-r/2a_0}\cos\theta$
2	1	±1	$\frac{1}{\sqrt{2\pi}} e^{\pm i\phi}$	$\frac{\sqrt{3}}{2}\sin\theta$	$\frac{1}{2\sqrt{6}\, a_0^{3/2}}\frac{r}{a_0} e^{-r/2a_0}$	$\frac{1}{8\sqrt{\pi}\, a_0^{3/2}}\frac{r}{a_0} e^{-r/2a_0}\sin\theta\, e^{\pm i\phi}$
3	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{2}{81\sqrt{3}\, a_0^{3/2}}\left(27-18\frac{r}{a_0}+2\frac{r^2}{a_0^2}\right) e^{-r/3a_0}$	$\frac{1}{81\sqrt{3\pi}\, a_0^{3/2}}\left(27-18\frac{r}{a_0}+2\frac{r^2}{a_0^2}\right) e^{-r/3a_0}$
3	1	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{6}}{2}\cos\theta$	$\frac{4}{81\sqrt{6}\, a_0^{3/2}}\left(6-\frac{r}{a_0}\right)\frac{r}{a_0} e^{-r/3a_0}$	$\frac{\sqrt{2}}{81\sqrt{\pi}\, a_0^{3/2}}\left(6-\frac{r}{a_0}\right)\frac{r}{a_0} e^{-r/3a_0}\cos\theta$
3	1	±1	$\frac{1}{\sqrt{2\pi}} e^{\pm i\phi}$	$\frac{\sqrt{3}}{2}\sin\theta$	$\frac{4}{81\sqrt{6}\, a_0^{3/2}}\left(6-\frac{r}{a_0}\right)\frac{r}{a_0} e^{-r/3a_0}$	$\frac{1}{81\sqrt{\pi}\, a_0^{3/2}}\left(6-\frac{r}{a_0}\right)\frac{r}{a_0} e^{-r/3a_0}\sin\theta\, e^{\pm i\phi}$
3	2	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{10}}{4}(3\cos^2\theta-1)$	$\frac{4}{81\sqrt{30}\, a_0^{3/2}}\frac{r^2}{a_0^2} e^{-r/3a_0}$	$\frac{1}{81\sqrt{6\pi}\, a_0^{3/2}}\frac{r^2}{a_0^2} e^{-r/3a_0}(3\cos^2\theta-1)$
3	2	±1	$\frac{1}{\sqrt{2\pi}} e^{\pm i\phi}$	$\frac{\sqrt{15}}{2}\sin\theta\cos\theta$	$\frac{4}{81\sqrt{30}\, a_0^{3/2}}\frac{r^2}{a_0^2} e^{-r/3a_0}$	$\frac{1}{81\sqrt{\pi}\, a_0^{3/2}}\frac{r^2}{a_0^2} e^{-r/3a_0}\sin\theta\cos\theta\, e^{\pm i\phi}$
3	2	±2	$\frac{1}{\sqrt{2\pi}} e^{\pm 2i\phi}$	$\frac{\sqrt{15}}{4}\sin^2\theta$	$\frac{4}{81\sqrt{30}\, a_0^{3/2}}\frac{r^2}{a_0^2} e^{-r/3a_0}$	$\frac{1}{162\sqrt{\pi}\, a_0^{3/2}}\frac{r^2}{a_0^2} e^{-r/3a_0}\sin^2\theta\, e^{\pm 2i\phi}$

Angular Probability Density

$$\Theta(\theta)^2\Phi(\phi)^2 \equiv \mathbf{Y}_l^{m_l *}\mathbf{Y}_l^{m_l}$$

n	l	m_l	$\Phi(\phi)$	$\Theta(\theta)$	$R(r)$	$\psi(r,\theta,\phi)$
1	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{2}{a_0^{3/2}}e^{-r/a_0}$	$\frac{1}{\sqrt{\pi}\,a_0^{3/2}}e^{-r/a_0}$
2	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{2\sqrt{2}\,a_0^{3/2}}\left(2-\frac{r}{a_0}\right)e^{-r/2a_0}$	$\frac{1}{4\sqrt{2\pi}\,a_0^{3/2}}\left(2-\frac{r}{a_0}\right)e^{-r/2a_0}$
2	1	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{6}}{2}\cos\theta$	$\frac{1}{2\sqrt{6}\,a_0^{3/2}}\frac{r}{a_0}e^{-r/2a_0}$	$\frac{1}{4\sqrt{2\pi}\,a_0^{3/2}}\frac{r}{a_0}e^{-r/2a_0}\cos\theta$
2	1	±1	$\frac{1}{\sqrt{2\pi}}e^{\pm i\phi}$	$\frac{\sqrt{3}}{2}\sin\theta$	$\frac{1}{2\sqrt{6}\,a_0^{3/2}}\frac{r}{a_0}e^{-r/2a_0}$	$\frac{1}{8\sqrt{\pi}\,a_0^{3/2}}\frac{r}{a_0}e^{-r/2a_0}\sin\theta\, e^{\pm i\phi}$
3	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{2}{81\sqrt{3}\,a_0^{3/2}}\left(27-18\frac{r}{a_0}+2\frac{r^2}{a_0^2}\right)e^{-r/3a_0}$	$\frac{1}{81\sqrt{3\pi}\,a_0^{3/2}}\left(27-18\frac{r}{a_0}+2\frac{r^2}{a_0^2}\right)e^{-r/3a_0}$
3	1	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{6}}{2}\cos\theta$	$\frac{4}{81\sqrt{6}\,a_0^{3/2}}\left(6-\frac{r}{a_0}\right)\frac{r}{a_0}e^{-r/3a_0}$	$\frac{\sqrt{2}}{81\sqrt{\pi}\,a_0^{3/2}}\left(6-\frac{r}{a_0}\right)\frac{r}{a_0}e^{-r/3a_0}\cos\theta$
3	1	±1	$\frac{1}{\sqrt{2\pi}}e^{\pm i\phi}$	$\frac{\sqrt{3}}{2}\sin\theta$	$\frac{4}{81\sqrt{6}\,a_0^{3/2}}\left(6-\frac{r}{a_0}\right)\frac{r}{a_0}e^{-r/3a_0}$	$\frac{1}{81\sqrt{\pi}\,a_0^{3/2}}\left(6-\frac{r}{a_0}\right)\frac{r}{a_0}e^{-r/3a_0}\sin\theta\, e^{\pm i\phi}$
3	2	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{10}}{4}(3\cos^2\theta-1)$	$\frac{4}{81\sqrt{30}\,a_0^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}$	$\frac{1}{81\sqrt{6\pi}\,a_0^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}(3\cos^2\theta-1)$
3	2	±1	$\frac{1}{\sqrt{2\pi}}e^{\pm i\phi}$	$\frac{\sqrt{15}}{2}\sin\theta\cos\theta$	$\frac{4}{81\sqrt{30}\,a_0^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}$	$\frac{1}{81\sqrt{\pi}\,a_0^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}\sin\theta\cos\theta\, e^{\pm i\phi}$
3	2	±2	$\frac{1}{\sqrt{2\pi}}e^{\pm 2i\phi}$	$\frac{\sqrt{15}}{4}\sin^2\theta$	$\frac{4}{81\sqrt{30}\,a_0^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}$	$\frac{1}{162\sqrt{\pi}\,a_0^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}\sin^2\theta\, e^{\pm 2i\phi}$

Unsöld's theorem

$$\sum_{m_l=-l}^{l}|\Theta_{l,m_l}|^2|\Phi_{m_l}|^2 = Constant$$

Angular Probability Density

$$l = 0,\ m_l = 0, \quad \Theta_{00} = \frac{1}{\sqrt{2}}, \Phi_0 = \frac{1}{\sqrt{2\pi}}$$

$$l = 1, m_l = 0, \quad \Theta_{10} = \frac{\sqrt{6}}{2}\cos\theta, \Phi_0 = \frac{1}{\sqrt{2\pi}}$$

$$l = 1, m_l = \pm1, \quad \Theta_{1\pm1} = \frac{\sqrt{3}}{2}\sin\theta, \Phi_{\pm1} = \frac{1}{\sqrt{2\pi}}e^{\pm i\phi}$$

$$l = 2, m_l = 0, \quad \Theta_{20} = \frac{\sqrt{10}}{4}(3\cos^2\theta - 1), \Phi_0 = \frac{1}{\sqrt{2\pi}}$$

$$l = 2, m_l = \pm1, \quad \Theta_{2\pm1} = \frac{\sqrt{15}}{2} sin\theta cos\theta, \Phi_{\pm1} = \frac{1}{\sqrt{2\pi}}e^{\pm i\phi}$$

$$l = 2, m_l = \pm2, \quad \Theta_{2\pm2} = \frac{\sqrt{15}}{4} sin^2\theta, \quad \Phi_{\pm2} = \frac{1}{\sqrt{2\pi}}e^{\pm 2i\phi}$$

Unsöld's theorem

$$\sum_{m_l=-l}^{l} |\Theta_{l,m_l}|^2 |\Phi_{m_l}|^2 = Constant$$

Angular Probability Density

$l = 0,\ m_l = 0, \quad \Theta_{00} = \frac{1}{\sqrt{2}}, \Phi_0 = \frac{1}{\sqrt{2\pi}}$

$l = 1, m_l = 0, \quad \Theta_{10} = \frac{\sqrt{6}}{2}\cos\theta, \Phi_0 = \frac{1}{\sqrt{2\pi}}$

$l = 1, m_l = \pm 1, \quad \Theta_{1\pm1} = \frac{\sqrt{3}}{2}\sin\theta, \Phi_{\pm1} = \frac{1}{\sqrt{2\pi}}e^{\pm i\phi}$

$l = 2, m_l = 0, \quad \Theta_{20} = \frac{\sqrt{10}}{4}(3\cos^2\theta - 1), \Phi_0 = \frac{1}{\sqrt{2\pi}}$

$l = 2, m_l = \pm 1, \quad \Theta_{2\pm1} = \frac{\sqrt{15}}{2} sin\theta cos\theta, \Phi_{\pm1} = \frac{1}{\sqrt{2\pi}}e^{\pm i\phi}$

$l = 2, m_l = \pm 2, \quad \theta_{2\pm2} = \frac{\sqrt{15}}{4} sin^2\theta, \quad \Phi_{\pm2} = \frac{1}{\sqrt{2\pi}}e^{\pm 2i\phi}$

Unsöld's theorem

$$\sum_{m_l=-l}^{l} |\Theta_{l,m_l}|^2 |\Phi_{m_l}|^2 = Constant$$

For $l = 0$,

$$\sum_{m_l=0}^{0} |\Theta_{0,m_l}|^2 |\Phi_{m_l}|^2 =$$

Angular Probability Density

$l = 0,\ m_l = 0, \quad \Theta_{00} = \frac{1}{\sqrt{2}}, \Phi_0 = \frac{1}{\sqrt{2\pi}}$

$l = 1, m_l = 0, \quad \Theta_{10} = \frac{\sqrt{6}}{2}\cos\theta, \Phi_0 = \frac{1}{\sqrt{2\pi}}$

$l = 1, m_l = \pm 1, \quad \Theta_{1\pm1} = \frac{\sqrt{3}}{2}\sin\theta, \Phi_{\pm1} = \frac{1}{\sqrt{2\pi}}e^{\pm i\phi}$

$l = 2, m_l = 0, \quad \Theta_{20} = \frac{\sqrt{10}}{4}(3\cos^2\theta - 1), \Phi_0 = \frac{1}{\sqrt{2\pi}}$

$l = 2, m_l = \pm 1, \quad \Theta_{2\pm1} = \frac{\sqrt{15}}{2} sin\theta cos\theta, \Phi_{\pm1} = \frac{1}{\sqrt{2\pi}}e^{\pm i\phi}$

$l = 2, m_l = \pm 2, \quad \Theta_{2\pm2} = \frac{\sqrt{15}}{4} sin^2\theta, \quad \Phi_{\pm2} = \frac{1}{\sqrt{2\pi}}e^{\pm 2i\phi}$

Unsöld's theorem

$$\sum_{m_l = -l}^{l} |\Theta_{l,m_l}|^2 |\Phi_{m_l}|^2 = Constant$$

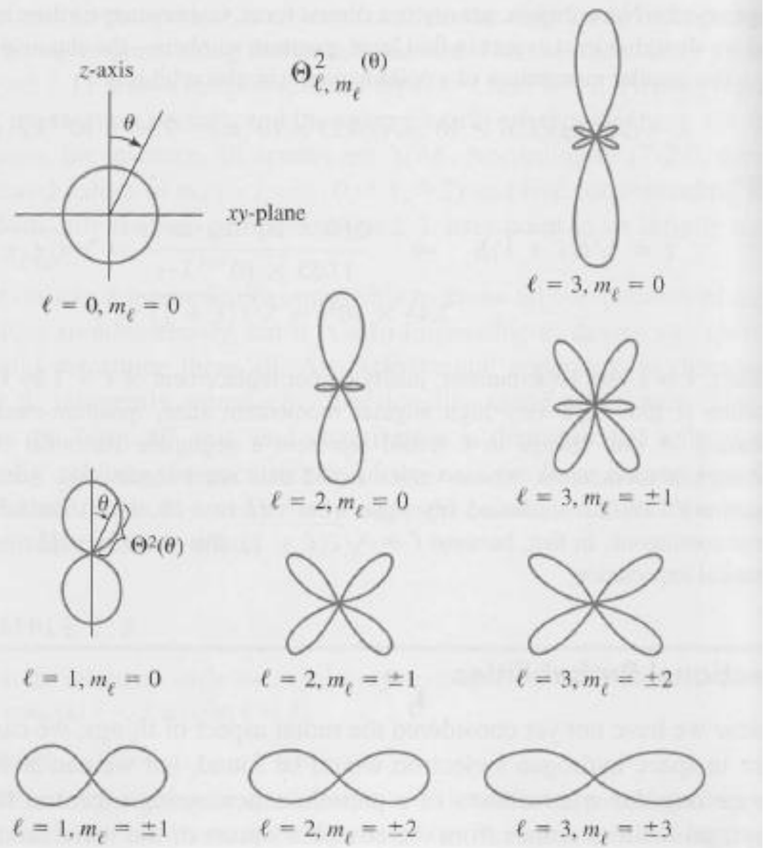
For $l = 0$,

$$\sum_{m_l = 0}^{0} |\Theta_{0,m_l}|^2 |\Phi_{m_l}|^2 = {\Theta_{00}}^2 {\Phi_0}^2 = \frac{1}{4\pi} = constant$$

Angular Probability Density

$$\Theta(\theta)^2\Phi(\phi)^2 \equiv \mathbf{Y}_l^{m_l *}\mathbf{Y}_l^{m_l}$$

Figure 7.13 Angular probability densities for a central force.



Normalization

$$|\psi_{n,l,m_l}|^2 = R(r)^2\Theta(\theta)^2\Phi(\phi)^2$$

$$\int |\psi_{n,l,m_l}|^2 \, dV = \int |\psi_{n,l,m_l}|^2 \, r^2 sin\theta \; dr d\theta d\phi$$

$$= \int_0^\infty R(r)^2 r^2 \, dr \int_0^\pi \Theta(\theta)^2 sin\theta \; d\theta \int_0^{2\pi} \Phi(\phi)^2 d\phi$$

Normalization

$$|\psi_{n,l,m_l}|^2 = R(r)^2\Theta(\theta)^2\Phi(\phi)^2$$

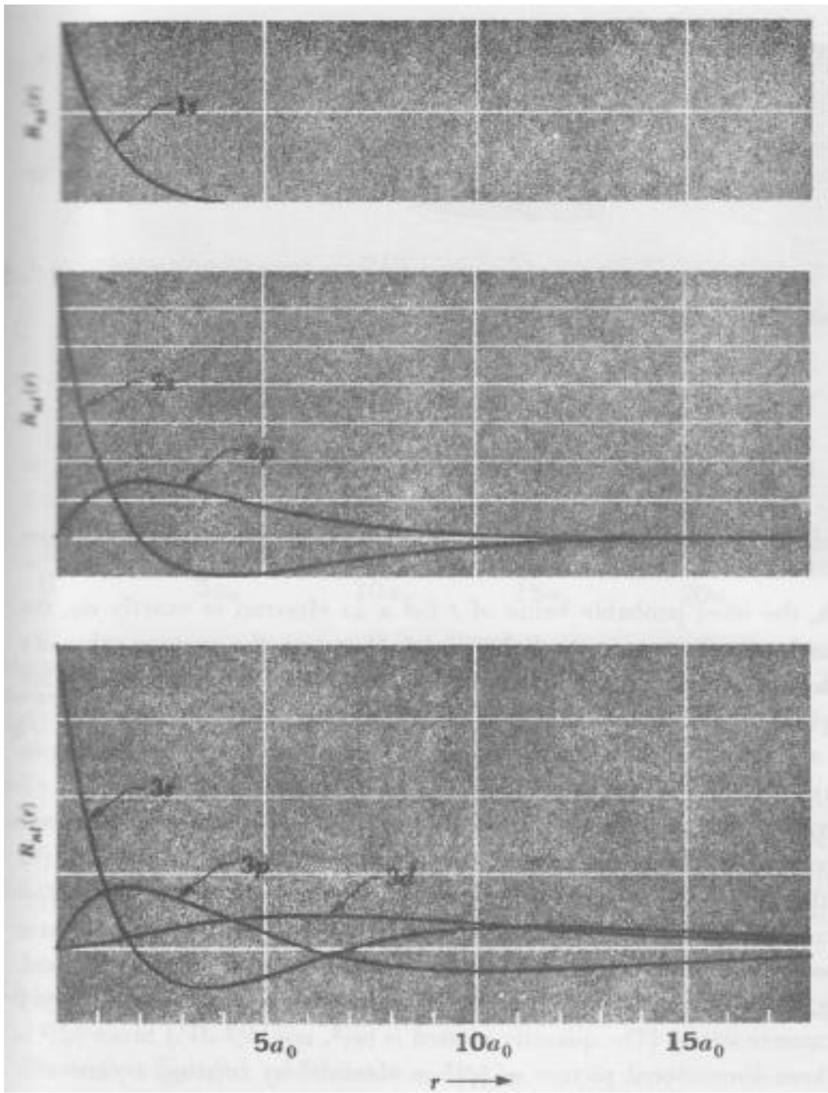
$$\int |\psi_{n,l,m_l}|^2\, dV = \int |\psi_{n,l,m_l}|^2\, r^2 sin\theta\ dr d\theta d\phi$$
$$= \int_0^\infty R(r)^2 r^2\, dr \int_0^\pi \Theta(\theta)^2 sin\theta\ d\theta \int_0^{2\pi} \Phi(\phi)^2 d\phi$$

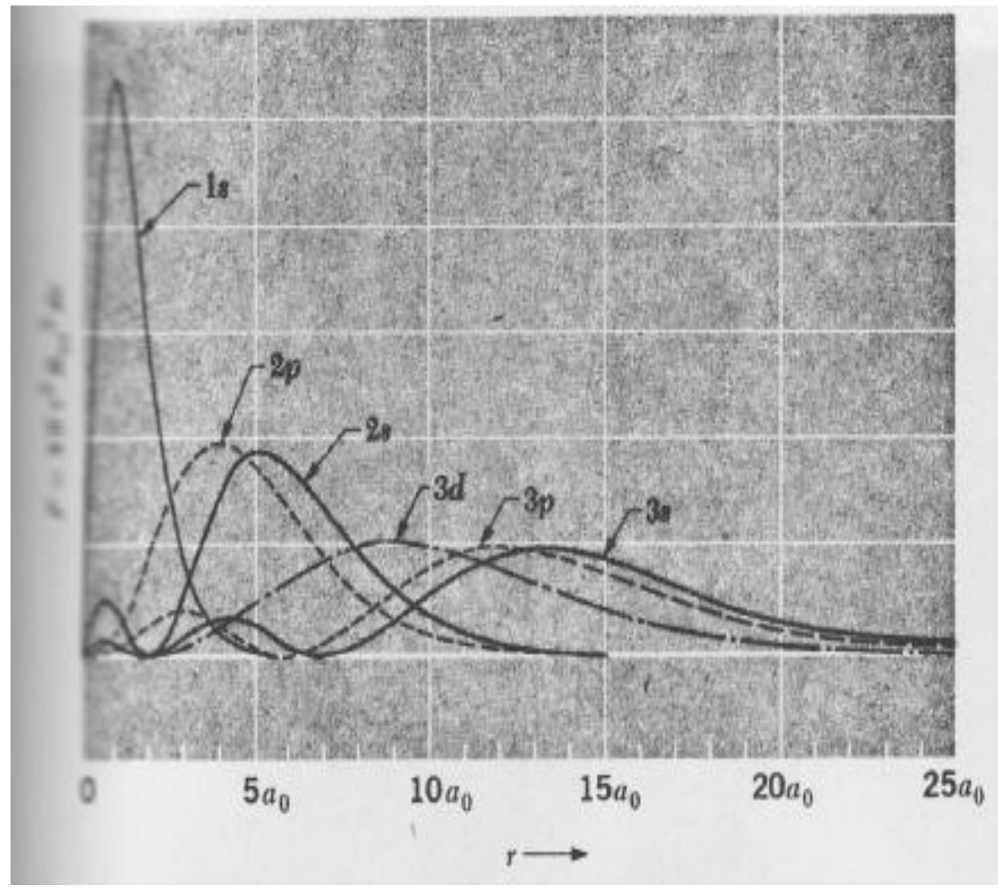
$$\begin{cases} \int_0^\infty R(r)^2 r^2\, dr = 1 \\ \int_0^\pi \Theta(\theta)^2 sin\theta\ d\theta \int_0^{2\pi} \Phi(\phi)^2 d\phi = 2\pi \int_0^\pi \Theta(\theta)^2 sin\theta\ d\theta = 1 \end{cases}$$

R(r) vs. $r^2 R^2(r)$

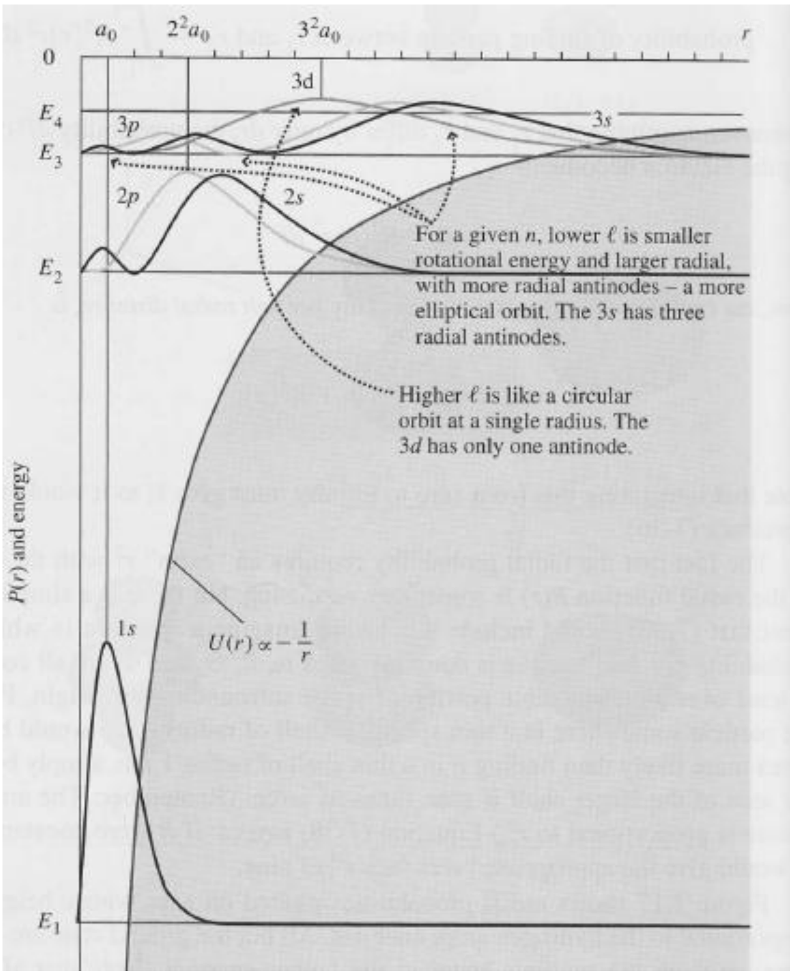
n	l	m_l	$\Phi(\phi)$	$\Theta(\theta)$	$R(r)$	$\psi(r,\theta,\phi)$
1	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{2}{a_0^{3/2}} e^{-r/a_0}$	$\frac{1}{\sqrt{\pi}\, a_0^{3/2}} e^{-r/a_0}$
2	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{2\sqrt{2}\, a_0^{3/2}}\left(2-\frac{r}{a_0}\right) e^{-r/2a_0}$	$\frac{1}{4\sqrt{2\pi}\, a_0^{3/2}}\left(2-\frac{r}{a_0}\right) e^{-r/2a_0}$
2	1	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{6}}{2}\cos\theta$	$\frac{1}{2\sqrt{6}\, a_0^{3/2}}\frac{r}{a_0} e^{-r/2a_0}$	$\frac{1}{4\sqrt{2\pi}\, a_0^{3/2}}\frac{r}{a_0} e^{-r/2a_0}\cos\theta$
2	1	±1	$\frac{1}{\sqrt{2\pi}} e^{\pm i\phi}$	$\frac{\sqrt{3}}{2}\sin\theta$	$\frac{1}{2\sqrt{6}\, a_0^{3/2}}\frac{r}{a_0} e^{-r/2a_0}$	$\frac{1}{8\sqrt{\pi}\, a_0^{3/2}}\frac{r}{a_0} e^{-r/2a_0}\sin\theta\, e^{\pm i\phi}$
3	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{2}{81\sqrt{3}\, a_0^{3/2}}\left(27-18\frac{r}{a_0}+2\frac{r^2}{a_0^2}\right) e^{-r/3a_0}$	$\frac{1}{81\sqrt{3\pi}\, a_0^{3/2}}\left(27-18\frac{r}{a_0}+2\frac{r^2}{a_0^2}\right) e^{-r/3a_0}$
3	1	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{6}}{2}\cos\theta$	$\frac{4}{81\sqrt{6}\, a_0^{3/2}}\left(6-\frac{r}{a_0}\right)\frac{r}{a_0} e^{-r/3a_0}$	$\frac{\sqrt{2}}{81\sqrt{\pi}\, a_0^{3/2}}\left(6-\frac{r}{a_0}\right)\frac{r}{a_0} e^{-r/3a_0}\cos\theta$
3	1	±1	$\frac{1}{\sqrt{2\pi}} e^{\pm i\phi}$	$\frac{\sqrt{3}}{2}\sin\theta$	$\frac{4}{81\sqrt{6}\, a_0^{3/2}}\left(6-\frac{r}{a_0}\right)\frac{r}{a_0} e^{-r/3a_0}$	$\frac{1}{81\sqrt{\pi}\, a_0^{3/2}}\left(6-\frac{r}{a_0}\right)\frac{r}{a_0} e^{-r/3a_0}\sin\theta\, e^{\pm i\phi}$
3	2	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{10}}{4}(3\cos^2\theta-1)$	$\frac{4}{81\sqrt{30}\, a_0^{3/2}}\frac{r^2}{a_0^2} e^{-r/3a_0}$	$\frac{1}{81\sqrt{6\pi}\, a_0^{3/2}}\frac{r^2}{a_0^2} e^{-r/3a_0}(3\cos^2\theta-1)$
3	2	±1	$\frac{1}{\sqrt{2\pi}} e^{\pm i\phi}$	$\frac{\sqrt{15}}{2}\sin\theta\cos\theta$	$\frac{4}{81\sqrt{30}\, a_0^{3/2}}\frac{r^2}{a_0^2} e^{-r/3a_0}$	$\frac{1}{81\sqrt{\pi}\, a_0^{3/2}}\frac{r^2}{a_0^2} e^{-r/3a_0}\sin\theta\cos\theta\, e^{\pm i\phi}$
3	2	±2	$\frac{1}{\sqrt{2\pi}} e^{\pm 2i\phi}$	$\frac{\sqrt{15}}{4}\sin^2\theta$	$\frac{4}{81\sqrt{30}\, a_0^{3/2}}\frac{r^2}{a_0^2} e^{-r/3a_0}$	$\frac{1}{162\sqrt{\pi}\, a_0^{3/2}}\frac{r^2}{a_0^2} e^{-r/3a_0}\sin^2\theta\, e^{\pm 2i\phi}$

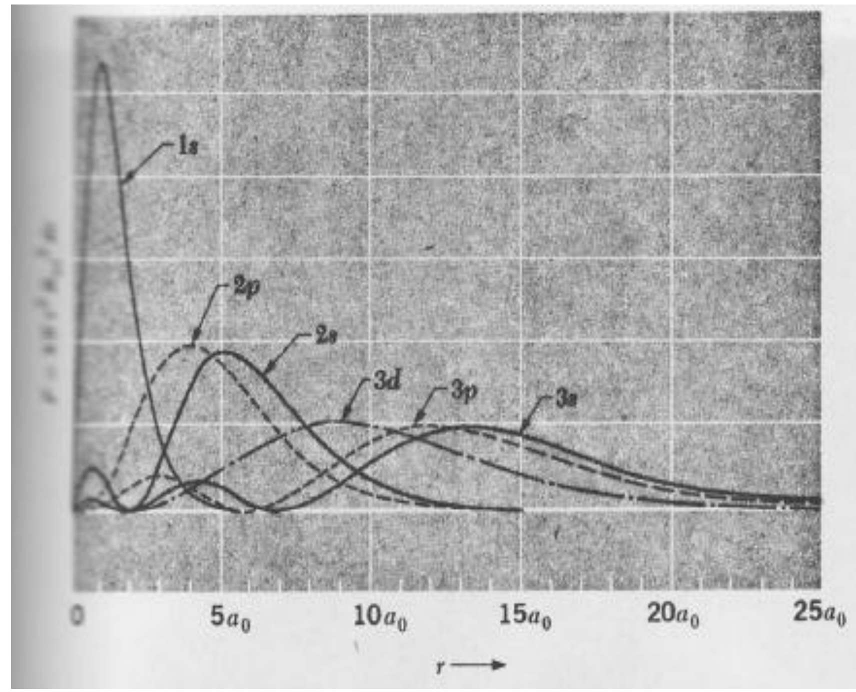
$R(r)$ vs. $r^2 R^2(r)$





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

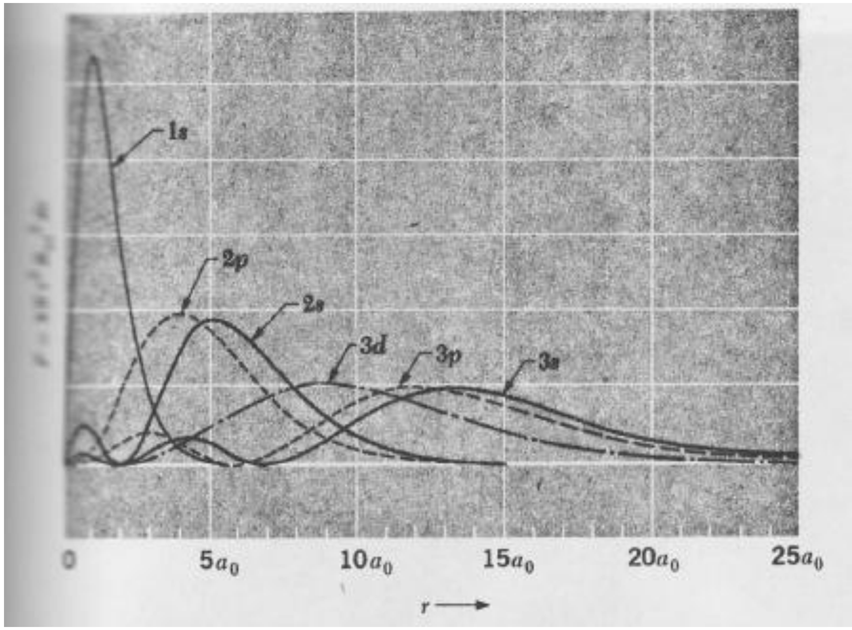

a_0
$2^2 a_0$
$3^2 a_0$
r
0
3d
E_4
3p
3s
E_3
2p
2s
For a given n, lower ℓ is smaller rotational energy and larger radial, with more radial antinodes – a more elliptical orbit. The 3s has three radial antinodes.
E_2
Higher ℓ is like a circular orbit at a single radius. The 3d has only one antinode.
$P(r)$ and energy
1s
$U(r) \propto -\frac{1}{r}$
E_1


1s
2p
2s
3d
3p
3s
0
$5a_0$
$10a_0$
$15a_0$
$20a_0$
$25a_0$
$r \longrightarrow$

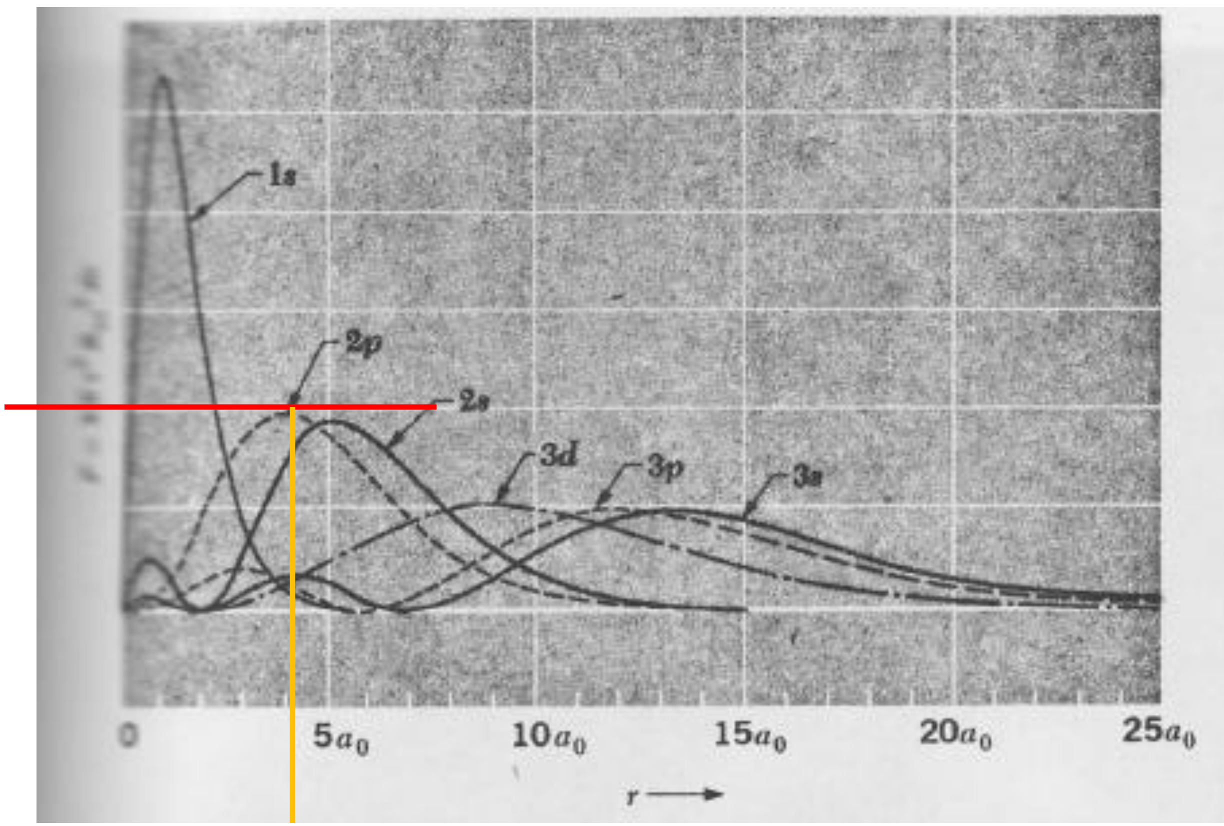
Most probable vs. expectation value

Expectation Value r $\langle r \rangle = \int_0^\infty r \cdot r^2 R_{n,l}(r)^2 dr$

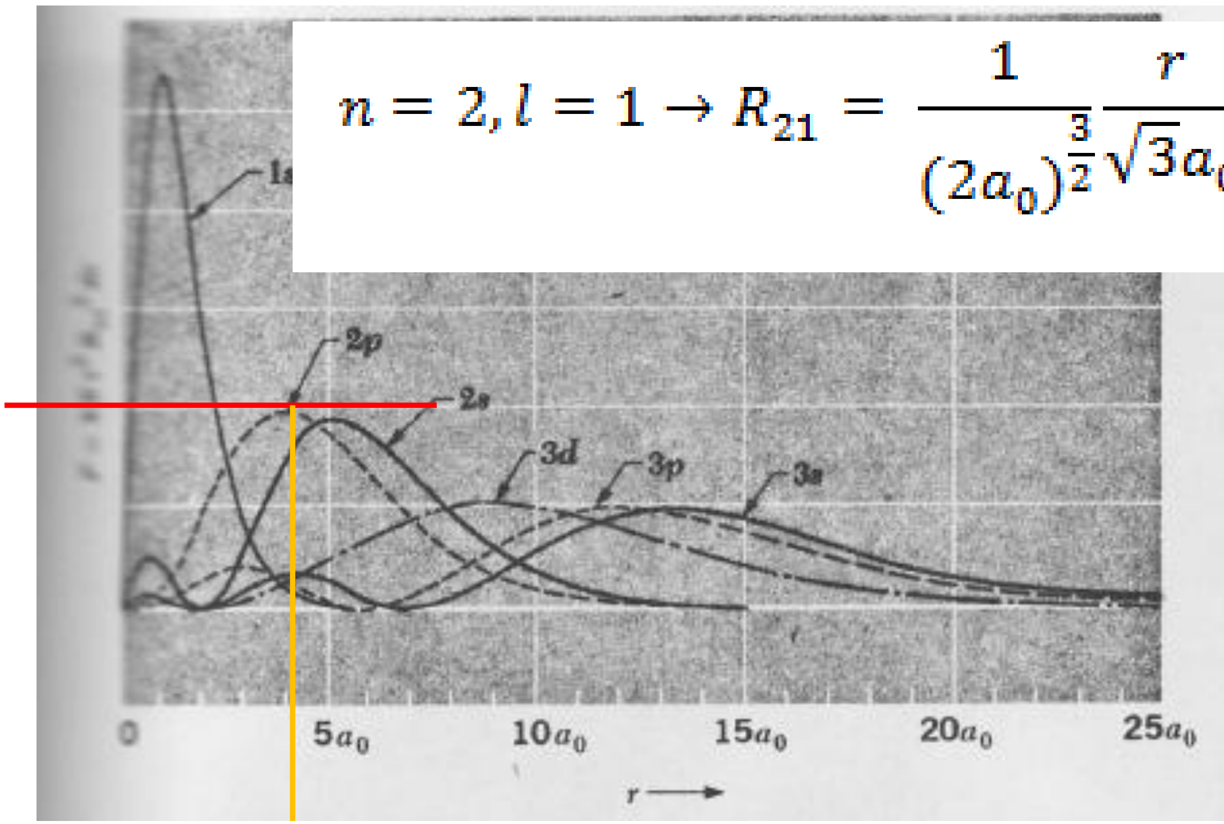
Most probable r Value $\frac{dP(r)}{dr} = \frac{d\, r^2 R_{n,l}(r)^2}{dr} = 0$



$P(r) \sim r^2 R^2(r)$



$P(r) \sim r^2 R^2(r)$



$$n = 2, l = 1 \rightarrow R_{21} = \frac{1}{(2a_0)^{\frac{3}{2}}} \frac{r}{\sqrt{3} a_0} e^{-\frac{r}{2a_0}}$$

Expected value

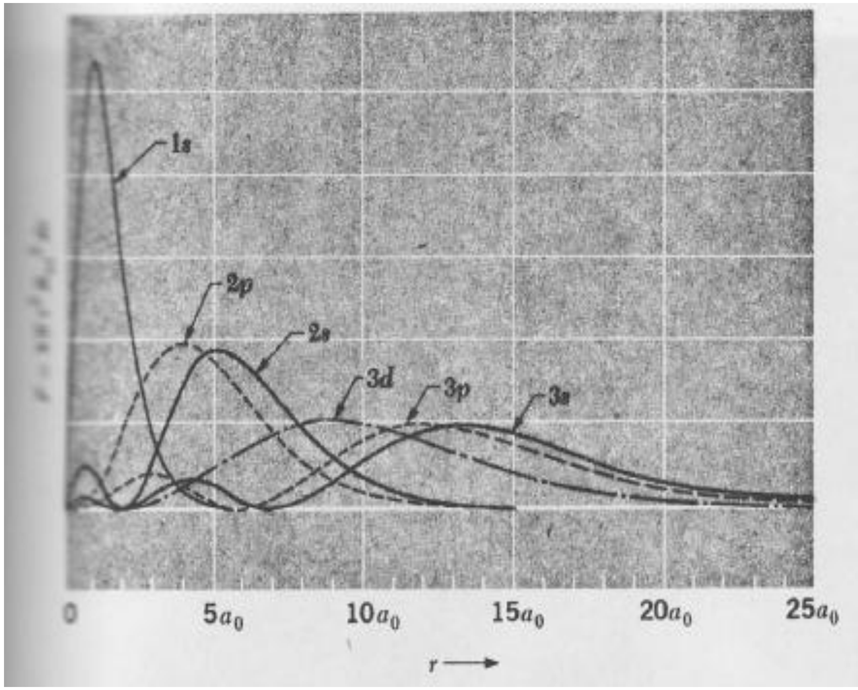
$$\langle r \rangle = \int_0^\infty r \cdot r^2 R_{n,l}(r)^2 dr$$

$$\int_0^\infty r \cdot r^2 \cdot \frac{1}{(2a_0)^3} \frac{r^2}{3a_0^2} e^{-\frac{r}{a_0}} dr$$

$$\int_0^\infty x^m e^{-bx} dr = \frac{m!}{b^{m+1}}$$

$$\frac{1}{3 \cdot 2^3 a_0^5} \int_0^\infty r^5 e^{-\frac{r}{a_0}} dr = \frac{1}{3 \cdot 2^3 a_0^5} 5!\, a_0^6 = 5\, a_0$$

Probability Density



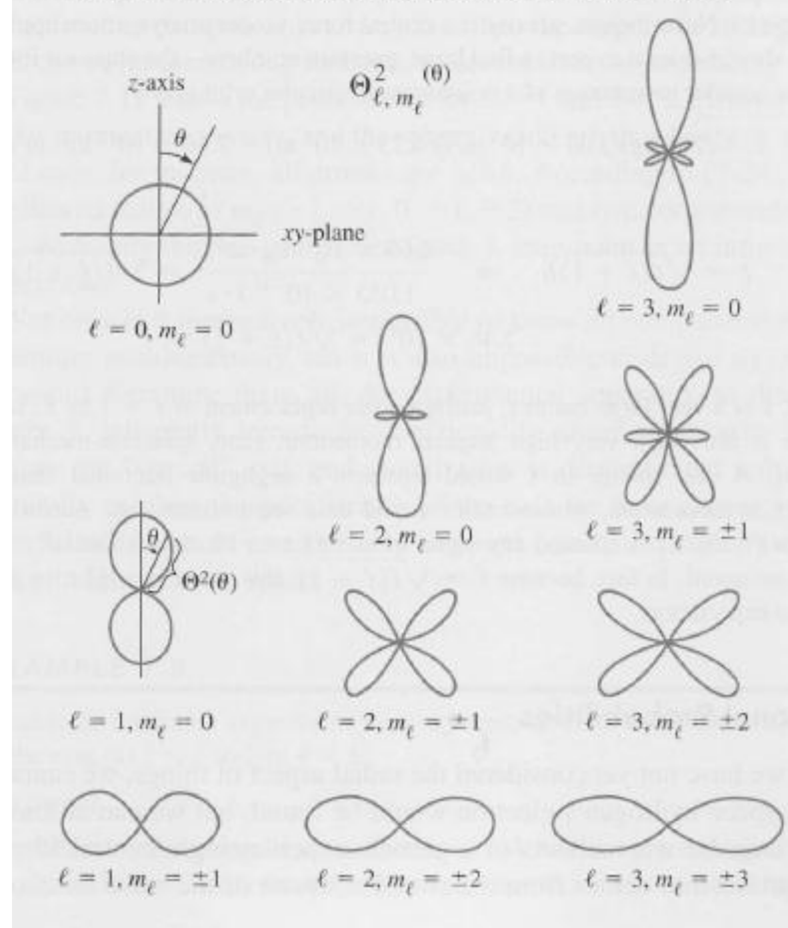
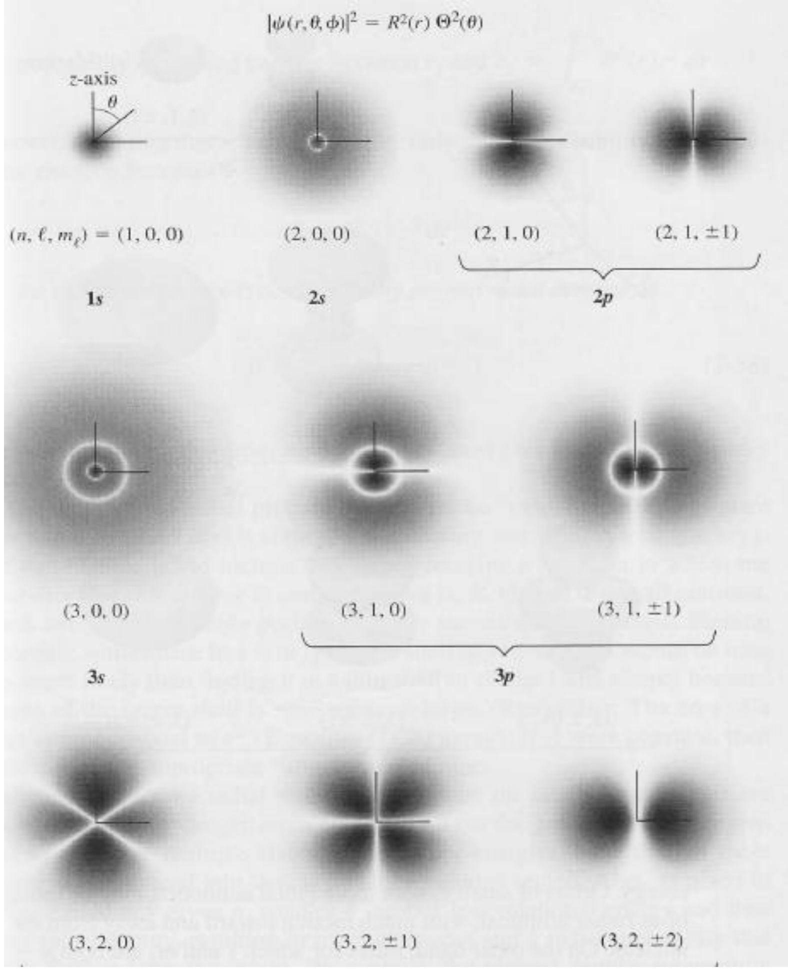
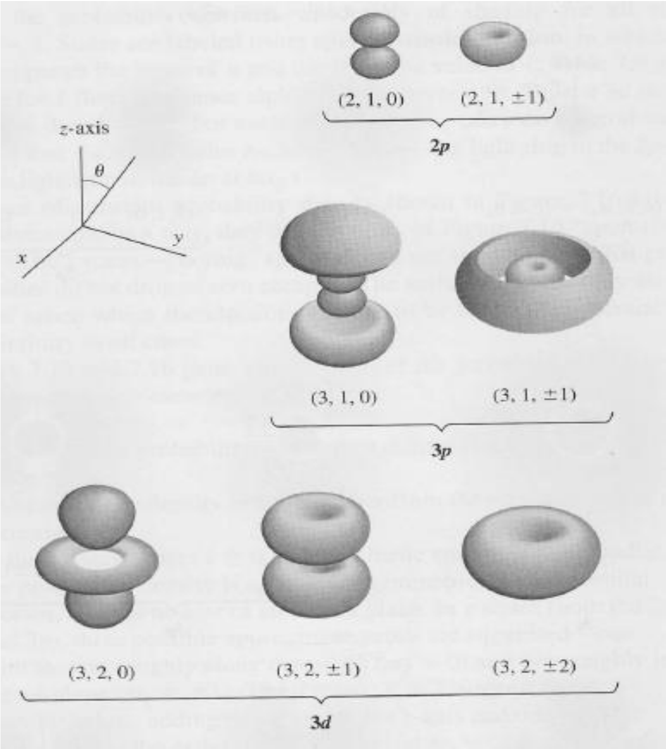


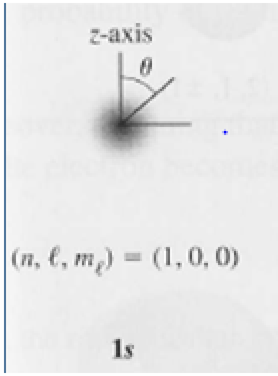
Figure 7.13 Angular probability densities for a central force.

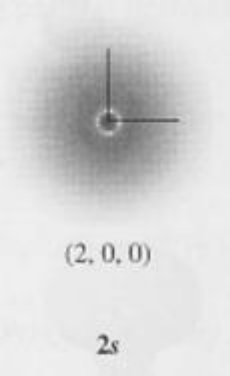
Probability Density

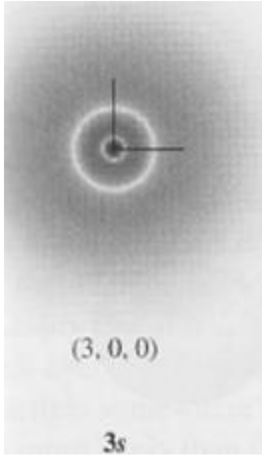




1s v. 2s vs. 3s



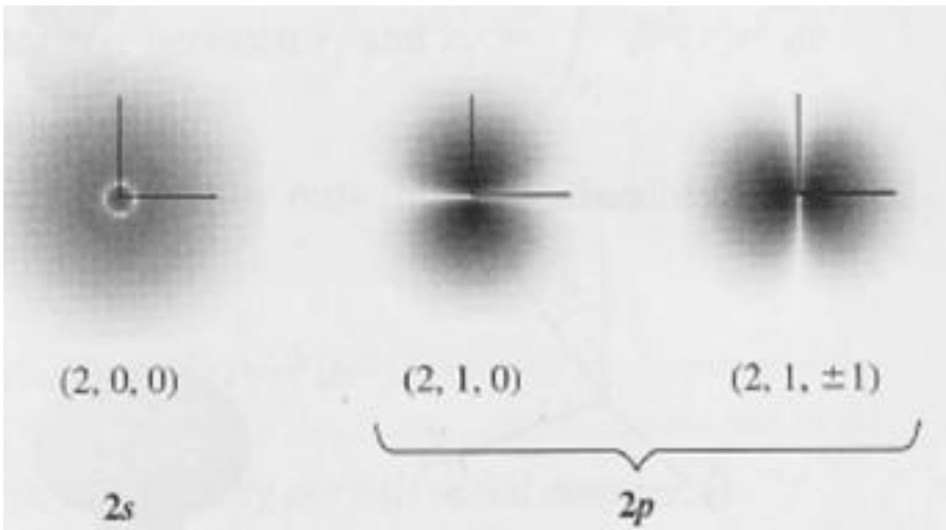


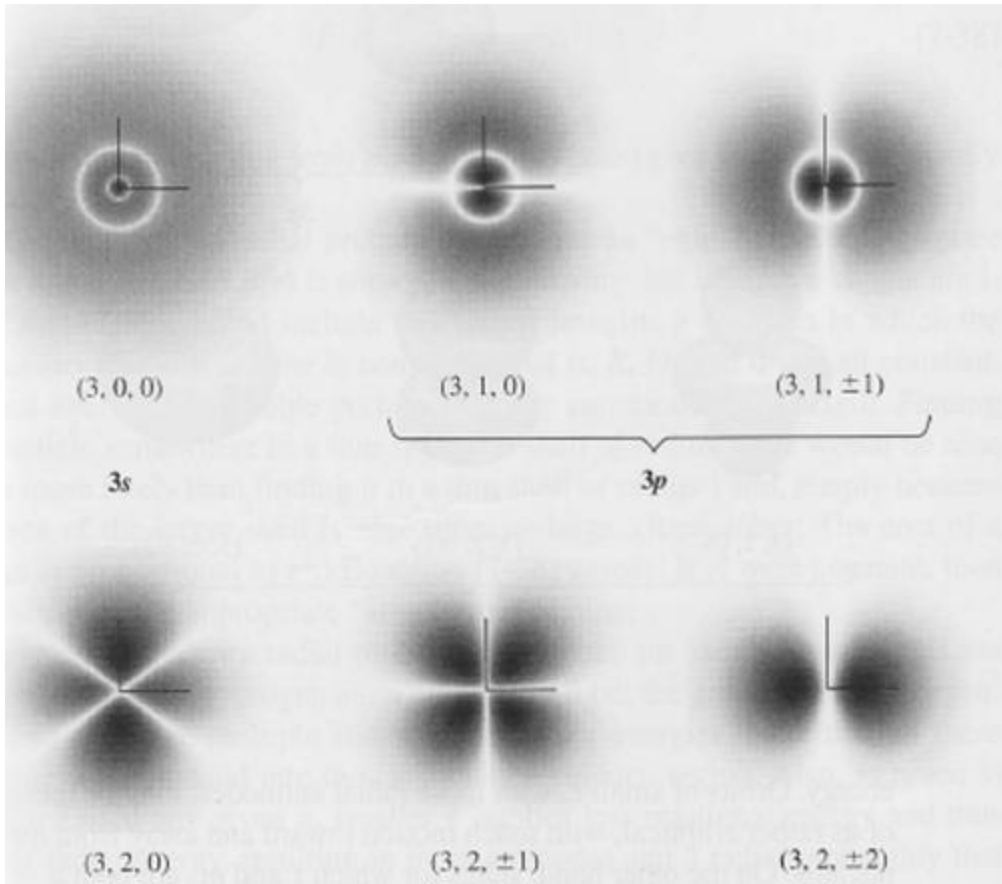


$$l = 0,\ m_l = 0, \quad \Theta_{00} = \frac{1}{\sqrt{2}}, \Phi_0 = \frac{1}{\sqrt{2\pi}}$$

$$l = 1, m_l = 0, \quad \Theta_{10} = \frac{\sqrt{6}}{2}\cos\theta, \Phi_0 = \frac{1}{\sqrt{2\pi}}$$

$$l = 2, m_l = 0, \quad \Theta_{20} = \frac{\sqrt{10}}{4}(3\cos^2\theta - 1), \Phi_0 = \frac{1}{\sqrt{2\pi}}$$


(2, 0, 0)
(2, 1, 0)
(2, 1, ±1)
2s
2p


(3, 0, 0)
(3, 1, 0)
(3, 1, ±1)
3s
3p
(3, 2, 0)
(3, 2, ±1)
(3, 2, ±2)