Angular Momentum and Central Forces

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Introduction to Angular Momentum and Central Forces

What is a Central Force?

- A particle that moves under the influence of a force towards a fixed origin (also called central field) has conserved physical observables such as energy, angular momentum, etc.
 - In a central force problem there is no external torque acting on the system
- "The law of conservation of angular momentum is a statement about the rotational symmetry of a system" (Kevin. F Brennan, Pg.130)

$$\frac{dL}{dt} = \frac{d}{dt}(r \times p) = \frac{dr}{dt} \times p + r \times \frac{dp}{dt} = 0$$

- In a given system if angular momentum is conserved then it is rotationally symmetric. i.e., the particle's wave function periodically ends in itself (can see in later slides)
- However, when an external field is applied to the system, the angular momentum is no longer symmetric. The applied force influences the particle to move in certain direction breaking the rotational symmetry.

Example of rotational symmetry

• For example, lets consider the electron and proton in a hydrogen atom. The central field would be the force they exert on each other pulling towards the centre of Mass G



- The angular momentum of the particle is a constant of motion (proved later on in the slides) the eigen states of the energy operator would be the same as the eigen states for the angular momentum.
- In this example, if there were interference from another particle (external field), the direction of movement of the particle is altered thus breaking the symmetry of space

What would you see in this lecture

- Angular momentum operator L commutes with the total energy Hamiltonian operator (H).
- Commutation relationship between different momentum operators
- Commutation of L with H
- Commutation of L² with H
- Calculating eigen values for L² with same eigen states as for H
- Calculating eigen values for Φ with L² operator
- Calculating eigen values for Θ with L² operator
- Spherical Harmonics to calculated eigen values for L and L² using m and l values
- Lowering and raising momentum operators changes the z-component by one quantum number

Angular momentum

• A particle at position r1 with linear momentum p has angular momentum,

$$\vec{L} = \vec{r} \times \vec{p}$$

Where r = r(x,y,z) and momentum vector is given by,

$$\vec{p} = \frac{\hbar}{i} \left[\frac{d}{dx}, \frac{d}{dy}, \frac{d}{dz} \right]$$

• Therefore angular momentum can be written as,

$$\vec{L} = \vec{r} \times \frac{\hbar}{i} \vec{\nabla}$$

Writing L in the matrix form and evaluating it gives the Lx, Ly and Lz components

$$\vec{L} = \frac{\hbar}{i} \begin{bmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ \frac{d}{dx} & \frac{d}{dy} & \frac{d}{dz} \end{bmatrix}$$

$$\vec{L} = \frac{\hbar}{i} \left[\left(y \frac{d}{dz} - z \frac{d}{dy} \right) \hat{i} + \left(z \frac{d}{dx} - x \frac{d}{dz} \right) \hat{j} + \left(x \frac{d}{dy} - y \frac{d}{dx} \right) \hat{k} \right]$$



Cont

Therefore,

$$\vec{L} = \frac{\hbar}{i} \left[(yp_z - zp_y)\hat{i} + (zp_x - x\frac{d}{dz})\hat{j} + (x\frac{d}{dy} - y\frac{d}{dx})\hat{k} \right]$$
$$\vec{L} = L_x\hat{i} + L_y\hat{j} + L_z\hat{k}$$

• In order to simplify the equation further we must consider the commutation of below,

$$\begin{bmatrix} L_x, y \end{bmatrix} = \left[\left(yp_z - zp_y \right), y \right] = -z \left[p_y, y \right] = +z(\hbar i) = i\hbar z$$
$$\begin{bmatrix} \left(yp_z - zp_y \right), y \end{bmatrix} = \left(yp_z - zp_y \right) * y - y * \left(yp_z - zp_y \right)$$
$$= y^2 p_z - z \frac{\hbar}{i} - zyp_y - y^2 p_z + yzp_y = iz\hbar$$
$$\begin{bmatrix} L_x, y \end{bmatrix} = iz\hbar$$

Commutation Properties

• Similarly we can show,

$$[L_x, p_y] = i\hbar p_z \qquad [L_x, x] = 0 \qquad [L_x, p_x] = 0$$

- If two operators do not commute, then from definition they cannot be found simultaneously, it can be shown that Lx and Ly do not commute therefore different components of angular momentum cannot be simultaneously determined. The commutation of Lx and Ly is given by,
- Similarly the commutation of other components is,

$$[L_x, L_y] = i\hbar L_z$$

 As it can be seen, the individual components of L (angular momentum) operator do not commute with each other therefore they cannot be simultaneously found

$$[L_{y}, L_{z}] = i\hbar L_{x} \qquad [L_{z}, L_{x}] = i\hbar L_{y} \qquad [L^{2}, L] = 0$$

L² operator

- A new operator L² is introduced because, this operator commutes with each individual components of L, however the components of L does not commute with each other.
- L² is given by, $L^2 = L^2_{x} + L^2_{y} + L^2_{z}$
- When a measurement is made, we can find the total angular momentum and only one other component at a time.
- For example, if a wave function is an eigenfunction of Lz then it is not an eigenfunction of Lx and Ly
- Taking measurement of angular momentum along Lz (applying an external field), shows the total angular momentum direction in figure below.
- When a particle is under the influence of a central (symmetrical) potential, then L commutes with potential energy V(r). If L commutes with kinetic energy, then L is a constant of motion.
- If L commutes with Hamiltonian operator (kinetic energy plus potential energy) then the angular momentum and energy can be known simultaneously.



Angular Momentum Constant of Motion

 Proof: To show if L commutes with H, then L is a constant of motion. General Case:

Let A is a time-independent operator, then

$$i\hbar \frac{d}{dt} [\psi^*(t)A\psi(t)] = i\hbar \left[\psi^*(t)A\frac{d}{dt}\psi(t)\right] + i\hbar \left[\frac{d}{dt}\psi^*(t)A\psi(t)\right] - i\hbar \frac{d\psi^*}{dt} = H\psi^* \quad i\hbar \frac{d\psi}{dt} = H\psi$$
$$i\hbar\psi^*A\frac{d\psi}{dt} + i\hbar \frac{d\psi^*}{dt}A\psi = \psi^*AH\psi - H\psi^*A\psi = \psi^*[A,H]\psi$$

• Integrating above equation through all space we get,

$$i\hbar \frac{d}{dt} \int (\psi^* A \psi) d^3 r = \int \psi^* (AH - HA) \psi d^3 r$$

But expectation value of A, $\int (\psi^* A \psi) d^3 r = \langle A \rangle$

Therefore,
$$i\hbar \frac{d(A)}{dt} = (AH - HA)$$

Since A is time independent, L.H.S is zero. Therefore when a time independent operator commutes with H, it's a constant of motion

L² commutation with H

- Similarly since L is time independent, it can be said that if L commutes with H, then the time rate of change of L is zero and it is constant of motion.
- Since L² is of high interest, it must be shown that L² commutes with H
- It is easier to prove the above in spherical coordinates, but first writing angular momentum in spherical coordinates we get, graphical representation of spherical coordinates $\vec{n} \frac{\hbar}{\nabla} \frac{\hbar}{\hat{\nabla}} \frac{\hbar}{\hat{\partial}} + \hat{\partial} \frac{1}{\hat{\partial}} \hat{\partial} + \hat{\partial} \frac{1}{\hat{\partial}} \hat{\partial} + \hat{\partial} \hat{\partial} \hat{\partial} + \hat{\partial} \hat{\partial} \hat{\partial} + \hat{\partial} \hat{\partial}$

$$p = \frac{n}{i}\nabla = \frac{n}{i}\left(\hat{r}\frac{\partial}{\partial r} + \hat{\phi}\frac{1}{r\sin\phi}\frac{\partial}{\partial\phi} + \hat{\phi}\frac{1}{r}\frac{\partial}{\partial\phi}\right)$$

• Where r, θ , Φ are written as, $\hat{r} = \sin\theta\cos\phi\hat{i} + \sin\theta\sin\phi\hat{j} + \cos\theta k$

• But
$$\vec{L} = \vec{r} \times \vec{p}$$

 $\hat{\phi} = -\sin\phi\hat{i} + \cos\phi\hat{j}$
 $\phi = \cos\theta\cos\phi\hat{i} + \cos\theta\sin\phi\hat{j} - \sin\theta k$

- Writing L in terms of radial coordinates we get, $\vec{L} = \vec{r} \times \vec{p} = r\vec{r} \times \frac{\hbar}{i} \vec{\nabla} = \frac{\hbar}{i} \left(\hat{\phi} \frac{\partial}{\partial \theta} \hat{\theta} \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} \right)$
- The i,j and k components of L are given as,

$$\vec{L} = \frac{\hbar}{i} \left[\left(-\sin\phi \frac{\partial}{\partial\theta} - \cot\theta \cos\phi \frac{\partial}{\partial\phi} \right) \hat{i} + (\cos\phi \frac{\partial}{\partial\theta} - \cot\theta \sin\phi \frac{\partial}{\partial\phi}) \hat{j} + \frac{\partial}{\partial\phi} \hat{k} \right]$$

Spherical Coordinates Vs Plane Coordinates

In spherical Coordinate System a point P is represented by three componets

 $0 \le r$ radius $0 \le \theta \le 180^{\circ}$ Theta $0 \le \varphi \le 180^{\circ}$ Phi

- Where r is the radius, the distance between origin and point P
- Theta is the angle between the line joining point P to the origin and z-axis
- Phi is the angle between is the angle between the x-axis and the line projection on the XY plane.
- <u>Click</u> to get back to the slides.



Spherical Coordinate System

Note: The θ used in the slides is represented by ϕ in the picture and like versa.

Calculating components of L²

• Given individual components of L given we can calculate L² components :

$$L_{x}^{2} = \left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right) * \left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)$$
$$= \sin\phi\frac{\partial}{\partial\theta}\sin\phi\frac{\partial}{\partial\theta} + \sin\phi\frac{\partial}{\partial\theta}\cot\theta\cos\phi\frac{\partial}{\partial\phi} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\sin\phi\frac{\partial}{\partial\theta}$$
$$+ \cot\theta\cos\phi\frac{\partial}{\partial\phi}\cot\theta\cos\phi\frac{\partial}{\partial\phi}$$
$$L_{y}^{2} = \left(\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right) * \left(\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)$$
$$= \cos\phi\frac{\partial}{\partial\theta}\cos\phi\frac{\partial}{\partial\theta} + \cos\phi\frac{\partial}{\partial\theta}\cot\theta\sin\phi\frac{\partial}{\partial\phi} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\cos\phi\frac{\partial}{\partial\theta}$$
$$+ \cot\theta\sin\phi\frac{\partial}{\partial\phi}\cot\theta\sin\phi\frac{\partial}{\partial\phi}$$

$$L_z^2 = \frac{\partial^2}{\partial \phi^2}$$

Calculating components for L² Cont'

• Adding the squares of Lx,Ly and Lz components we get,

$$L^{2} = \frac{1}{\sin^{2}\theta} \frac{\partial^{2}}{\partial\phi^{2}} + \cot\theta \frac{\partial}{\partial\theta} + \frac{\partial^{2}}{\partial^{2}\theta}$$

• $\cot\theta = \cos \theta / \sin \theta$ taking $1 / \sin \theta$ out of the last two terms we get

$$L^{2} = \frac{1}{\sin^{2}\theta} \frac{\partial^{2}}{\partial\phi^{2}} + \frac{1}{\sin\theta} \left[\cos\theta \frac{\partial}{\partial\theta} + \sin\theta \frac{\partial}{\partial\theta} \frac{\partial}{\partial\theta} \right]$$

• $d/dt(\sin \theta) = \cos \theta$ replacing it in the above equation

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

• The last two terms of R.H.S in the form $(\frac{d}{dx}x)y + x(\frac{d}{dx})y = \frac{d}{dx}(xy)$, by simplifying it we get

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

 As it can be seen that L and L² is independent of *r*, therefore it commutes with any function of *r* or its derivative. Potential energy V(r) is a function of *r*. Therefore V(r) commutes with both L and L²

L^2 commutation with the Hamiltonian Operator

- The L² operator needs to commute with the kinetic energy operator in order to commute with Hamiltonian operator as Hamiltonian operator is the sum of potential and kinetic energy.
- The kinetic energy operator in terms of L² and r is given as,

$$T = \frac{p^2}{2m} = \frac{L^2}{2mr^2} - \frac{h^2}{2mr^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right)$$

- Since potential energy operator is dependent on radial component and kinetic energy is dependent only on L² operator and radial component, L² commutes with H operator because an operator can commute with another independent operator or with itself.
- Therefore angular momentum square operator commutes with the total energy Hamiltonian operator. With similar argument angular momentum commutes with Hamiltonian operator as well.

$$[H, L^2] = 0, \qquad [H, L] = 0$$

 When a measurement is made on a particle (given its eigen function), now we can simultaneously measure the total energy and angular momentum values of that particle.

$$H\Psi = E\Psi, \qquad L^2\Psi = \lambda h^2\Psi$$

Eigen value calculation with L² operator

• The Hamiltonian equation acting on wave function ψ can be given as,

$$\left[\frac{L^2}{2mr^2} - \frac{h^2}{2mr^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + V(r)\right]\Psi = E\Psi$$

- As angular momentum operator is only a function of θ and Φ and the rest of the Hamiltonian is a function of r, therefore we can split the wave function into its radial component and angular components R(r) and Y(θ,Φ) respectively. For notational purposes it is represented as R and Y.
- When L² acts upon the eigen function we obtain the eigen value as given below,

$$L^{2}\Psi = L^{2}R(r)Y(\theta,\phi) = R(r)L^{2}Y(\theta,\phi) = R(r)\lambda h^{2}Y(\theta,\phi) = \lambda h^{2}\Psi$$

- Where λ is the wavelength of the paticle
- Therefore, when Hamiltonian operator acts on the wave function, the L² operator gives the above eigen value. The above H operator equation can be rewritten as,

$$-\frac{h^2}{2mr^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)RY + \frac{\lambda h^2}{2mr^2}RY + VRY = ERY$$

L² operation on Y

- The only operator that has effect on Y is the L² operator, once it has been operated its merely a multiplication of the eigen value with itself, therefore Y can be eliminated from the above equation.
- Therefore the eigen value equation for L² is,

$$\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) Y = -\lambda Y$$

• Angular momentum operator has θ and Φ dependence and since Y is just a function of θ and Φ as well, we can separate Y(θ , Φ) into two components,

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

• Substituting Y into the above equation we get,

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

Splitting Y into components

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

- Because either sides of the equation above are independent of each other, the only way they can equal each other is if it were a constant. By equating the above two equations to a constant, we can obtain the solutions for each individual components separately.
- Therefore, $-\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = m^2$, $\frac{d^2\Phi}{d\phi^2} + m^2\Phi = 0$
- The above differential equation can be solved to obtain an exponential solution for Φ as

$$\Phi \sim e^{im\phi}, \ m = 0, \pm 1, \pm 2, \pm 3, \dots$$

 The above solution indicates that, the system is periodic with rotational symmetry, i.e. when the particle moves in a complete circle it ends back into itself in Φ component. Therefore with a period of 2π the waveform above repeats itself at multiples of m.

Eigen value of Φ function

• The Φ function which is completely dependent on ϕ is an eigenfunction of I_z because the I_z operator is defined as

$$L_{z}\Phi = \frac{\hbar}{i}\frac{\partial}{\partial\phi}$$

• Therefore when I_z operator acts on Φ , we get the original function back along with eigenvalue of the wave-function,

$$L_z \Phi = \frac{\hbar}{i} \frac{\partial}{\partial \phi} e^{im\phi} = m\hbar e^{im\phi}$$

- The eigenvalue obtained is mħ, this shows that the z component of angular momentum of a particle in the influence of central force is quantized, therefore the values obtained are discrete.
- After obtaining the solution for Φ function, lets try to obtain the solution for Θ function, this is however complex compared to the Φ function, the differential equation for Θ function is,

$$\frac{1}{\sin\theta} \frac{d}{d\theta} \left(\sin\theta \frac{d\Theta}{d\theta} \right) + \lambda\Theta - \frac{m^2}{\sin^2\theta} \Theta = 0$$

Solution for Θ function

• The equation for Θ function is (same as in previous page),

$$\frac{1}{\sin\theta} \frac{d}{d\theta} \left(\sin\theta \frac{d\Theta}{d\theta} \right) + \lambda\Theta - \frac{m^2}{\sin^2\theta} \Theta = 0 \qquad \text{eq.1}$$

• This differential equation is solved by using change of variables as given,

$$\xi = \cos \theta, \quad d\xi = -\sin \theta \, d\theta, \quad F(\xi) = \Theta(\theta),$$
 eq.2

• After substituting $\sin^2\theta = 1-\xi^2$ and the eq.2 into the differential equation eq.1 we get,

$$\frac{1}{\sin\theta} \frac{d}{d\theta} \left(\frac{\sin^2\theta}{\sin\theta} \frac{d\Theta}{d\theta} \right) + \lambda\Theta - \frac{m^2}{\sin^2\theta} \Theta = 0 \qquad \frac{d}{d\xi} \left[(1 - \xi^2) \frac{dF}{d\xi} \right] - \frac{m^2F}{1 - \xi^2} + \lambda F = 0$$
eq.3

• **Case 1** when the constant m² is equal to zero, the above equation becomes,

$$\frac{d}{d\xi} \left[\left(1 - \xi^2 \right) \frac{dF}{d\xi} \right] + \lambda F = 0$$

Solution Cont'

• The above equation can be further simplified to,

$$\left[\frac{d}{d\xi}(1-\xi^2)\right]\frac{dF}{d\xi} + \left[\left(1-\xi^2\right)\frac{d}{d\xi}\left(\frac{dF}{d\xi}\right)\right] + \lambda F = 0$$

$$-2\xi\frac{dF}{d\xi} + (1-\xi^2)\frac{d^2F}{d\xi^2} + \lambda F = 0$$

• The above equation is in the form of Legendre equation. The general form of Legendre equation is given as

$$(1 - x2)y'' - 2xy' + l(l+1)y = 0.$$

• The polynomials obtained from Legendre equation form an orthonormal set. The general solution for a Legendre equation is given as,

$$y = \sum_{n=0}^{\infty} a_n x^n,$$

• The coefficient a_{n+2} is given by,

$$a_{n+2} = rac{n(n+1) - l(l+1)}{(n+1)(n+2)}a_0,$$

Solution Cont'

- Applying the Legendre equation to our equation, we can see that x = ξ; y" = F" and λ = l(l+1).
- Therefore the general solution for the equation is,

 $F(\xi) = \sum a_{k}\xi^{k}$

The summation coefficient also known as recursion relationship because the new coefficient a_{k+2} is dependent on its previous coefficient a_k, is given as

$$a_{k+2} = a_k \frac{k(k+1) - \lambda}{(k+1)(k+2)}$$
 0\infty

• The series must terminate at a finite value of k or the ratio a_{k+2}/a_k approaches k/k+2, the solution diverges from $\theta = 0$ or π and will no longer would be the eigen value of L². Therefore if the terminate the recursion at value *l*, such that *l* is the last term in the summation we get

$$0 = a_l \frac{l(l+1) - \lambda}{(l+1)(l+2)}$$
$$l(l+1) = \lambda$$

• With m²=0 eq.3a becomes

$$\frac{1}{\sin\theta} \frac{d}{d\theta} \left(\sin\theta \frac{d\Theta}{d\theta} \right) = -\lambda\Theta = -l(l+1)\Theta \quad \text{eq.4}$$

Operation of L^2 on Θ

• When L² operator acts on Θ (function of θ) we get,

$$L^{2}\Theta = -\hbar^{2} \left[\frac{1}{\sin^{2}\theta} \frac{d^{2}}{d\phi^{2}} + \frac{1}{\sin\theta} \frac{d}{d\theta} \left(\sin\theta \frac{d}{d\theta} \right) \right] \Theta$$

Since Θ is independent of φ, the derivative of Θ w.r.t to φ is zero therefore L² operating on Θ becomes,

$$L^{2}\Theta = -\hbar^{2} \left[\frac{1}{\sin\theta} \frac{d}{d\theta} \left(\sin\theta \frac{d}{d\theta} \right) \right] \Theta$$

• But from eq.4 the above equation can be written as,

$$L^2\Theta = h^2 \lambda \Theta = h^2 l(l+1)\Theta$$

L² operating on Θ gave the original function Θ back modified with a scalar constant. Therefore Θ is also an eigenfunction of L² with eigen value h² *l*(*l*+1). Where *l* is called an orbital angular-momentum quantum number. Explained in later slides

Eigenvalues and Orbital Quantum Numbers

- Different values of *l* and its corresponding eigen values Pg.142
- The eigen values are given by the formula *l*(*l*+1), where *l* is any positive integer including zero.
- The state of the atom (or eigenstate) are expanded into linear combinations of one electron functions. The spatial components of these electron functions are called atomic orbitals.
- As studied in chemistry s, p, d and f are the orbitals occupied by the electrons, as shown in the picture.
- s, p, d and f are characterized by the orbital quantum numbers as shown in the table above.

Table 3.1.1 Values of <i>l</i> and its corresponding Eigenvalues		
l	Eigenvalue	Spectroscopic State
0	0	S
1	$2\hbar^2$	р
2	$6\hbar^2$	d
3	$12\hbar^2$	f
•		alphabetic
		from
l	$/(l+1)\hbar^2$	here



Spherical Harmonics

• The eq.3 is redefined in special harmonics. Special Harmonics are the angular portion of the solution to Laplace's equations in spherical coordinates. The notation for special Harmonics is given by $Y_{Im}(\theta, \phi)$ and is given by,

$$Y_{im}(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} (-1)^{m} e^{im\phi} P_{i}^{m}(\cos\theta)$$

- For each value of *l* there are 2 *l* +1 spherical harmonics given by the values of *m*, which range in integer steps from -*l* to + *l*. They all have the same angular momentum.
- The φ dependent part of $Y_{lm}(\theta, \varphi)$ is still given by $e^{im\varphi}$. Therefore $Y_{lm}(\theta, \varphi)$ is still an eigenfunction of l_z with an eigenvalue of m \hbar and also L².
- The total angular momentum of the particle is given by,

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

 The picture to the right shows the magnitude of the l_z component and L component



Spherical Coordinates Cont'

• Few spherical Harmonics are given by

$$Y_{00} = \frac{1}{\sqrt{4\pi}},$$

$$Y_{10} = \sqrt{\frac{3}{4\pi}} \cos \theta,$$

$$Y_{1,\pm 1} = \mp \sqrt{\frac{3}{8\pi}} e^{\pm i\phi} \sin \theta$$

- Example Spherical Harmonics for $l = 2, -l \le m \le l$ with possible total angular momentum values chosen along z-axis z
- The values on circular rim represent the total momentum values, whereas the values on the z-axis represent the m values.



Spherical Harmonics Cont'

 Like Legendre Polynomials, spherical harmonics for a complete basis set. All the basis components are orthogonal and completely span the space. The orthogonality condition for spherical coordinates is given as,

$$\int\limits_{0}^{2\pi}\int_{0}^{\pi}Y_{lm}^{*}(heta,\phi)Y_{l',m'}(heta,\phi)d\Omega=\delta_{ll'}\delta_{mm'}$$

• As described above, the angular part of the wave function $Y_{lm}(\theta, \phi)$ is an eigenfunction for operators l_z and L². Their eigen values are,

$$L^{2}Y_{lm} = h^{2}l(l+1)Y_{lm}$$
$$L_{z}Y_{lm} = mhY_{lm}$$

Angular momentum raising and lowering operators

 The angular momentum operators can be used to define the raising and lowering operators. The notations are L₋ and L₊ used for lowering and raising respectively. They are given as,

$$L_{+} = L_{x} + iL_{y}, \qquad L_{-} = L_{x} - iL_{y}$$

• The L_x and L_v components given in the earlier slides is,

$$\overline{L_x} = \frac{\hbar}{i} \left[\left(-\sin\phi \frac{\partial}{\partial\theta} - \cot\theta \cos\phi \frac{\partial}{\partial\phi} \right) \right]$$
$$L_y = \frac{\hbar}{i} (\cos\phi \frac{\partial}{\partial\theta} - \cot\theta \sin\phi \frac{\partial}{\partial\phi})$$
$$\hbar \left[-\cos\phi \frac{\partial}{\partial\theta} - \cot\theta \sin\phi \frac{\partial}{\partial\phi} \right]$$

$$L_{x} + iL_{y} = \frac{\hbar}{i} \left[-\sin\phi \frac{\partial}{\partial\theta} - \cot\theta \cos\phi \frac{\partial}{\partial\phi} + i\cos\phi \frac{\partial}{\partial\theta} - i\cot\theta \sin\phi \frac{\partial}{\partial\phi} \right]$$

$$=\hbar \big[(\cos\phi + i\sin\phi)\big]\frac{\partial}{\partial\theta} + i\cot\theta(\cos\phi + i\sin\phi)\frac{\partial}{\partial\phi}\big]$$

Raising and lowering operator Cont'

• But $e^{j\Phi} = \cos \Phi + i \sin \Phi$, Therefore the final expression for the raising operator is,

$$L_{+} = \hbar e^{i\phi} \left(\frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right),$$

• Similarly we can show, the lowering operator with $e^{-i\Phi} = \cos \Phi - i \sin \Phi$, is

$$L_{-} = -\hbar e^{-i\phi} \left(\frac{\partial}{\partial \theta} - i \cot \theta \frac{\partial}{\partial \phi} \right)$$

• When the raising and lowering operator are implemented on $Y_{lm}(\theta, \phi)$, the only change it is going to bring is on the m value which represents the z component by one as shown in l = 2 example above

$$L_{_{+}}Y_{_{lm}} = h\sqrt{(l-m)(l+m+1)}Y_{_{l,m+1}}(\theta,\phi),$$

$$L_{_{-}}Y_{_{lm}} = h\sqrt{(l+m)(l-m+1)}Y_{_{l,m-1}}(\theta,\phi)$$

Review

- For a spherically symmetric potential V(r), angular momentum is constant of motion.
- In a central force problem only one component and the magnitude of angular momentum can be found.
- $Y(\theta, \phi)$ can be further split into independent components $\Theta(\theta)$ and $\Phi(\phi)$
- $\Phi(\phi)$ is an eigen function of Iz operator
- $\Theta(\theta)$ is an eigen function of L² operator
- The eigen values of Iz and L² operator are given by m and I values
- Therefore the total angular momentum, z component and total energy can be simultaneously found in a central force problem.



- Brennan, K.F, "The Physics of Semiconductors: With Applications to Optoelectronic Devices", Cambridge University Press 1999.
- <u>http://www.astro.cf.ac.uk/undergrad/module/PX3104/tp3/node4.html</u>
- <u>http://www.spenvis.oma.be/spenvis/help/background/magfield/legendre.html</u>
- <u>http://en.wikipedia.org/wiki/Electron_configuration</u>
- <u>http://en.wikipedia.org/wiki/Spherical_coordinate_system#Spherical_coordinate_system</u>
- <u>http://www.abdn.ac.uk/physics/px3509/hndt-3.pdf</u>
- <u>http://mathworld.wolfram.com/SphericalHarmonic.html</u>