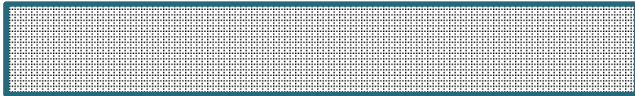


# Quantum Theory of Angular Momentum

## Goals

1. Understand how to use different coordinate systems in QM (cartesian, spherical,...)
2. Derive the quantum mechanical properties of Angular Momentum
3. Use the resulting theory to treat spherically symmetric problems in three dimensions
  - Calculating the Hydrogen atom energy levels will be our target goal



$$\psi(x, y, z)$$

Vector operators are really three operators

$$\vec{r} = x\hat{i} + y\hat{j} + z\hat{k}$$

where

$$\left\{ \begin{array}{l} -\infty < x < \infty \\ -\infty < y < \infty \\ -\infty < z < \infty \end{array} \right.$$

Scalar Operators

$x, y, z$

Ordinary Vectors

$\hat{i}, \hat{j}, \hat{k}$

Coordinate system not unique:

– For example, we could use spherical coordinates if it helpful in solving the problem.

$$\vec{r} = r\vec{e}_r(\theta, \phi)$$

Scalar Operators

$r, \theta, \phi$

Vector Operator

$\vec{e}_r(\theta, \phi)$

$$\vec{e}_r(\theta, \phi) = \sin \theta \cos \phi \hat{i} + \sin \theta \sin \phi \hat{j} + \cos \theta \hat{k}$$

You can never go wrong with Cartesian Coordinates.

- In all other coordinate systems, the unit vectors are also operators
  - so must be treated carefully

For each point in space there is a position eigenstate

- How we want to label these points is up to us:

$$\psi \equiv \psi(x, y, z)$$

$$\psi \equiv \psi(r, \theta, \phi)$$

$$\psi \equiv \psi(\rho, z, \phi)$$

} Different ways  
to refer to  
the same state

## Wavefunctions

- Wavefunctions are defined in the usual way as:

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |\psi(x, y, z)| dx dy dz = 1$$

$$\int_0^{\infty} r^2 dr \int_0^{\pi} \sin \theta d\theta \int_0^{2\pi} d\phi |\psi(r, \theta, \phi)| = 1$$

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

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

$$z = r \cos \theta$$

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

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

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



The three-dimensional momentum vector operator is:

$$\vec{P} = \hat{i}p_x + \hat{j}p_y + \hat{k}p_z$$

The three-dimensional Hamiltonian is

$$H = \frac{\vec{P} \cdot \vec{P}}{2m} + V(\vec{r})$$

In Cartesian components, this becomes:

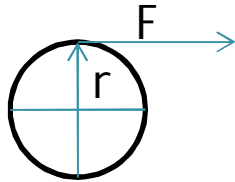
$$H = \frac{p_x^2 + p_y^2 + p_z^2}{2m} + V(\vec{r})$$

$$H = -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + V(x, y, z)$$

$$H = -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r})$$

In spherical coordinate

$$H = -\frac{\hbar^2}{2m} \nabla_{r,\theta,\phi}^2 + V(\vec{r})$$



The torque is the reason for rotational motion

$$L = mrv = mr^2(v/r) = I\omega$$

Conserved if  $T_{\text{net}}=0$ ,  $T=\text{Torque} = r \times F$   
 $I = \text{moment of inertia}$

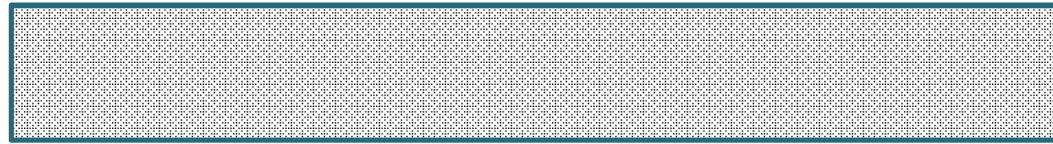
$$T = \frac{\Delta L}{\Delta t}$$

$$W = \int T \cdot d\theta$$

Rotational energy

$$T\theta = I\alpha\theta = I \frac{\omega}{t} \left( \frac{1}{2} \omega t \right) = \frac{1}{2} I\omega^2$$

$$= \frac{(I\omega)^2}{2I} = \frac{L^2}{2I}$$



The force is the reason for the linear motion

$$P = mv$$

Conserved if  $F_{\text{net}}=0$

$$F = \frac{\Delta P}{\Delta t}$$

$$W = \int F \cdot dx$$

Work = The change in kinetic energy

$$Fd = mad = m \frac{v}{t} \cdot \left( \frac{1}{2} vt \right) = \frac{1}{2} mv^2$$

Kinetic energy

# Angular Momentum

The angular momentum operator is defined as:

$$\vec{L} = \vec{r} \times \vec{p} \quad \text{or} \quad \vec{L} = -i\hbar(\vec{r} \times \vec{\nabla})$$

It is a vector operator:

In Cartesian coordinate:

$$\vec{L} = L_x \hat{i} + L_y \hat{j} + L_z \hat{k}$$

According to the definition of the cross product, the components are given by:

$$L_x = yp_z - zp_y$$

$$L_y = zp_x - xp_z$$

$$L_z = xp_y - yp_x$$



$$\hat{L}_x = -i\hbar \left( y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right)$$

$$\hat{L}_y = -i\hbar \left( z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right)$$

$$\hat{L}_z = -i\hbar \left( x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right)$$

In spherical coordinate:

$$\begin{aligned}\vec{r} \times \vec{\nabla} &= \det \begin{vmatrix} e_r & e_\theta & e_\phi \\ r & 0 & 0 \\ \frac{\partial}{\partial r} & \frac{1}{r} \frac{\partial}{\partial \theta} & \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \end{vmatrix} \\ &= -e_\theta \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} + e_\phi \frac{\partial}{\partial \theta} \\ \vec{L} &= -i\hbar \left( -e_\theta \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} + e_\phi \frac{\partial}{\partial \theta} \right)\end{aligned}$$

For simplicity use the following relation to calculate  $L^2$  in spherical coordinate

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

Please note that

$$\begin{aligned}\frac{d}{dx} &= \frac{\partial r}{\partial x} \frac{\partial}{\partial r} + \frac{\partial \theta}{\partial x} \frac{\partial}{\partial \theta} + \frac{\partial \phi}{\partial x} \frac{\partial}{\partial \phi} & \frac{d}{dx} &= \sin \theta \cos \phi \frac{\partial}{\partial r} + \frac{\cos \theta \cos \phi}{r} \frac{\partial}{\partial \theta} - \frac{\sin \phi}{r \sin \theta} \frac{\partial}{\partial \phi} \\ \frac{d}{dy} &= \frac{\partial r}{\partial y} \frac{\partial}{\partial r} + \frac{\partial \theta}{\partial y} \frac{\partial}{\partial \theta} + \frac{\partial \phi}{\partial y} \frac{\partial}{\partial \phi} & \frac{d}{dy} &= \sin \theta \sin \phi \frac{\partial}{\partial r} + \frac{\cos \theta \sin \phi}{r} \frac{\partial}{\partial \theta} + \frac{\cos \phi}{r \sin \theta} \frac{\partial}{\partial \phi} \\ \frac{d}{dz} &= \frac{\partial r}{\partial z} \frac{\partial}{\partial r} + \frac{\partial \theta}{\partial z} \frac{\partial}{\partial \theta} + \frac{\partial \phi}{\partial z} \frac{\partial}{\partial \phi} & \frac{d}{dz} &= \cos \theta \frac{\partial}{\partial r} - \frac{\sin \theta}{r} \frac{\partial}{\partial \theta}\end{aligned}$$


As you will see in the H.W


$$L_z = -i\hbar \frac{\partial}{\partial \phi}$$

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

# Commutation Relations

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

if  $[\hat{A}, \hat{B}] = 0$   The two operator A and B are commute

if  $[\hat{A}, \hat{B}] \neq 0$   The two operator A and B are not commute

The commutation relations for the angular momentum component are given by:

In the H.W you will see

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

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

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

they are just a  
consequence of

$$[x_i, p_j] = i\hbar \delta_{ij}$$

Compact notations:

$$[L_i, L_j] = i\hbar L_k \varepsilon_{ijk}$$

$$[x_i, L_j] = i\hbar x_k \varepsilon_{ijk}$$

$$[p_i, L_j] = i\hbar p_k \varepsilon_{ijk}$$

$$\varepsilon_{ijk} = \begin{cases} 0 & \text{if any two indices are the same} \\ 1 & \text{cyclic permutations of x,y,z (or 1,2,3)} \\ -1 & \text{cyclic permutations of z,y,x (or 3,2,1)} \end{cases}$$

Any three operators which obey these relations are considered as 'generalized angular momentum operators'

The components of angular momentum do not commute this means:

In the context of an experiment this translates to the statement that components of angular momentum observables can not be measured "simultaneously".

In a theoretical framework this is expressed in the fact that these operators do not have common eigenfunctions

In the HW you will see that:

$$[L^2, L_x] = 0$$

$$[L^2, L_y] = 0$$

$$[L^2, L_z] = 0$$

Please note that  $[A, BC] = [A, B]C + B[A, C]$

Where: 
$$L^2 = L_x^2 + L_y^2 + L_z^2$$

This means that simultaneous eigenstates of  $L^2$  and  $L_z$  exist

## Particle in a Ring: Wave function of $L_z$

$$-\frac{\hbar^2}{2m} \cdot \frac{d^2\psi(x)}{dx^2} = E\psi(x)$$

$$-\frac{\hbar^2}{2mR^2} \cdot \frac{d^2\psi(x)}{d\phi^2} = E\psi(x)$$

$$\phi = x / R$$

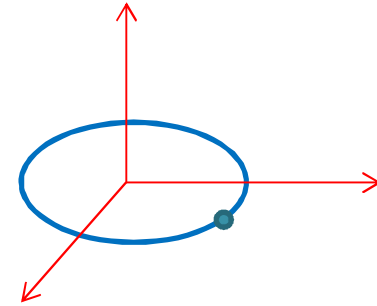
$$dx = R d\phi$$

From classical Mechanics

The kinetic energy of a body rotating in the xy-plane  
Can be expressed as

$$E = \frac{L_z^2}{2I}$$

$$I = mR^2$$



$$\frac{d^2\psi(\phi)}{d\phi^2} + m\psi(\phi) = 0$$

$$m \equiv 2IE / \hbar^2$$

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

Single value condition for the wave function

$$\psi(\phi + 2\pi) = \psi(\phi)$$

$$e^{im(\phi+2\pi)} = e^{im\phi}$$

This require that

$$e^{2\pi im} = 1$$



The wave function to be periodic,  
the value of m must be real.  
(complex m would result  
exponential solution)

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

**m is called magnetic quantum number**

A measurement of the z-component of the orbital angular momentum  
Can only yield the values  $0, \pm \hbar, \pm 2 \hbar, \dots$  because the z-axis can be chosen  
Along an arbitrary direction, we see that the component of **the orbital angular  
Momentum about any axis is quantized.**

As you will see in the H.W  $A = \frac{1}{\sqrt{2\pi}}$

So, 
$$\psi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}$$

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The eigenfunctions of the ring form an orthonormal set:

$$\int_0^{2\pi} \psi_m^*(\phi) \psi_n(\phi) d\phi = \delta_{mn}$$

You will prove this relation in the H.W

The eigenfunctions form a complete set, so that any function  $f(\phi)$  define in the interval  $0 \leq \phi \leq 2\pi$  Can be expanded as

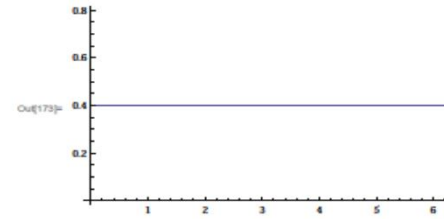
$$f(\phi) = \sum_{m=-\infty}^{\infty} a_m \psi_m(\phi)$$
$$a_m = \int_0^{2\pi} \psi_m^*(\phi) f(\phi) d\phi$$

The eigenfunctions satisfy

$$\sum_{m=-\infty}^{\infty} \psi_m^*(\phi') \psi_m(\phi) = \delta(\phi - \phi')$$

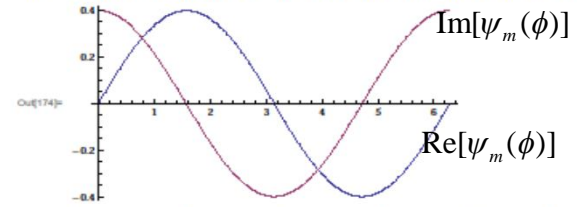
m=0

```
In[173]= Plot[1/Sqrt[2 Pi], {x, 0, 2 Pi}]
```



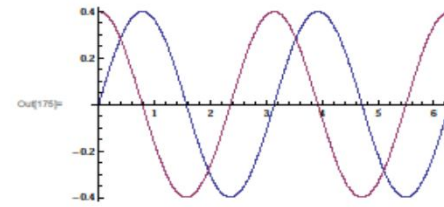
m=1

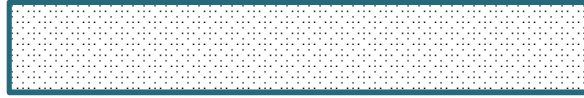
```
In[174]= Plot[{(1/Sqrt[2 Pi]) * Sin[x], (1/Sqrt[2 Pi]) * Cos[x]}, {x, 0, 2 Pi}]
```



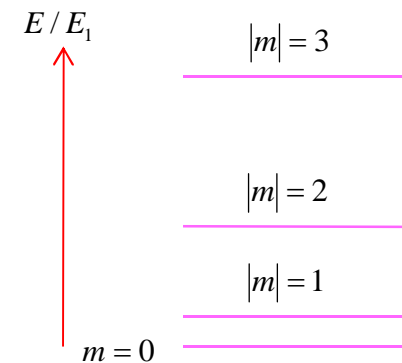
m=2

```
In[175]= Plot[{(1/Sqrt[2 Pi]) * Sin[2 x], (1/Sqrt[2 Pi]) * Cos[2 x]}, {x, 0, 2 Pi}]
```






$$E_{|m|} = \frac{\hbar^2}{2I} m^2$$



All eigen values are twofold (doubly) degenerate.

The eigenstate corresponding to  $+|m|$  and  $-|m|$  states have the same energy, so this system is degenerate.

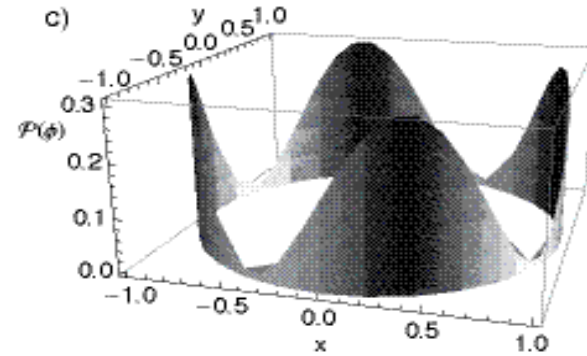
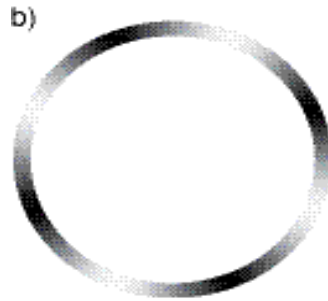
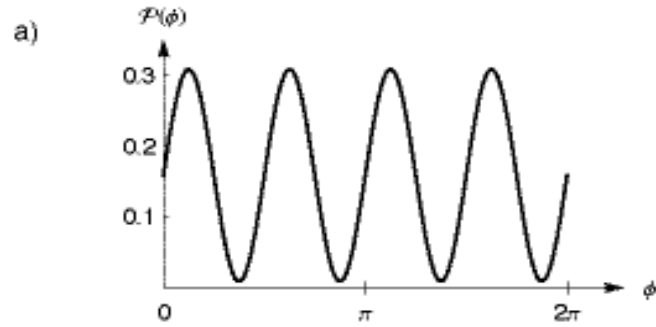
The  $\pm m$  degeneracy of the energy eigenstates corresponds to  $L_z = +m\hbar$  and  $L_z = -m\hbar$ . That is, the two degenerate states represent states with opposite components of the Angular momentum along the z-axis.


$$P_m(\phi) = |\psi_m(\phi)|^2$$

$$P_m(\phi) = \left| \frac{1}{\sqrt{2\pi}} e^{im\phi} \right|^2 = \frac{1}{2\pi}$$

Which is a constant independent on the quantum number  $m$ .  
However there is spatial dependence in the probability density for  
Superposition states.  
As you will see in H.W 7.

Graph shows the probability density of problem 7.  
The plot in one, two, and three dimensions.  
As we see the probability change with the angle.



Since the states  $\psi_m, \psi_{-m}$

Have the same energy, the probability of measuring the energy  $E_{|m|}$   
Is the sum

$$P_{E_{|m|}} = \left| \int_0^{2\pi} \psi_m^*(\phi) \Psi(\phi) \right|^2 + \left| \int_0^{2\pi} \psi_{-m}^*(\phi) \Psi(\phi) \right|^2$$

On the other hand the state  $\psi_m$  uniquely specifies the orbital angular momentum Component along the z-direction, so the probability of measuring the angular Momentum component is

$$P_{L_z=m\hbar} = \left| \int_0^{2\pi} \psi_m^*(\phi) \Psi(\phi) \right|^2$$