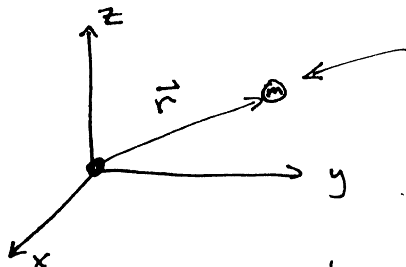
Angular Momentum

This is the basic framework for how we understand particles (e.g. electrons) flying around other particles (e.g. nuclei).

We'll start by pinning down the nucleus at the origin of the coordinate system, and using the electron's coordinates:



particle of mass m at:

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

$\hat{i}, \hat{j}, \& \ \hat{k}$ are unit vectors

Velocity: $\vec{v} = \frac{\partial}{\partial t}\vec{r} = \hat{i}\frac{\partial x}{\partial t} + \hat{j}\frac{\partial y}{\partial t} + \hat{k}\frac{\partial z}{\partial t}$

velocity components: $v_x = \frac{\partial x}{\partial t}$ $\quad v_y = \frac{\partial y}{\partial t}$ $\quad v_z = \frac{\partial z}{\partial t}$

Linear Momentum is defined using the particle's mass:

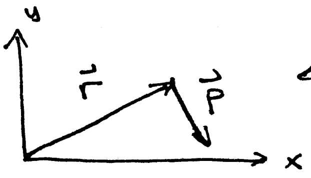
$$\vec{p} = m\vec{v} \quad : \quad p_x = mv_x, \ p_y = mv_y, \ p_z = mv_z$$

Angular Momentum references the origin of the coordinate system

$$\vec{L} = \vec{r} \times \vec{p} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix}$$

$$= (yp_z - zp_y)\hat{i} + (zp_x - xp_z)\hat{j} + (xp_y - yp_x)\hat{k}$$

$\vec{L}$ is perpendicular to the plane defined by $\vec{r}$ & $\vec{p}$



$\vec{L}$ will be in the z direction in this example

Torque (the angular equivalent of force)

$$\vec{F} = \frac{d\vec{p}}{dt} \leftarrow m\frac{d\vec{v}}{dt} = m\vec{a}$$

$$\vec{\tau} = \vec{r} \times \vec{F}$$

a proof of this:

$$\frac{d}{dt}(\vec{L}) = \frac{d}{dt}(\vec{r} \times \vec{p})$$

$$= \frac{d\vec{r}}{dt} \times \vec{p} + \vec{r} \times \frac{d\vec{p}}{dt}$$

$$= \vec{v} \times \vec{p} + \vec{r} \times \frac{d\vec{p}}{dt}$$

$\vec{v}$ & $\vec{p}$ are parallel, so the cross product is zero!

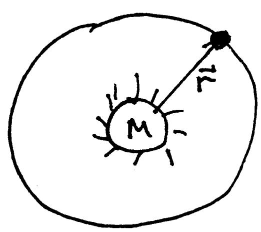
$$\therefore \quad \frac{d}{dt}(\vec{L}) = \vec{r} \times \frac{d\vec{p}}{dt}$$

$$= \vec{r} \times \vec{F}$$

Angular momentum is conserved $\left(\frac{d\vec{L}}{dt} = 0\right)$ when the torque on a particle is zero.

Consider the solar system

$$\vec{F} = G\frac{Mm}{r^2}\hat{r} \leftarrow \text{points along } \vec{r}$$



$\vec{r} \times \vec{F} = 0$ because $\vec{F}$ & $\vec{r}$ are parallel so $\frac{d\vec{L}}{dt} = 0$

$\therefore$ $\vec{L}$ is a constant

There are two kinds of angular momentum in Quantum Mech:

Orbital Angular Momentum: $\vec{L}$ (results from motion of particles in space around each other)

Spin Angular Momentum: $\vec{S}$ (an intrinsic property of particles $\rightarrow$ there's no direct classical analogy)

Mapping from classical → Quantum with operators:

$$L_x = y p_z - z p_y \longrightarrow -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$
$$L_y = z p_x - x p_z \longrightarrow -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$
$$L_z = x p_y - y p_x \longrightarrow -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

classical definitions

QM analogies (note: $\hbar$ has units of angular momentum)

We can ask questions about total angular momentum:

$$\hat{L}^2 = |\vec{L}|^2 = \vec{L}\cdot\vec{L} = L_x^2 + L_y^2 + L_z^2$$

As well as individual components: $\hat{L}_z$

As we try to figure out wavefunctions, we'll need to get a set of commutation relations:

$$\left.\begin{aligned} [\hat{L}_x, \hat{L}_y] &= i\hbar\hat{L}_z \\ [\hat{L}_y, \hat{L}_z] &= i\hbar\hat{L}_x \\ [\hat{L}_z, \hat{L}_x] &= i\hbar\hat{L}_y \end{aligned}\right\}$$

proof of these will be in the Homework

← Note the cyclic behavior!

A very important consequence of these is:

$$[\hat{L}^2, \hat{L}_x] = [\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2, \hat{L}_x] = \underbrace{[\hat{L}_x^2, \hat{L}_x]}_{=0} + [\hat{L}_y^2, \hat{L}_x] + [\hat{L}_z^2, \hat{L}_x]$$

To do the others, we'll need:

$$[\hat{A}\hat{B}, \hat{C}] = [\hat{A}, \hat{C}]\hat{B} + \hat{A}[\hat{B}, \hat{C}]$$

add 0

proof:
$$\begin{aligned}[\hat{A}\hat{B}, \hat{C}] &= (\hat{A}\hat{B}\hat{C} - \hat{C}\hat{A}\hat{B}) + (\hat{A}\hat{C}\hat{B} - \hat{A}\hat{C}\hat{B}) \\ &= (\hat{A}\hat{B}\hat{C} - \hat{A}\hat{C}\hat{B}) + (\hat{A}\hat{C}\hat{B} - \hat{C}\hat{A}\hat{B}) \\ &= \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}\end{aligned}$$

$$[\hat{L}^2, \hat{L}_x] = [L_y, L_x]L_y + L_y[L_y, L_x] + [L_z, L_x]L_z + L_z[L_z, L_x].$$

$$= -i\hbar L_z L_y - i\hbar L_y L_z + i\hbar L_y L_z + i\hbar L_z L_y$$

$$[\hat{L}^2, \hat{L}_x] = 0$$

Consequences of these commutation relations

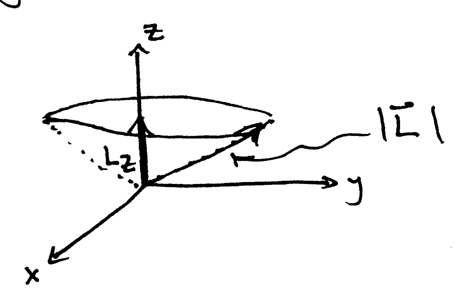
1. Only one component of $\vec{L}$ can be measured simultaneously:

$$\left.\begin{matrix}[L_x, L_y]\\ [L_z, L_x]\\ [L_y, L_z]\end{matrix}\right\} \neq 0 \leftarrow$$ so these operators can't share eigenstates.

2. $\hat{L}^2 = |\vec{L}|^2$ along with 1 component of $\vec{L}$ (usually $\hat{L}_z$) can be specified by the same Quantum state:

$$[\hat{L}^2, \hat{L}_z] = 0$$

A geometric picture of this:



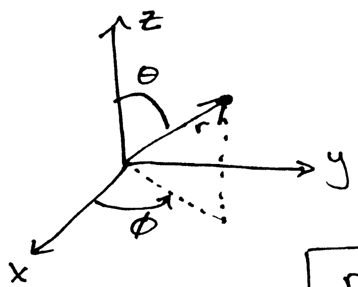
$\vec{L}$ lies somewhere on a cone defined by total angular momentum $|\vec{L}|$ and the z-component of angular momentum, $\hat{L}_z$, but we can't specify where on that cone it lies!

3. $\hat{L}^2$ & $\hat{L}_z$ share common eigenfunctions (with different eigenvalues)

$$\left.\begin{matrix}\hat{L}^2 Y = bY\\ \hat{L}_z Y = cY\end{matrix}\right]$$ what are the functions?

Finding the Eigenfunctions for rotation

In Cartesian coordinates this is a nearly impossible task, but it is much simpler in spherical coordinates



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

$$r^2 = x^2 + y^2 + z^2$$
$$\cos\theta = \frac{z}{r}$$
$$\tan\phi = y/x$$

We need to express these operators:

$$\begin{cases} \hat{L}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \\ \hat{L}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \\ \hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \end{cases}$$

in spherical coordinates, so we need $\frac{\partial}{\partial x}$, $\frac{\partial}{\partial y}$ & $\frac{\partial}{\partial z}$ in spherical coordinates.

chain rule expressions!

$$\frac{\partial}{\partial x} = (\sin\theta\cos\phi)\frac{\partial}{\partial r} + \left(\frac{\cos\theta\cos\phi}{r}\right)\frac{\partial}{\partial\theta} - \left(\frac{\sin\phi}{r\sin\theta}\right)\frac{\partial}{\partial\phi}$$

$$\frac{\partial}{\partial y} = (\sin\theta\sin\phi)\frac{\partial}{\partial r} + \left(\frac{\cos\theta\sin\phi}{r}\right)\frac{\partial}{\partial\theta} + \left(\frac{\cos\phi}{r\sin\theta}\right)\frac{\partial}{\partial\phi}$$

$$\frac{\partial}{\partial z} = (\cos\theta)\frac{\partial}{\partial r} - \left(\frac{\sin\theta}{r}\right)\frac{\partial}{\partial\theta}$$

$$\therefore \quad \hat{L}_x = i\hbar\left[\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right]$$

$$\hat{L}_y = -i\hbar\left[\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right]$$

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

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

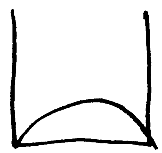
Where we're going with this:

$$\hat{L}^2 \, Y(\theta, \phi) = b \, Y(\theta, \phi)$$
$$\hat{L}_z \, Y(\theta, \phi) = c \, Y(\theta, \phi)$$

$Y(\theta, \phi)$ is a wavefunction in <u>angles</u> that describes <u>rotation</u> around a fixed point.

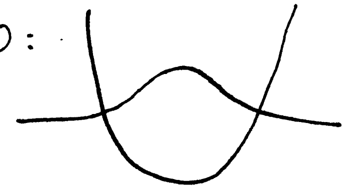
What are good <u>boundary</u> <u>conditions</u>?

P-I-B



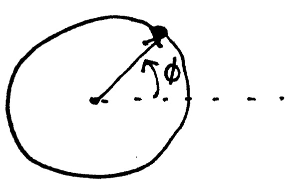
$\psi(0) = 0 \qquad \psi(a) = 0$

HO:



$\psi(x \to \pm\infty) = 0$

For rotational motion, the idea is to find wave functions for a particle moving in a circular orbit



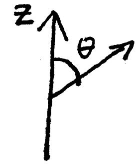
$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \phi}$$

a <u>momentum</u> on the ϕ angle

If the wavefunction is going to be <u>continuous</u>, then when it comes back after a full rotation it must have the same value:

$$Y(\theta, \phi + 2\pi) = Y(\theta, \phi)$$

There <u>isn't</u> a similar condition on θ, which is only defined from $0 \to \pi$



$\theta = 0$ pointing up

$\theta = \pi$ pointing down!

These are different positions, so there's no boundary on θ.

So: $\hat{L}_x, \hat{L}_y, \hat{L}_z$ only depend on θ & ϕ (not on r)

On to the real problem:

$$\hat{L}_z Y(\theta,\phi) = b\, Y(\theta,\phi)$$
$$\hat{L}^2 Y(\theta,\phi) = c\, Y(\theta,\phi)$$

Seperability: $Y(\theta,\phi) = S(\theta)\,T(\phi)$

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

$$\hat{L}_z Y(\theta,\phi) = -i\hbar \frac{\partial}{\partial\phi} S(\theta)T(\phi) = b\, S(\theta)T(\phi$$

$$-i\hbar\, \cancel{S(\theta)} \frac{\partial T(\phi)}{\partial\phi} = b\, \cancel{S(\theta)}\, T(\phi)$$

} split derivative

$$\frac{1}{T(\phi)}\, dT(\phi) = \frac{ib}{\hbar}\, d\phi$$

$$\ln T(\phi) = \frac{ib}{\hbar}\phi \quad (+ \text{ constant})$$

$$T(\phi) = e^{c}\, e^{ib\phi/\hbar} = A\, e^{ib\phi/\hbar}$$

Boundary condition told us that $T(\phi+2\pi) = T(\phi)$

$$A e^{ib\phi/\hbar}\, e^{ib2\pi/\hbar} = A e^{ib\phi/\hbar}$$

$$\therefore\; e^{ib2\pi/\hbar} = 1$$

$$\cos\left(\frac{2\pi b}{\hbar}\right) + i \sin\left(\frac{2\pi b}{\hbar}\right) = 1$$

this is true only when $\frac{2\pi b}{\hbar} = 2\pi m$ where $m = 0, \pm 1, \pm 2, \ldots$

So: $b = m\hbar$ and therefore $T(\phi) = A e^{im\phi}$

with $m = 0, \pm 1, \pm 2, \ldots$

To normalize this:

$$1 = \int_0^{2\pi} A^* e^{-im\phi} A e^{+im\phi} \, d\phi$$

$$= A^* A \int_0^{2\pi} 1 \, d\phi = A^* A \, 2\pi$$

$$\therefore \quad A = \frac{1}{\sqrt{2\pi}}$$

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

$$Y(\theta, \phi) = \frac{1}{\sqrt{2\pi}} S(\theta) e^{im\phi}$$

Now we need to consider $S(\theta)$

$$\hat{L}^2 Y(\theta,\phi) = c\, Y(\theta,\phi) = \frac{c}{\sqrt{2\pi}} e^{im\phi} S(\theta)$$

$$-\hbar^2 \left(\frac{\partial^2}{\partial\theta^2} + \cot\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right) \cancel{\frac{1}{\sqrt{2\pi}}} e^{im\phi} S(\theta)$$

$$= c \cancel{\frac{1}{\sqrt{2\pi}}} e^{im\phi} S(\theta)$$

$$-\hbar^2 \left(\frac{\partial^2}{\partial\theta^2} + \cot\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}(-m^2) \right) \cancel{e^{im\phi}} S(\theta) = c \, \cancel{e^{im\phi}} S(\theta)$$

$$\frac{d^2 S}{d\theta^2} + \frac{\cos\theta}{\sin\theta} \frac{dS}{d\theta} + \left(\frac{c}{\hbar^2} - \frac{m^2}{\sin^2\theta} \right) S = 0$$

The solutions match the Associated Legendre Eqn:

$$\frac{d^2 S}{d\theta^2} + \frac{\cos\theta}{\sin\theta} \frac{dS}{d\theta} + \left(l(l+1) - \frac{m^2}{\sin^2\theta} \right) S = 0$$

$$\frac{c}{\hbar^2} \longrightarrow l(l+1) \longrightarrow c = \hbar^2 l(l+1)$$

The conditions under which we can use the associated Legendre equation are

$$l = 0, 1, 2, \ldots \quad \underline{\text{and}} \quad |m| \le l$$

$$= -l, -l+1, \ldots 0 \ldots l-1, l$$

$$m = 0, \pm 1 \ldots \pm l$$

$$S_{lm}(\theta) = B\, P_l^{|m|}(\cos\theta)$$

$P_l^{|m|}$ are the Associated Legendre Polynomials

if $(x = \cos\theta)$

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

$P_0^0(x) = 1$ $\qquad$ $P_0^0(\cos\theta) = 1$

$P_1^0(x) = x$ $\qquad$ $P_1^0(\cos\theta) = \cos\theta$

$P_1^1(x) = (1-x^2)^{1/2}$ $\qquad$ $P_1^1(\cos\theta) = \sin\theta$

$P_2^0(x) = \frac{1}{2}(3x^2-1)$ $\qquad$ $P_2^0(\cos\theta) = \frac{1}{2}(3\cos^2\theta - 1)$

$P_2^1(x) = 3x(1-x^2)^{1/2}$ $\qquad$ $P_2^1(\cos\theta) = 3\cos\theta\sin\theta$

$P_2^2(x) = 3 - 3x^2$ $\qquad$ $P_2^2(\cos\theta) = 3\sin^2\theta$

$$S_{lm}(\theta) = \underbrace{\left[\frac{2l+1}{2} \frac{(l-|m|)!}{(l+|m|)!}\right]^{1/2}}_{\text{normalization factor}} P_l^{|m|}(\cos\theta)$$

So now we've arrived at the angular wavefunctions:

$$\hat{L}_z \, Y_l^m(\theta, \phi) = \hbar m \, Y_l^m(\theta, \phi)$$

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

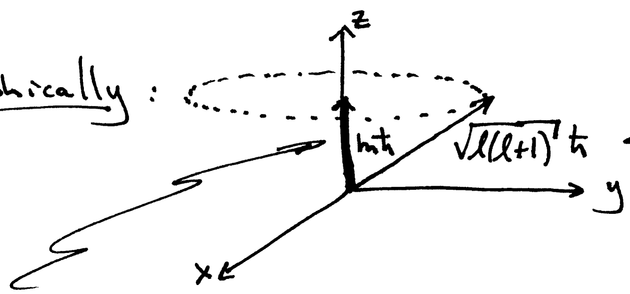
$l = 0, 1, 2 \ldots \leftarrow$ angular momentum QN

$m = 0, \pm 1, \pm 2 \ldots \pm l \leftarrow$ azimuthal QN

$Y_l^m(\theta, \phi)$ are called the <u>spherical harmonics</u>

$$Y_l^m(\theta, \phi) = \frac{1}{\sqrt{2\pi}} \left[\frac{2l+1}{2} \frac{(l-|m|)!}{(l+|m|)!} \right]^{1/2} P_l^{|m|}(\cos\theta) \, e^{im\phi}$$

Graphically:

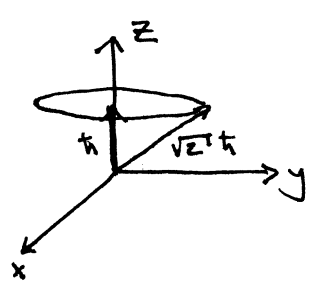


$\leftarrow$ <u>length</u> of angular momentum vector is <u>quantized</u> (only some angular momenta are allowed)

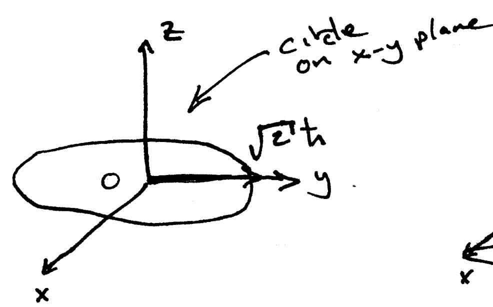
L_z is <u>z-projection</u> of the total angular momentum.

For any given l, only some m-values or z-projections can be observed. Consider $l = 1$ case:

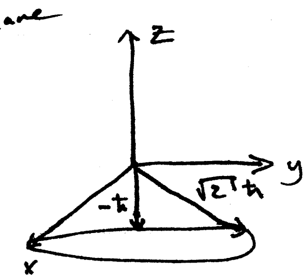
$\hat{L}^2 \, Y_1^m = 2\hbar^2 \, Y_1^m \longrightarrow |L^2| = \sqrt{2}\,\hbar \leftarrow$ <u>length</u>



$l=1, m=1$



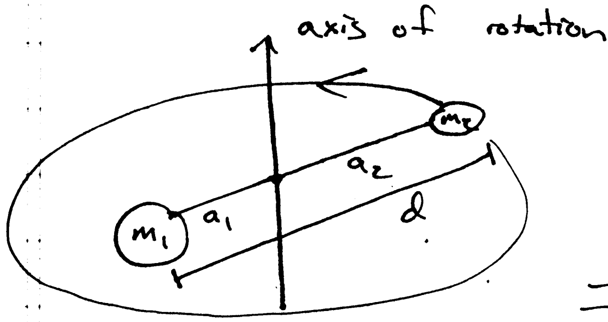
$l=1, m=0$



$l=1, m=-1$

Practical application of angular momentum

Rotational Spectroscopy



The Moment of inertia

$$I = \sum_i m_i a_i^2 \leftarrow$$ square of distance from axis of rotation

If the rotation is around the center of mass:

$$m_1 a_1 = m_2 a_2$$

$$a_2 = \frac{m_1}{m_2} a_1 \qquad\qquad a_1 = \frac{m_2}{m_1} a_2$$

$$* \quad \boxed{a_1 a_2 = \frac{m_1}{m_2} a_1^2 \qquad\qquad a_1 a_2 = \frac{m_2}{m_1} a_2^2}$$

$$I = m_1 a_1^2 + m_2 a_2^2$$

put μ in front

$$= \mu \left(\frac{m_1 (m_1 + m_2)}{m_1 m_2} a_1^2 + \frac{m_2 (m_1 + m_2)}{m_1 m_2} a_2^2 \right)$$

$$= \mu \left(\frac{m_1 + m_2}{m_2} a_1^2 + \frac{m_1 + m_2}{m_1} a_2^2 \right)$$

$$= \mu \left(a_1^2 + \frac{m_1}{m_2} a_1^2 + a_2^2 + \frac{m_2}{m_1} a_2^2 \right)$$

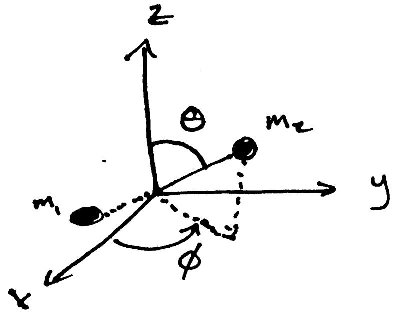
use * above

$$= \mu \left(a_1^2 + a_1 a_2 + a_2^2 + a_1 a_2 \right)$$

$$= \mu \left(a_1^2 + 2 a_1 a_2 + a_2^2 \right) = \mu (a_1 + a_2)^2$$

$$I = \mu d^2 \leftarrow$$ moment of inertia for a diatomic

The rotation can be understood in 3d with spherical coordinates, $(V(r,\theta,\phi) = 0)$



$$\vec{r} = |\vec{r}_1 - \vec{r}_2| = d = \text{fixed}$$

$$\hat{H} = \frac{\hat{p}^2}{2\mu} = \frac{-\hbar^2}{2\mu}\nabla^2$$

$$= \frac{-\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + \frac{L^2}{2\mu r^2}$$

r is held fixed at d, so we can ignore all $\frac{\partial}{\partial r}$ terms in the Hamiltonian

$$\hat{H} = \frac{1}{2\mu d^2}\hat{L}^2 \quad \longleftarrow \text{ rotational } \hat{H} \text{ has only } \hat{L}^2 \text{ as the operator}$$

$$\hat{H}\psi = E\psi$$

$$\frac{1}{2\mu d^2}\hat{L}^2\psi = E\psi$$

$$\hat{L}^2\psi = 2\mu d^2 E\psi$$

but we know what the eigen functions of $\hat{L}^2$ are

(← we (by convention) use J to talk about molecular rotations)

$$\hat{L}\, Y_J^m(\theta,\phi) = \hbar^2 J(J+1)\, Y_J^m(\theta,\phi)$$

$$\therefore \quad \hat{H}\, Y_J^m(\theta,\phi) = \frac{1}{2\mu d^2}\hat{L}^2 Y_J^m(\theta,\phi) = \underbrace{\frac{\hbar^2}{2\mu d^2} J(J+1)}_{E_J}\, Y_J^m(\theta,\phi)$$

$$E_J = \frac{\hbar^2}{2\mu d^2} J(J+1) \quad \longleftarrow \text{ energies don't depend on } m.$$

$$= \frac{\hbar^2}{2I} J(J+1) \quad , \quad J = 0, 1, 2, \ldots$$

- The interesting thing is that each <u>level</u> (J) has a degeneracy of $2J+1$

<u>level</u>	<u>states</u> (all have same E)	<u>degeneracy</u>
$J=0$	$m=0$	1
$J=1$	$m=-1,0,+1$	3
$J=2$	$m=-2,-1,0,+1,+2$	5
$J=3$	$m=-3,-2,-1,0,+1,+2,+3$	7
⋮		

- Also, there's <u>no</u> <u>zero point</u> energy for rotational motion, and energy levels get farther apart as J increases

$E_2 = 3\hbar^2/I$

$E_1 = \hbar^2/I$

$E_0 = 0 \longleftarrow$ we can have non-rotating molecules!

<u>Selection rules</u> for pure rotational transitions

Rotational transitions are typically in the microwave region of the spectrum.

The selection rules are governed by the dipole integral

$$\vec{M} = \langle Y_{J'}^{m'} | \hat{\mu} | Y_J^m \rangle$$

dipole operator

final rotational state

initial rotational state

$$= \int_0^{\pi} \sin\theta \, d\theta \int_0^{2\pi} d\phi \; Y_{J'}^{m'}(\theta,\phi)^* \, \hat{\mu} \, Y_J^m(\theta,\phi)$$

$$\hat{\mu} = \mu_x \hat{\imath} + \mu_y \hat{\jmath} + \mu_z \hat{k} = \mu_0 (\sin\theta\cos\phi\,\hat{\imath} + \sin\theta\sin\phi\,\hat{\jmath} + \cos\theta\,\hat{k})$$

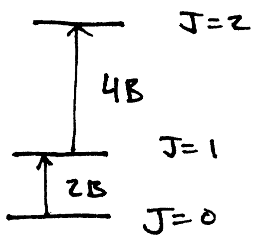
cartesian components of molecular dipole

These integrals are not hard to do, but they are tedious, so what we find, are rules (just like the $\Delta n = \pm 1$ for vibrational motion):

1. Molecule must have a permanent dipole ($\mu_0 \neq 0$)
2. $\Delta J = \pm 1$
3. $\Delta m = 0, \pm 1$

→ These are called the selection rules for rotational spectra.

$$B = \frac{h}{8\pi^2 I} = \underline{\text{rotational}}\ \underline{\text{constant}}$$



$$h\nu = \Delta E = E_{J+1} - E_J$$

$$= \frac{\hbar^2}{2I}\left[(J+1)(J+2) - J(J+1)\right]$$

$$= \frac{h^2}{8\pi^2 I}\left[J^2+3J+2 - J^2 - J\right]$$

$$= \frac{h^2}{8\pi^2 I}\left[2(J+1)\right]$$

$$\therefore \quad \nu = \underbrace{\frac{h}{8\pi^2 I}}_{B}\, 2(J+1) = 2(J+1)B$$

B is usually reported in frequency units [Hz or MHz) or sometimes in cm^{-1}

$$B\,[Hz] = \frac{h}{8\pi^2 I}$$

$$B\,[MHz] = \frac{h}{8\pi^2 I} \times 10^{-6}$$

$$B\,[cm^{-1}] = \frac{h}{8\pi^2 c I}$$

rotational spectra give us structural information:

$$B \rightarrow I \rightarrow d \leftarrow \text{Bond } \underline{\text{length}}$$