

Lecture 18. Introduction to Angular Momentum

Classical examples:

1. Orbital angular momentum

$$L = \mathbf{p} \mathbf{b}$$

\mathbf{b} = impact parameter

\mathbf{p} = linear momentum

$$L = \mu v b$$

2. Rotation in the xy -plane about a point: $\hat{L} = r p \hat{k}$

3. General definition:

$$\vec{L} = \vec{r} \times \vec{p} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} = (y p_z - z p_y) \hat{i} + (z p_x - x p_z) \hat{j} + (x p_y - y p_x) \hat{k} = L_x \hat{i} + L_y \hat{j} + L_z \hat{k}$$

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

Cyclic permutation of $x \rightarrow y \rightarrow z$ results in $L_x \rightarrow L_y \rightarrow L_z$

Quantum mechanical operators:

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

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

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

Commutators:

$$\begin{aligned}
[\hat{L}_x, \hat{L}_y] &= \hat{L}_x \hat{L}_y - \hat{L}_y \hat{L}_x \\
&= (y\hat{p}_z - z\hat{p}_y)(z\hat{p}_x - x\hat{p}_z) - (z\hat{p}_x - x\hat{p}_z)(y\hat{p}_z - z\hat{p}_y) \\
&= y\hat{p}_z z\hat{p}_x - \{y\hat{p}_z x\hat{p}_z + z\hat{p}_y z\hat{p}_x\} + z\hat{p}_y x\hat{p}_z \\
&\quad - z\hat{p}_x y\hat{p}_z + \{z\hat{p}_x z\hat{p}_y + x\hat{p}_z y\hat{p}_z\} - x\hat{p}_z z\hat{p}_y \\
&= y\hat{p}_z z\hat{p}_x + z\hat{p}_y x\hat{p}_z - z\hat{p}_x x\hat{p}_z - x\hat{p}_z z\hat{p}_y \\
&= \hat{p}_z z y \hat{p}_x - z \hat{p}_z y \hat{p}_x + z \hat{p}_z x \hat{p}_y - \hat{p}_z z x \hat{p}_y \\
&= [\hat{p}_z, z] y \hat{p}_x + [z, \hat{p}_z] x \hat{p}_y \\
&= -[z, \hat{p}_z] y \hat{p}_x + [z, \hat{p}_z] x \hat{p}_y \\
&= i\hbar (x \hat{p}_y - y \hat{p}_x) \\
&= i\hbar \hat{L}_z
\end{aligned}$$

Cyclic permutation:

$$[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z \rightarrow [\hat{L}_y, \hat{L}_z] = i\hbar \hat{L}_x \rightarrow [\hat{L}_z, \hat{L}_x] = i\hbar \hat{L}_y$$

What about the squared operators?

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

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

$$\begin{aligned}
[\hat{L}_y^2, \hat{L}_x] &= \hat{L}_y^2 \hat{L}_x - \hat{L}_x \hat{L}_y^2 \\
&= \hat{L}_y^2 \hat{L}_x - \hat{L}_y \hat{L}_x \hat{L}_y + \hat{L}_y \hat{L}_x \hat{L}_y - \hat{L}_x \hat{L}_y^2 \\
&= \hat{L}_y [\hat{L}_y, \hat{L}_x] + [\hat{L}_y, \hat{L}_x] \hat{L}_y \\
&= -i\hbar \hat{L}_y \hat{L}_z - i\hbar \hat{L}_z \hat{L}_y
\end{aligned}$$

Similarly, you can show that

$$[\hat{L}_z^2, \hat{L}_x] = i\hbar \hat{L}_z \hat{L}_y + i\hbar \hat{L}_y \hat{L}_z$$

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

Here is a physical explanation of the incompatibility of all the components of the angular momentum vector. Imagine a particle moving in a circular orbit with angular momentum L . Suppose you knew all three components of the L precisely. For example, suppose L_z has some definite value, and that $L_x = L_y = 0$. In other words, suppose L points along the z -axis precisely. Then the particle is confined to the xy plane. Then you know that z and p_z are both zero. This violates the uncertainty principle.

$$\text{Cyclically: } [\hat{L}^2, L_y] = 0 = [\hat{L}^2, L_z]$$

We choose L^2 and L_z as a compatible pair of observables..

Having determined what are the compatible operators, we now ask what are their eigenfunctions and eigenvalues. That is, we wish to solve the following equations:

$$\begin{aligned}\hat{L}_z Y &= bY \\ \hat{L}^2 Y &= cY\end{aligned}$$

The natural coordinates to use are spherical polar coordinates.

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

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

In these coordinates, the operators become

$$\begin{aligned}\hat{L}_z &= -i\hbar \frac{\partial}{\partial \phi} \\ \hat{L}^2 &= -\hbar^2 \left(\frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right)\end{aligned}$$

Since \hat{L}_z depends only on ϕ , and since Y is an eigenfunction of both \hat{L}_z and \hat{L}^2 , it follows that Y must be separable in θ and ϕ :

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

Normalization:

$$\begin{aligned}\int_0^\pi |S(\theta)|^2 \sin \theta d\theta &= 1 \\ \int_0^{2\pi} |T(\phi)|^2 d\phi &= 1\end{aligned}$$

Boundary conditions:

$$S(\theta) = S(\theta + \pi)$$

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

Eigenfunctions and eigenvalues of \hat{L}_z

$$-i\hbar \frac{dT}{d\phi} = bT(\phi)$$

$$\frac{dT}{T} = ib\hbar d\phi$$

$$T(\phi) = Ae^{ib\phi/\hbar}$$

Boundary condition:

$$Ae^{ib\phi/\hbar} = Ae^{ib(\phi+2\pi)/\hbar}$$

$$1 = e^{2i\pi b/\hbar}$$

But $e^{2i\pi} = 1 \Rightarrow b/\hbar = m$, where $m=0$ or an integer.

$$T(\phi) = Ae^{im\phi}$$

$$\hat{L}T(\phi) = m\hbar T(\phi)$$

Normalization:

$$\int_0^{2\pi} |T_m(\phi)|^2 d\phi = 1$$

$$2\pi|A|^2 = 1$$

$$|A| = \frac{1}{\sqrt{2\pi}}$$

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

All ϕ values are equally probable.

Orthogonality:

$$\int_0^{2\pi} T_m(\phi)T_n(\phi)d\phi = \delta_{mn}$$

Eigenfunctions and eigenvalues of \hat{L}^2

$$\begin{aligned}\hat{L}^2 ST &= cST \\ \hat{L}^2 e^{im\phi} S(\theta) &= ce^{im\phi} S(\theta) \\ &= -\hbar^2 \left(\frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right) S(\theta) e^{im\phi} \\ &= -\hbar^2 \left(S'' + \cot \theta S' - \frac{m^2}{\sin^2 \theta} S \right)\end{aligned}$$

Canceling out the ϕ dependence (which is separable!), we get the equation

$$S'' + \cot \theta S' - \frac{m^2}{\sin^2 \theta} S = -\frac{c}{\hbar^2} S$$

Transformation of variable:

$$\begin{aligned}x &\equiv w \equiv \cos \theta, \\ -1 &\leq w \leq 1 \\ G(w) &= S(\theta) \\ dw &= -\sin \theta d\theta\end{aligned}$$

After expressing the first and second derivatives of S in terms of the derivatives of G, we readily get

$$(1-w^2)G'' - 2wG' + \left[\frac{c}{\hbar^2} - \frac{m^2}{1-w^2} \right] G = 0.$$

This equation is identical to the associated Legendre equation if we make the identification

$$c = l(l+1)\hbar^2,$$

where l is zero or a positive integer.

Show that is a Sturm-Liouville equation. Its solutions are the associated Legendre polynomials,

$$S_{l,m}(\theta) = \left[\left(\frac{2l+1}{2} \right) \frac{(l-|m|)!}{(l+|m|)!} \right]^{1/2} P_l^{|m|}(\cos \theta)$$

Orthogonality:

$$\int_0^\pi S_l^m(\theta) S_k^m(\theta) \sin \theta d\theta = \int_{-1}^1 G_l^m(x) G_k^m(x) dx = \delta_{kl}$$

Note what this condition does *not* say.

Generating functions:

$$P_l(x) = \frac{1}{2^l l!} \frac{d^l}{dx^l} (x^2 - 1)^l$$

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

Recursion relations:

$$(2l+1)P_l(x) = \frac{d}{dx} (P_{l+1} - P_{l-1})$$

$$(l+1)P_l(x) = \frac{dP_{l+1}}{dx} - x \frac{dP_l}{dx}$$

$$xP_l^{|m|}(x) = \cos \theta P_l^{|m|}(\cos \theta) = \frac{1}{2l+1} \{ (l-|m|+1)P_{l+1}^{|m|} + (l+|m|)P_{l-1}^{|m|} \}$$

$$\sqrt{1-x^2} P_l^{|m|}(x) = \sin \theta P_l^{|m|}(\cos \theta)$$

$$= \frac{1}{2l+1} \{ P_{l+1}^{|m|+1} + P_{l-1}^{|m|} \} = \frac{1}{2l+1} \{ (l+|m|)(l+|m|-1)P_{l-1}^{|m|-1} - (l-|m|)(l-|m|+2)P_{l+1}^{|m|-1} \}$$

Lecture 19. Model Problems Involving Angular Momentum

Particle on a Ring

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

$$\hat{H} = \frac{\hat{L}_z^2}{2\mu R^2} = \frac{\hat{L}_z^2}{2I} = -\frac{\hbar^2}{2I} \frac{d^2}{d\phi^2}$$

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

$$\hat{H}T_m = \frac{m^2\hbar^2}{2I} T_m$$

$$E_m = \frac{m^2\hbar^2}{2I}$$

There is no zero-point energy. Levels are spaced quadratically and are two-fold degenerate (except for $m = 0$).

Free Rotor

In this case we must use the full three-dimensional angular momentum.

$$\hat{H} = \frac{\hat{L}^2}{2I}$$

$$Y_{lm}(\theta, \phi) = S_{l,|m|}(\theta, \phi) T_m(\phi) \propto Y_{l,|m|}(\theta, \phi) e^{im\phi}$$

$$\hat{H}Y_{lm} = \frac{l(l+1)\hbar^2}{2I} Y_{lm}$$

In dealing with rotation, it is conventional to label the quantum number by J rather than l .

The energy levels are again spaced quadratically, and here the degeneracy is $2J+1$.

The length of the J vector is given by $\sqrt{J(J+1)}\hbar$. For large J ,

$$\sqrt{J(J+1)} = J \sqrt{1 + \frac{1}{J}} \approx J \left(1 + \frac{1}{2J} \right) = J + \frac{1}{2}$$

The angle between the angular momentum vector and the z-axis is given by

$$\cos\alpha = \frac{M_J}{\sqrt{J(J+1)}}$$

The same formulism describes a particle confined to move on the surface of a sphere.

What are the expectation values of the components of \vec{J} ?

We already know that $\langle J_z \rangle = M_J \hbar$. This means that $\langle J_z^2 \rangle = M_J^2 \hbar^2$. It follows that

$$\langle J_x^2 + J_y^2 \rangle = [J(J+1) - M_J^2] \hbar^2$$

By symmetry $\langle J_x^2 \rangle = \langle J_y^2 \rangle$

Later we will prove that $\langle J_x \rangle = \langle J_y \rangle = 0$.

It follows that the polar angle of \vec{J} is completely unknown. This leads to a physical picture of the \vec{J} vector precessing about the z-axis at an angle of inclination equal to α .

Physical picture of the rotor:

1. Suppose $M_J = J$. This means that J is roughly parallel to the z-axis, and the molecule rotates in the xy-plane. The azimuthal angle of \vec{J} is given by

$$\cos \alpha = \frac{M_J}{J} = \frac{J}{J} = 1$$

For $J=1$, $Y_{11} \propto \sin \theta$, $\alpha = 45^\circ$, and the probability density is concentrated near the equator. The same picture applies for $M_J = -J$, except that the molecule rotates in the opposite direction. The probability distribution is given by

$$p(\theta)d\theta = |Y_{JM}(\theta, \phi)|^2 \sin \theta d\theta \propto \sin^3 \theta$$

The most probable θ is given by

$$\frac{dp}{d\theta} \propto \sin^2 \theta \cos \theta = 0 \Rightarrow \theta = \pi/2$$

2. Suppose $M_J = 0$. In this case, J lies in the xy-plane, $\alpha = 0$, and the molecule rotates in a plane containing the z axis. This plane precesses about the z-axis because the direction of J in the xy plane is completely unknown. For $J=1$, $Y_{10} \propto \cos \theta$, and the probability density is concentrated near the poles.

$$p(\theta)d\theta = |Y_{JM}(\theta, \phi)|^2 \sin \theta d\theta \propto \cos^2 \theta \sin \theta$$

The most probable θ is given by

$$\frac{dp}{d\theta} \propto \cos^3 \theta - 2 \sin^2 \theta \cos \theta = 0$$

$$\tan^2 \theta = 1/2 \Rightarrow \theta = 35.3^\circ$$

Note that the angle of the greatest probability density is not necessarily the most probable angle. This is where the Jacobian is crucial.

Practical considerations for a rotating linear molecule:

The energy levels are given by $E_J = \frac{J(J+1)\hbar^2}{2\mu R^2} = hcBJ(J+1)$, where B is called the rotational constant and has the units of wave numbers.

Statistical mixtures: The Boltzmann population is given as usual by

$$P_J = \frac{g_J e^{-E_J/kT}}{\sum_J g_J e^{-E_J/kT}}$$

where the degeneracy is $g_J = 2J + 1$.

The denominator is called a partition function and has the value

$$Q = \sum_J (2J+1) e^{-hcBJ(J+1)/kT} \approx \int_0^\infty e^{-hcBJ(J+1)/kT} (2J+1) dJ = \frac{kT}{hcB}$$

The population of level J is therefore

$$P_J \approx \frac{hcB}{kT} (2J+1) e^{-hcBJ(J+1)/kT}$$

The most probable J is calculated by taking the maximum of P_J :

$$\begin{aligned} \frac{dP_J}{dJ} &= 0 \\ 2 - \frac{hcB}{kT} (2J_m + 1)^2 &= 0 \\ J_m &= \sqrt{\frac{kT}{2hcB}} - \frac{1}{2} \end{aligned}$$

Remember that kT at 300 K is 208 cm^{-1} . Here are some examples at 300 K:

Molecule	B(cm ⁻¹)	P ₀	J _m	P _{J_m}
H ₂	60.8	0.29	1	0.49
I ₂	0.037	0.00018	53	0.011

We can also describe a rotational wave packet and pendular states.

$$\psi(\theta, \phi, t) = \sum_J c_J Y_{J, M_J}(\theta, \phi) e^{-E_J t / \hbar}$$

Prove that the (full) revival time of such a wave packet is given by $\frac{1}{2Bc}$

Alignment.

We define the alignment of a molecule by

$$A = \langle \cos^2 \theta \rangle = \int_0^\pi \int_0^{2\pi} Y_{JM}^*(\theta, \phi) \cos^2 \theta Y_{JM}(\theta, \phi) \sin \theta d\theta d\phi$$

If you don't remember the normalization constant, you can work it out at the same time:

$$A = \frac{\int_0^\pi |P_J^M(\cos \theta)|^2 \cos^2 \theta \sin \theta d\theta}{\int_0^\pi |P_J^M(\cos \theta)|^2 \sin \theta d\theta} = \frac{\int_{-1}^1 |P_J^M(x)| x^2 dx}{\int_{-1}^1 |P_J^M(x)|^2 dx}$$

J=1, M=0

$$A = \frac{\int_{-1}^1 x^4 dx}{\int_{-1}^1 x^2 dx} = \frac{2/5}{2/3} = 3/5$$

J=1, M=1, -1

$$A = \frac{\int_{-1}^1 (1-x^2)x^2 dx}{\int_{-1}^1 (1-x^2) dx} = \frac{2/3 - 2/5}{2 - 2/3} = 1/5$$

$$A = \left(\frac{1}{3}\right)\left(\frac{3}{5}\right) + \left(\frac{2}{3}\right)\left(\frac{1}{5}\right) = \frac{1}{3}$$

Lecture 20. Ladder Operators

Definition of the ladder operators:

$$\begin{aligned}\hat{L}_+ &= \hat{L}_x + i\hat{L}_y \\ \hat{L}_- &= \hat{L}_x - i\hat{L}_y\end{aligned}$$

Commutation properties:

$$\hat{L}_+\hat{L}_- = (\hat{L}_x + i\hat{L}_y)(\hat{L}_x - i\hat{L}_y) = \hat{L}_x^2 + \hat{L}_y^2 + i(\hat{L}_y\hat{L}_x - \hat{L}_x\hat{L}_y) = \hat{L}_x^2 + \hat{L}_y^2 - i[\hat{L}_x, \hat{L}_y] = \hat{L}_x^2 + \hat{L}_y^2 + \hbar\hat{L}_z = \hat{L}^2 - \hat{L}_z^2 + \hbar\hat{L}_z$$

Prove the following:

$$\begin{aligned}[\hat{L}_+, \hat{L}_-] &= 2\hbar\hat{L}_z \\ [\hat{L}_z, \hat{L}_\pm] &= \hbar\hat{L}_\pm \\ [\hat{L}^2, \hat{L}_\pm] &= 0\end{aligned}$$

Suppose that the following are true:

$$\begin{aligned}\hat{L}_z Y &= bY \\ \hat{L}^2 Y &= cY\end{aligned}$$

Question: Is $\hat{L}_+ Y$ also an eigenfunction of \hat{L}_z and \hat{L}^2 ? Find out by operating on the function:

$$\begin{aligned}\hat{L}_z(\hat{L}_+ Y) &= (b + \hbar)(\hat{L}_+ Y) \\ \hat{L}^2(\hat{L}_+ Y) &= c(\hat{L}_+ Y)\end{aligned}$$

The first result follows from the commutator property, $\hat{L}_z\hat{L}_+ = \hat{L}_+\hat{L}_z + \hbar\hat{L}_+$.

Conclusion: It is indeed an eigenfunction of both, with the same eigenvalue of \hat{L}^2 but with an eigenvalue of \hat{L}_z that is increased by \hbar . That is why \hat{L}_+ is called a raising operator.

By induction we deduce that

$$\begin{aligned}\hat{L}_z(\hat{L}_+^n Y) &= (b + n\hbar)(\hat{L}_+^n Y) \\ \hat{L}^2(\hat{L}_+^n Y) &= c(\hat{L}_+^n Y)\end{aligned}$$

We can also prove that \hat{L}_- is a lowering operator. Prove the following:

$$\begin{aligned}\hat{L}_z(\hat{L}_-Y) &= (b - \hbar)(\hat{L}_+Y) \\ \hat{L}^2(\hat{L}_-Y) &= c(\hat{L}_-Y)\end{aligned}$$

And by induction:

$$\begin{aligned}\hat{L}_z(\hat{L}_-^n Y) &= (b - n\hbar)(\hat{L}_-^n Y) \\ \hat{L}^2(\hat{L}_-^n Y) &= c(\hat{L}_-^n Y)\end{aligned}$$

Question: Is there any bound on n?

$$\hat{L}_z^2(\hat{L}_\pm Y) = \hat{L}_z[\hat{L}_z(\hat{L}_\pm Y)] = \hat{L}_z[(b \pm \hbar)\hat{L}_\pm Y] = (b \pm \hbar)^2 \hat{L}_\pm Y$$

By induction:

$$\hat{L}_z^2(\hat{L}_\pm^n Y) = (b \pm n\hbar)^2 \hat{L}_\pm^n Y$$

But $\langle \hat{L}_z^2 \rangle \leq \langle \hat{L}^2 \rangle$. Therefore, $(b \pm n\hbar)^2 \leq c$.

We conclude that

$$b_{\max} \leq \sqrt{c} \quad \text{with eigenfunction } Y_{\max}$$

$$b_{\min} \geq -\sqrt{c} \quad \text{with eigenfunction } Y_{\min}$$

That is,

$$\hat{L}_+ Y_{\max} = 0$$

$$\hat{L}_- Y_{\min} = 0$$

The reason is that

$$\hat{L}_z(\hat{L}_+ Y_{\max}) = (b_{\max} + \hbar)(\hat{L}_+ Y_{\max})$$

But this cannot be true unless one of the factors is zero.

It therefore follows that $\hat{L}_- \hat{L}_+ Y_{\max} = 0$.

But we already know that $\hat{L}_- \hat{L}_+ Y = (\hat{L}^2 - \hat{L}_z^2 - \hbar \hat{L}_z)Y$

It follows that

$$\begin{aligned}(c - b_{\max}^2 - \hbar b_{\max}) Y_{\max} &= 0 \\ c - b_{\max}^2 - \hbar b_{\max} &= 0 \\ c &= b_{\max}^2 + \hbar b_{\max}\end{aligned}$$

Similarly,

$$\hat{L}_+ \hat{L}_- Y_{\min} = 0 \Rightarrow c = b_{\min}^2 - \hbar b_{\min}$$

Therefore

$$b_{\max}^2 + \hbar b_{\max} = b_{\min}^2 - \hbar b_{\min}$$

Solving the quadratic equation for b_{\max} gives

$$\begin{aligned}b_{\max} &= \frac{1}{2}[-\hbar \pm (\hbar - 2b_{\min})] \\ &= -b_{\min} \text{ or } b_{\min} - \hbar\end{aligned}$$

We reject the second solution because we know that $b_{\max} > b_{\min}$. Therefore $b_{\max} = -b_{\min}$

Now suppose that we apply the lowering operator N times:

$$Y_{\min} \propto \hat{L}_-^N Y_{\max} \Rightarrow b_{\max} - b_{\min} = N\hbar$$

Combining these two results gives $b_{\min} = -N\hbar/2$ and $b_{\max} = N\hbar/2$

Setting $l = N/2$ gives $b_{\max} = l\hbar$ and $b_{\min} = -l\hbar$, where J is an integer or half integer.

We also conclude that $c = b_{\max}^2 + \hbar b_{\max} = l(l+1)\hbar^2$.

What are the expectation values of \hat{L}_x and \hat{L}_y ? From the definitions of \hat{L}_+ and \hat{L}_- we readily show that

$$\begin{aligned}\hat{L}_x &= \frac{1}{2}(\hat{L}_+ + \hat{L}_-) \\ \hat{L}_y &= \frac{1}{2i}(\hat{L}_+ - \hat{L}_-)\end{aligned}$$

But $\langle lm | \hat{L}_{\pm} | lm \rangle \propto \langle lm | l, m \pm 1 \rangle = 0 \Rightarrow \langle \hat{L}_x \rangle = \langle \hat{L}_y \rangle = 0$.

What are the expectation values of \hat{L}_x^2 and \hat{L}_y^2 ?

$$\begin{aligned}\hat{L}_x^2 &= \frac{1}{4}(\hat{L}_+ + \hat{L}_-)(\hat{L}_+ + \hat{L}_-) = \frac{1}{4}(\hat{L}_+^2 + \hat{L}_-^2 + \hat{L}_+ \hat{L}_- + \hat{L}_- \hat{L}_+) = \frac{1}{4}\hat{L}_+^2 + \frac{1}{4}\hat{L}_-^2 + \frac{1}{4}(\hat{L}^2 - \hat{L}_z^2 + \hbar\hat{L}_z) + \frac{1}{4}(\hat{L}^2 - \hat{L}_z^2 - \hbar\hat{L}_z) \\ &= \frac{1}{4}\hat{L}_+^2 + \frac{1}{4}\hat{L}_-^2 + \frac{1}{2}(\hat{L}^2 - \hat{L}_z^2)\end{aligned}$$

It follows that

$$\langle \hat{L}_x^2 \rangle = \frac{1}{2}\langle \hat{L}^2 \rangle - \frac{1}{2}\langle \hat{L}_z^2 \rangle = \frac{1}{2}\hbar^2[l(l+1) - m^2] = \langle \hat{L}_y^2 \rangle$$

Now let's solve for the eigenfunctions. We start by invoking separability in θ and ϕ :

$$Y_{ll}(\theta, \phi) = \frac{1}{\sqrt{2\pi}} e^{il\phi} S_{ll}(\theta)$$

The equation we wish to solve is

$$\hat{L}_+ Y_{ll} = 0.$$

Using the transformation from Cartesian to polar coordinates, you can show that

$$\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y = \hbar e^{\pm i\phi} \left(\frac{\partial}{\partial \theta} \pm i \cot \theta \frac{\partial}{\partial \phi} \right)$$

Our equation is therefore

$$\begin{aligned}e^{il\phi} S'_{ll} + i \cot \theta S_{ll} (ile^{il\phi}) &= 0 \\ S'_{ll} &= l \cot \theta S_{ll}\end{aligned}$$

You can verify that the solution is

$$S_{ll}(\theta) = C_{ll} \sin^l \theta$$

Proof: $\frac{d}{d\theta}(\sin^l \theta) = l(\sin^{l-1} \theta) \cos \theta = l \cot \theta \sin^l \theta$

You can work out the normalization and get

$$Y_{ll}(\theta, \phi) = \frac{1}{\sqrt{2\pi}} e^{il\phi} (-1)^l \sqrt{\frac{(2l+1)!}{2}} \frac{1}{2^l l!} \sin^l \theta$$

Finally, we can apply the lowering operator to get all the other eigenfunctions:

$$Y_{lm} = C_{lm} \hat{L}_-^{l-m} Y_{ll} = C_{lm} \left[-\hbar e^{-i\phi} \left(\frac{\partial}{\partial \theta} - i \cot \theta \frac{\partial}{\partial \phi} \right) \right]^{l-m} Y_{ll}$$

What are the coefficients? Let

$$\hat{L}_+ |lm\rangle = C_+ |l, m+1\rangle$$

When we learn about Hermitian operators, we will be able to show that

$$\langle lm | \hat{L}_- = \langle l, m+1 | C_+^*$$

It follows that

$$\langle lm | \hat{L}_- \hat{L}_+ |lm\rangle = \langle l, m+1 | C_+^* C_+ |l, m+1\rangle = |C_+|^2$$

But

$$\hat{L}_- \hat{L}_+ = \hat{L}^2 - \hat{L}_z^2 - \hat{L}_z \hbar$$

Therefore

$$\langle lm | \hat{L}^2 - \hat{L}_z^2 - \hat{L}_z \hbar |lm\rangle = [l(l+1) + m^2 - m] \hbar^2$$

By sign (and phase convention),

$$C_+ = [l(l+1) - m(m+1)]^{1/2} \hbar$$

Similarly,

$$C_- = [l(l+1) - m(m-1)]^{1/2} \hbar$$