Orbital Angular Momentum in Three Dimensions

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The Angular Momentum Operators in Spherical Polar Coordinates

The angular momentum operator $\vec{L} = \vec{r} \times \vec{p} = -i\hbar \vec{r} \times \vec{\nabla}$.

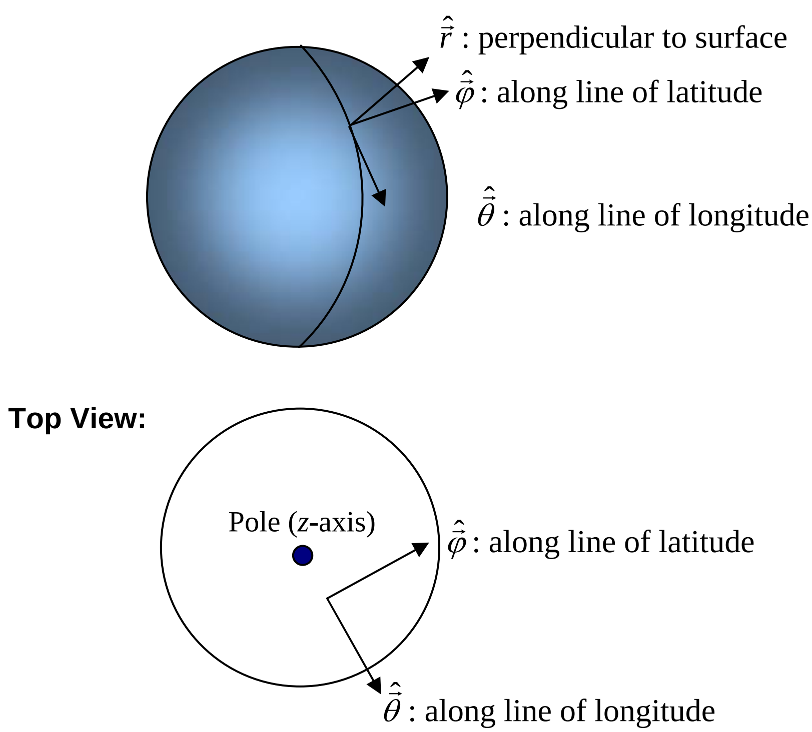
In spherical polar coordinates,

$$\begin{aligned} x &= r\sin\theta\cos\phi \\ y &= r\sin\theta\sin\phi \\ z &= r\cos\theta \\ ds^2 &= dr^2 + r^2 d\theta^2 + r^2\sin^2\theta d\phi^2 \end{aligned}$$

the gradient operator is

$$\vec{\nabla} = \hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial \theta} + \hat{\phi}\frac{1}{r\sin\theta}\frac{\partial}{\partial \phi}$$

where now *the little hats denote unit vectors*: $\hat{r}$ is radially outwards, $\hat{\theta}$ points along a line of longitude away from the north pole (and therefore in the direction of increasing θ) and $\hat{\phi}$ points along a line of latitude in an anticlockwise direction as seen looking down on the north pole (that is, in the direction of increasing ϕ).



The three unit vectors in the spherical polar system

Here $\hat{r},\ \hat{\theta},\ \hat{\phi}$ form an orthonormal local basis, and

$$\hat{r}\times\hat{\theta}=\hat{\phi},\quad \hat{r}\times\hat{\phi}=-\hat{\theta}\,,$$

as should be clear from the diagram.

So

$$\vec{r}\times\vec{\nabla}=\hat{\phi}\frac{\partial}{\partial\theta}-\hat{\theta}\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}\,.$$

(Explicitly, $\hat{\phi}=\left(-\sin\phi,\cos\phi,0\right)$ and $\hat{\theta}=\left(\cos\theta\cos\phi,\cos\theta\sin\phi,-\sin\theta\right)$.)

The vector $\hat{\phi}$ has zero component in the *z*-direction, the vector $\hat{\theta}$ has component $-\sin\theta$ in the *z*-direction, so we can immediately conclude that

$$L_z=\left(\vec{r}\times\vec{p}\right)_z=-\left(i\hbar\vec{r}\times\vec{\nabla}\right)_z=-i\hbar\frac{\partial}{\partial\phi}$$

just as in the two-dimensional case.

The operator

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

To evaluate this expression, we use $\hat{\phi}^2=1,\quad \hat{\theta}^2=1,\quad \hat{\phi}\cdot\hat{\theta}=0$ *but* we must also check the effects of the differential operators in the first expression on the variables in the second, *including the unit vectors*.

From the explicit coordinate expressions for the unit vectors, or by staring at the diagram, you should be able to establish the following: $\partial\hat{\phi}/\partial\theta=0,\quad \partial\hat{\theta}/\partial\theta$ is in the *r*-direction, $\partial\hat{\phi}/\partial\phi$ is a horizontal unit vector pointing inwards perpendicular to $\hat{\phi}$, and having component $-\cos\theta$ in the $\hat{\theta}$-direction, $\partial\hat{\theta}/\partial\phi=\hat{\phi}\cos\theta$.

Therefore, the *only* "differentiation of a unit vector" term that contributes to L^2 is $\hbar^2\hat{\theta}\frac{1}{\sin\theta}\cdot\frac{\partial\hat{\phi}}{\partial\phi}\frac{\partial}{\partial\theta}=-\hbar^2\cot\theta\frac{\partial}{\partial\theta}$. The $\hat{\phi}\frac{\partial}{\partial\theta}$ acting on the $\sin\theta$ in $-\hat{\theta}\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}$ contributes nothing because $\hat{\phi}\cdot\hat{\theta}=0$.

Hence

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

Now, we know that L^2 and L_z have a common set of eigenkets (since they commute) and we've already established that those of L_z are $\Phi_m(\phi) = e^{im\phi}/\sqrt{2\pi}$, with m an integer, so the eigenkets of L^2 must have this same ϕ dependence, so they must be of the form $\Theta_l^m(\theta)\Phi(\phi)$, where $\Theta_l^m(\theta)$ is a (suitably normalized) solution of the equation

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\sin\theta\frac{d\Theta_l^m(\theta)}{d\theta} - \frac{m^2}{\sin^2\theta}\Theta_l^m(\theta) = -l(l+1)\Theta_l^m(\theta)$$

more conveniently written

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

To summarize: the solutions to this differential equation, with integer $l, m, |m| \le l,$ will (together with $\Phi_m(\phi)$) give the complete set of eigenstates of L^2, L_z in the coordinate representation.

Finding the *m* = *l* Eigenket of L^2, L_z

Recall now that for the simple harmonic oscillator, the easiest wave function to find was that of the ground state, the solution of the simple *linear* equation $\hat{a}\psi_0 = 0$ (as well as being a solution of the quadratic Schrödinger equation, of course). The other state wave functions could then be found by applying the creation operator in differential form the necessary number of times.

A similar strategy works here: we can easily find the *highest* state on the *l* ladder, $m = l$, the state $|l,l\rangle$, since it satisfies the linear equation $L_+|l,l\rangle = 0,$ where $L_+ = L_x + iL_y$. We just need to cast this equation in coordinate form. In Cartesian coordinates, $L_+ = -i\hbar\left(\hat{r}\times\vec{\nabla}\right)_+$, and we've already shown that $\vec{r}\times\vec{\nabla} = \hat{\phi}\frac{\partial}{\partial\theta} - \hat{\theta}\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}$.

Therefore

$$\left(\vec{r}\times\vec{\nabla}\right)_+ = \hat{\phi}_+\frac{\partial}{\partial\theta} - \hat{\theta}_+\frac{1}{\sin\theta}\frac{\partial}{\partial\phi},$$

and using $\hat{\phi} = (-\sin\phi, \cos\phi, 0)$, $\hat{\theta} = (\cos\theta\cos\phi, \cos\theta\sin\phi, -\sin\theta)$ we see that $\hat{\phi}_+$, the component of $\hat{\phi}$ in the + direction, is $\hat{\phi}_+ = \hat{\phi}_x + i\hat{\phi}_y = ie^{i\phi}$, and similarly $\hat{\theta}_+ = \cos\theta e^{i\phi}$.

So

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

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

and $L_+|l,l\rangle = 0$ becomes

$$\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right)\Theta_l^l(\theta)e^{il\phi} = 0.$$

That is,

$$\left(\frac{d}{d\theta} - l\cot\theta\right)\Theta_l^l(\theta) = 0.$$

The solution to this equation is

$$\Theta_l^l(\theta) = N(\sin\theta)^l$$

where N is the normalization constant. The $m \neq l$ wave functions are generated by applying the lowering operator L_-.

Normalizing the $m = l$ Eigenket

The standard notation for the normalized eigenkets $|l,m\rangle$ is $Y_l^m(\theta,\phi) = \Theta_l^m(\theta)\Phi_m(\phi)$. These functions, being eigenkets of Hermitian operators with different eigenvalues, must satisfy

$$\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi} Y_{l'}^{m'*}(\theta,\phi)Y_l^m(\theta,\phi)\sin\theta d\theta d\phi = \int Y_{l'}^{m'*}(\theta,\phi)Y_l^m(\theta,\phi)d\Omega = \delta_{l'l}\delta_{m'm}.$$

So, our first job is to normalize $\Theta_l^l(\theta) = N(\sin\theta)^l$ (taking $\Phi_l(\phi) = e^{il\phi}/\sqrt{2\pi}$ already normalized)

$$|N|^2\int_0^{\pi}(\sin\theta)^{2l+1}d\theta = 1$$

The integral can be evaluated using the substitution $\mu = \cos\theta$ to give $\int_{-1}^{1}(1-\mu^2)^l d\mu$, then making the further substitution $u = \frac{1}{2}(1-\mu)$ to give $2^{2l+1}\int_0^1 u^l(1-u)^l du$, which can be integrated by parts to give

$$|N|^2 \, 2^{2l+1} (l!)^2 / (2l+1)! = 1 .$$

Therefore

$$Y_l^l(\theta,\phi) = (-1)^l \left(\frac{(2l+1)!}{4\pi} \right)^{1/2} \frac{1}{2^l l!} (\sin\theta)^l e^{il\phi} = c_l (\sin\theta)^l e^{il\phi}$$

where we have fixed the sign in accord with the standard convention, and we will denote the rather cumbersome normalization constant by c_l.

Notice that for large values of l, this function is heavily weighted around the equator, as we would expect—for a given total angular momentum one gets a maximum component in the z-direction when the motion is concentrated in the x, y plane. This looks like a Bohr orbit.

Finding the Rest of the Eigenkets: the Details

Now that $|l,l\rangle$ is normalized, we can automatically produce correctly normalized $|l,m\rangle$'s, since we know the matrix element of the lowering operator between normalized states. We don't have to do any more integrals.

For example, $L_-|l,l\rangle = \hbar\sqrt{2l}\,|l,l-1\rangle$, equivalently (the $\hbar$'s of course cancel)

$$Y_l^{l-1}(\theta,\phi) = \frac{(-1)}{\sqrt{2l}} e^{-i\phi} \left(\frac{\partial}{\partial\theta} - i\cot\theta \frac{\partial}{\partial\phi} \right) Y_l^l .$$

That is,

$$\begin{aligned} Y_l^{l-1}(\theta,\phi) &= c_l e^{-i\phi} \left(\frac{\partial}{\partial\theta} - i\cot\theta \frac{\partial}{\partial\phi} \right) \sin^l\theta \cdot e^{il\phi} \\ &= -c_l e^{i(l-1)\phi} \sqrt{2l} \sin^{l-1}\theta \cos\theta \end{aligned}$$

(both terms giving equal contributions).

Note that this function is actually *zero* on the equator, but for large l it peaks close to the equator (on both sides).

In principle, we can reapply this differential operator over and over to generate all the $|l,m\rangle$ states, but this gets very messy. However, there is a neat theorem concerning the lowering operator that makes it all straightforward:

$$L_- e^{im\phi} f(\theta) = e^{i(m-1)\phi} \left(\sin^{1-m}\theta \frac{d}{d(\cos\theta)} \sin^m\theta \right) f(\theta)$$

Exercise: prove this.

So

$$L_- e^{il\phi}\sin^l\theta = e^{i(l-1)\phi}\left(\sin^{1-l}\theta\frac{d}{d(\cos\theta)}\sin^l\theta\right)\sin^l(\theta)$$

and applying the operator again,

$$\begin{aligned}(L_-)^2 e^{il\phi}\sin^l\theta &= L_- e^{i(l-1)\phi}\left(\sin^{1-l}\theta\frac{d}{d(\cos\theta)}\sin^l\theta\right)\sin^l(\theta)\\ &= e^{i(l-2)\phi}\left(\sin^{2-l}\theta\frac{d}{d(\cos\theta)}\sin^{l-1}\theta\right)\cdot\left(\sin^{1-l}\theta\frac{d}{d(\cos\theta)}\sin^l\theta\right)\sin^l(\theta)\\ &= e^{i(l-2)\phi}\left(\sin^{2-l}\theta\frac{d^2}{d^2(\cos\theta)}\sin^l\theta\right)\sin^l(\theta).\end{aligned}$$

So the point of introducing this odd-looking representation of the lowering operator is that the $\sin^{1-l}\theta$ term in the middle is exactly *canceled* when the operator is applies twice, and similar cancellations occur on repeating the operation, giving the (relatively) simple representation:

$$Y_l^m(\theta,\phi) = c_l\sqrt{\frac{(l+m)!}{(2l)!(l-m)!}}e^{im\phi}\sin^{-m}\theta\frac{d^{l-m}}{d(\cos\theta)^{l-m}}\sin^{2l}\theta$$

(Where did all those factorials come from? They're the product of all the inverse square root factors in $|l,m-1\rangle = \frac{1}{\sqrt{(l+m)(l-m+1)}}L_-|l,m\rangle$ for the number of lowerings necessary.)

Note that for $m = 0$ the function is

$$Y_l^0(\theta,\phi) = c_l\sqrt{\frac{1}{(2l)!}}\frac{d^l}{d(\cos\theta)^l}\sin^{2l}\theta,$$

and in fact not a function of ϕ at all. This isn't surprising, since it has zero angular momentum about the *z*-direction, the appropriate $\Phi(\phi)$ is just constant.

For $m = -l$, the differentiation becomes trivial, because, writing $\cos\theta = \mu$, the differentiation becomes $\frac{d^{2l}}{d\mu^{2l}}(1-\mu^2)^l$ and only the μ^{2l} term survives, giving

$$Y_l^{-l}(\theta,\phi) = (-1)^l c_l e^{-il\phi} \sin^l \theta .$$

Of course, this could also have been found from the linear equation $L_-|l,-l\rangle = 0$, and we could have equally generated all the states by applying L_+ to this state. In fact, this gives a different—but of course equivalent—expression for the $Y_l^m(\theta,\phi)$:

$$Y_l^m(\theta,\phi) = (-1)^m c_l \sqrt{\frac{(l-m)!}{(2l)!(l+m)!}} e^{im\phi} \sin^m \theta \frac{d^{l+m}}{d(\cos\theta)^{l+m}} \sin^{2l} \theta$$

(from Messiah, page 522).

Relating the Y_l^m's to the Legendre Functions

The *Legendre polynomials* $P_n(\cos\theta)$ are defined by:

$$P_n(\cos\theta) = \frac{1}{2^n n!} \frac{d^n}{d(\cos\theta)^n} \sin^{2n} \theta, \quad \text{or}$$

$$P_n(\mu) = \frac{1}{2^n n!} \frac{d^n}{d\mu^n} (1-\mu^2)^n$$

where $\mu = \cos\theta$, so $d\mu = -\sin\theta d\theta$. From this form, it is easy to show that $P_n(1) = 1$ (all n differentiations must take out a $(1-\mu^2)$ factor to give a nonzero contribution), and $P_n(\mu)$ must have n zeros in the interval (−1, 1). $P_n(\mu)$ alternates between an even function and an odd function.

The normalization of the $P_n(\mu)$'s is

$$\int_{-1}^{1} (P_n(\mu))^2 d\mu = \left(\frac{1}{2^n n!}\right)^2 \int_{-1}^{1} \frac{d^n}{d\mu^n}(\mu^2-1)^n \frac{d^n}{d\mu^n}(\mu^2-1)^n d\mu$$

$$= (-1)^n \left(\frac{1}{2^n n!}\right)^2 \int_{-1}^{1} (\mu^2-1)^n \frac{d^{2n}}{d\mu^{2n}}(\mu^2-1)^n d\mu$$

$$= (2n)! \left(\frac{1}{2^n n!}\right)^2 \int_{-1}^{1} (\mu^2-1)^n d\mu$$

$$= \frac{2}{2n+1}$$

where in that last line we used the result for the integral obtained earlier in this lecture for normalizing Y_l^l.

Doing the same repeated integration by parts for two different Legendre polynomials proves they are orthogonal,

$$\int_{-1}^{1} P_m(\mu) P_n(\mu)\, d\mu = 0, \quad m \neq n.$$

The *associated Legendre functions* are defined (for *n* and *m* zero or positive integers, $n \geq m$) by:

$$\begin{aligned} P_n^m(\mu) &= \left(1-\mu^2\right)^{m/2} \frac{d^m}{d\mu^m} P_n(\mu) \\ &= (-1)^n \frac{\left(1-\mu^2\right)^{m/2}}{2^n n!} \frac{d^{n+m}}{d\mu^{n+m}} \left(1-\mu^2\right)^n. \end{aligned}$$

Following Messiah in requiring $Y_l^0(0,0)$ be real and positive, we find

$$Y_l^0(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta)$$

where the coefficient just reflects the differing normalization conventions. Similarly, the spherical harmonics with nonzero *m* are proportional to the associated Legendre functions (the odd ones are *not* polynomials in $\cos\theta$, despite Shankar p. 337, since they include odd powers of $\sin\theta$),

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

The Spherical Harmonics as a Basis

We have found explicit expressions for the spherical harmonics: an orthonormal set of eigenfunctions of L^2 and L_z defined on the surface of a sphere,

$$\int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} Y_{l'}^{m'*}(\theta,\phi) Y_l^m(\theta,\phi) \sin\theta\, d\theta\, d\phi = \int Y_{l'}^{m'*}(\theta,\phi) Y_l^m(\theta,\phi)\, d\Omega = \delta_{l'l}\delta_{m'm}.$$

They form a *complete* set:

$$\sum_{l=0}^{\infty} \sum_{m=-l}^{l} |l,m\rangle\langle l,m| = I$$

or

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y_l^{m*}(\theta,\phi)Y_l^m(\theta',\phi') = \delta(\cos\theta-\cos\theta')\delta(\phi-\phi') = \delta(\Omega-\Omega')$$

in the notation of Messiah, where Ω refers to a point on the spherical surface.

(Formal proof of the completeness is given in Byron and Fuller, *Mathematics of Classical and Quantum Physics*.)

The above equation could also be written

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l} \langle\theta,\phi|l,m\rangle\langle l,m|\theta',\phi'\rangle = \langle\theta,\phi|\theta',\phi'\rangle = \delta(\cos\theta-\cos\theta')\delta(\phi-\phi')$$

where the ket $|\theta',\phi'\rangle$ is to be understood as a localized ket, the spherical-surface version of $|x\rangle$, normalized by its δ-function inner product with the bra $\langle\theta,\phi|$, exactly analogous to $\langle x|x'\rangle = \delta(x-x')$, bearing in mind that the infinitesimal area element is $-d(\cos\theta)d\phi$, (a positive quantity in the relevant interval, 0 to π).

This completeness means that any reasonable function on the surface of the sphere can be expressed as a sum over spherical harmonics with appropriate coefficients, in other words the spherical generalization of a Fourier series.

In fact, L^2 is equivalent to ∇^2 on the spherical surface, so the Y_l^m are the eigenfunctions of the operator ∇^2. Just as in one dimension the eigenfunctions of d^2/dx^2 have the spatial dependence of the eigenmodes of a vibrating string, the spherical harmonics have the spatial dependence of the eigenmodes of a vibrating spherical balloon. Of course, to describe the displacement of the balloon skin (which must be real!) with these eigenfunctions, we can no longer use the eigenfunctions of the *z*-component of angular momentum, since they are complex except in the trivial zero case. We must rearrange the eigenfunctions of L^2, for example replacing the pair $e^{i\phi}, e^{-i\phi}$ with $\cos\phi, \sin\phi$. These real solutions, essentially $\frac{1}{\sqrt{2}}\left(|l,l\rangle \pm |l,-l\rangle\right)$, have l nodal lines (zeroes) of longitude. Moving down one notch in $|m|$, the (real) state with $|m| = l-1$ has $l-1$ longitudinal nodes, but has added a *latitudinal* node: the equator. Then $|m| = l-2$ has $l-2$ longitudinal nodes, 2 latitudinal nodal lines—*there are always l nodal lines total*.

Some of these modes of vibration have been observed in the sun after a sunspot storm. The spherical harmonics are also used in analyzing the cosmic background radiation.

Some Low Order Spherical Harmonics

Let's look in more detail at the lowest order spherical harmonics. For the first few, the normalization of the highest state $|l,l\rangle$ is pretty easy to do from scratch: factoring out the ϕ dependence as before, $Y_l^m(\theta,\phi)=\Theta_l^m(\theta)\Phi_m(\phi)$, and taking the normalized $\Phi_m(\phi)=e^{im\phi}/\sqrt{2\pi}$, the θ normalization for $|l,l\rangle$ is just $|N|^2\int\limits_0^\pi(\sin\theta)^{2l+1}d\theta=1$, easily accomplished for $l=0,1,2$.

All we then need is $L_\pm=\pm\hbar e^{\pm i\phi}\left(\frac{\partial}{\partial\theta}\pm i\cot\theta\frac{\partial}{\partial\phi}\right)$, $L_-|l,m\rangle=\hbar\sqrt{l(l+1)-m(m-1)}|l,m-1\rangle$, and finally the *sign convention* that $Y_l^0(0,0)$ be real and positive.

With a few elementary steps, it can be established that:

$$
\begin{aligned}
Y_0^0 &= \frac{1}{\sqrt{4\pi}}\\
Y_1^1 &= -\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\phi}\\
Y_1^0 &= \sqrt{\frac{3}{4\pi}}\cos\theta\\
Y_1^{-1} &= \sqrt{\frac{3}{8\pi}}\sin\theta e^{-i\phi}
\end{aligned}
$$

$$
Y_2^2=\sqrt{\frac{15}{32\pi}}\sin^2\theta e^{2i\phi},\quad Y_2^1=-\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{i\phi},\quad Y_2^0=\sqrt{\frac{5}{16\pi}}\left(3\cos^2\theta-1\right)
$$
$$
Y_2^{-2}=\sqrt{\frac{15}{32\pi}}\sin^2\theta e^{-2i\phi},\quad Y_2^{-1}=\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{-i\phi}
$$

It is often useful to write the Y_l^m in terms of Cartesian coordinates,

$$(x,y,z)=(r\sin\theta\cos\phi,\ r\sin\theta\sin\phi,\ r\cos\theta)$$

so

$$
Y_1^1(x,y,z)=-\sqrt{\frac{3}{8\pi}}\cdot\frac{x+iy}{r},\quad Y_1^0(x,y,z)=\sqrt{\frac{3}{4\pi}}\cdot\frac{z}{r},\quad Y_1^{-1}(x,y,z)=\sqrt{\frac{3}{8\pi}}\cdot\frac{x-iy}{r}
$$

and

$$Y_2^2 = \sqrt{\frac{15}{32\pi}} \frac{(x+iy)^2}{r^2}, \quad Y_2^1 = -\sqrt{\frac{15}{8\pi}} \frac{(x+iy)z}{r^2}, \quad Y_2^0 = \sqrt{\frac{5}{16\pi}} \frac{(3z^2-1)}{r^2}, \text{ etc.}$$

The Y_1^m as a Basis of the l = 1 Subspace

The Y_1^m are the $l = 1$ eigenstates of L^2 and L_z. But what if we'd chosen to look for the common eigenstates of L^2 and L_x instead? What $l = 1$ state has zero angular momentum component in the direction of the x-axis? Clearly it will be $\sqrt{\frac{3}{4\pi}} \cdot \frac{x}{r}$, in other words the previous Y_1^0 with z replaced by x, because after all, our labeling of axes was arbitrary.

Now,

$$\sqrt{\frac{3}{4\pi}} \cdot \frac{x}{r} \quad \text{is just} \quad (1/\sqrt{2})(-Y_1^1 + Y_1^{-1}).$$

In fact, *any* $l = 1$ state, with a specified component in *any* direction, can be written as

$$\alpha_1 |1,1\rangle + \alpha_0 |1,0\rangle + \alpha_{-1} |1,-1\rangle = \sum \alpha_m |1,m\rangle .$$

This can be seen as follows: an $l = 1$ state has to be *linear* in $x/r,\ y/r,\ z/r$ (any quadratic term would give rise to $e^{2i\phi}$ about an appropriate axis, call that the z-axis, so $m = 2$ and l must be 2 or greater), and any such state can be written as a linear combination of

$$(x+iy)/\sqrt{2}r,\ (x-iy)/\sqrt{2}r,\ z/r .$$

The bottom line, then, is that the Y_1^m do indeed provide a *complete* basis for the $l = 1$ space of eigenstates of L^2.

Representing the Rotation Operator Within the l = 1 Subspace

Recall that we originally introduced the angular momentum operator $\vec{J}$ by defining it as the generator of infinitesimal rotations when acting on any wave function, including multicomponent wave functions. We found, using the commutativity properties of ordinary rotations, that the vector components of $\vec{J}$ had to satisfy $[J_x, J_y] = i\hbar J_z$, etc., and from that we deduced the possible sets of eigenvalues of the commuting pair of operators $\vec{J}^2, J_z$ were $j(j+1)\hbar^2$ for $\vec{J}^2$, with j an integer of half an odd integer, and for each such j the allowed eigenvalues of J_z were $m\hbar, \quad m = -j, -j+1, \ldots, +j.$

Back to the $l = 1$ angular wave functions: we have established that any such function can be written $\alpha_1 |1,1\rangle + \alpha_0 |1,0\rangle + \alpha_{-1} |1,-1\rangle = \sum \alpha_m |1,m\rangle$, and so is a vector in a three-dimensional space spanned by the set $|1,m\rangle$, $m = 1, 0, -1$. In other words, the wave function is a three-component object. The angular momentum operator must therefore be *a matrix operator in this three-dimensional space*, such that, by definition, the effect of an infinitesimal rotation on the multicomponent wave function is:

$$R\left(\delta\vec{\theta}\right)\psi_{l=1}(\theta,\phi) = e^{-\frac{i}{\hbar}\delta\vec{\theta}.\hat{\vec{J}}}\begin{pmatrix}\alpha_1\\ \alpha_0\\ \alpha_{-1}\end{pmatrix} = \begin{pmatrix}\alpha'_1\\ \alpha'_0\\ \alpha'_{-1}\end{pmatrix}$$

The unitary rotation operator acting in the $l = 1$ subspace, $U\left(R\left(\vec{\theta}\right)\right) = e^{-\frac{i\vec{\theta}\cdot\vec{J}}{\hbar}}$, has to be a 3×3 matrix. The standard notation for its matrix elements is:

$$D^{(1)}_{m'm}\left(R\left(\vec{\theta}\right)\right) = \langle 1, m'| e^{-\frac{i\vec{\theta}\cdot\vec{J}}{\hbar}} |1, m\rangle$$

so the rotated ket is

$$\alpha'_{m'} = \sum_{m',m} D^{(1)}_{m'm}\alpha_m, \quad \text{or } \alpha' = D\alpha$$

To evaluate this matrix explicitly, we must expand the exponential and we need the matrix elements of $J_z,\ J_+,\ J_-$ between the states $|1, m\rangle$ —which we already know.

Now, the basis of the three-dimensional space is just the common eigenkets of $\vec{J}^2$, J_z, in this case identical to $\vec{L}^2,\ L_z$. We know the matrix elements of $J_z,\ J_+,\ J_-$ between states $|j, m\rangle$ from the earlier lecture, so it is simple to find the matrix representations of the components of *J* in this space:

$$J^{(1)}_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix}0 & 1 & 0\\ 1 & 0 & 1\\ 0 & 1 & 0\end{pmatrix},\quad J^{(1)}_y = \frac{i\hbar}{\sqrt{2}}\begin{pmatrix}0 & -1 & 0\\ 1 & 0 & -1\\ 0 & 1 & 0\end{pmatrix},\quad J^{(1)}_z = \hbar\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1\end{pmatrix}.$$

We have added the superscript (1) because this representation of the infinitesimal rotation operators is specific to $j = 1$ (representations for general values of *j* are as $(2j+1)\times(2j+1)$ matrices, reflecting the dimensionality of the space spanned by the $2j + 1$ distinct *m* values).

Expanding the exponential is not difficult, because by inspection $\left(J^{(1)}_z/\hbar\right)^3 = \left(J^{(1)}_z/\hbar\right)$, so from spherical symmetry $\left(\hat{\vec{n}}\cdot\vec{J}^{(1)}/\hbar\right)^3 = \left(\hat{\vec{n}}\cdot\vec{J}^{(1)}/\hbar\right)$ for a unit vector in any direction. The result is:

$$D^{(1)}\left(R\left(\vec{\theta}\right)\right)=e^{-\frac{i\theta\hat{\vec{n}}\cdot\vec{J}}{\hbar}}=I+\left(\cos\theta-1\right)\left(\frac{\hat{\vec{n}}\cdot\vec{J}}{\hbar}\right)^{2}-i\sin\theta\left(\frac{\hat{\vec{n}}\cdot\vec{J}}{\hbar}\right).$$

One other point we should note: at the end of the linear algebra lecture, we discussed rotations about the z-axis in ordinary (x, y, z) space. Obviously, if we label a point in the (x, y) plane using the complex number $x + iy$, a rotation by an angle θ about the z-axis will move the point in such a way that the new label is $e^{i\theta}\left(x+iy\right)$. The angle in this case has the opposite sign to that given by the operator above: the reason is that when we write the eigenstate as $-\sqrt{\frac{3}{8\pi}}\cdot\frac{x+iy}{r}$, this is a *function* of position in the plane, not a point in the plane, so for the reasons discussed at the beginning of the first Angular Momentum lecture, the sign is opposite.