221A Lecture Notes

Spherical Harmonics

1 Oribtal Angular Momentum

The orbital angular momentum operator is given just as in the classical mechanics,

$$\vec{L} = \vec{x} \times \vec{p}. \tag{1}$$

From this definition and the canonical commutation relation between the position and momentum operators, it is easy to verify the commutation relation among the components of the angular momentum,

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k. \tag{2}$$

When using the position representation, the action of the angular momentum on any state is given by a differential operator

$$\langle\vec{x}|\vec{L}|\psi\rangle = \vec{x} \times \frac{\hbar}{i}\vec{\nabla}\langle\vec{x}|\psi\rangle = \vec{x} \times \frac{\hbar}{i}\vec{\nabla}\psi(\vec{x}). \tag{3}$$

Loosely, we can write

$$\vec{L} = \vec{x} \times \frac{\hbar}{i}\vec{\nabla}, \tag{4}$$

but you have to be careful on what this differential operator is acting on. If you act on a position ket instead of a bra,

$$\vec{L}|\vec{x}\rangle = -\vec{x} \times \frac{\hbar}{i}\vec{\nabla}|\vec{x}\rangle. \tag{5}$$

Whenever I write the orbital angular momentum operator as a differential operator in this note, it is understood that it acts on a position bra instead of ket.

With this caveat in mind, we can rewrite the orbital angular momentum operator in the polar coordinates. Following the usual definitions

$$\begin{aligned} x &= r\sin\theta\cos\phi, \\ y &= r\sin\theta\sin\phi, \\ z &= r\cos\theta, \end{aligned} \tag{6}$$

we can rewrite the derivatives using the chain rule,

$$\begin{aligned}
\begin{pmatrix} \partial_r \\ \partial_\theta \\ \partial_\phi \end{pmatrix} &= \begin{pmatrix} \partial_r x & \partial_r y & \partial_r z \\ \partial_\theta x & \partial_\theta y & \partial_\theta z \\ \partial_\phi x & \partial_\phi y & \partial_\phi z \end{pmatrix} \begin{pmatrix} \partial_x \\ \partial_y \\ \partial_z \end{pmatrix} \\
&= \begin{pmatrix} \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \\ r\cos\theta\cos\phi & r\cos\theta\sin\phi & -r\sin\theta \\ -r\sin\theta\sin\phi & r\sin\theta\cos\phi & 0 \end{pmatrix} \begin{pmatrix} \partial_x \\ \partial_y \\ \partial_z \end{pmatrix}. \qquad (7)
\end{aligned}$$

We invert the matrix and find

$$\begin{pmatrix} \partial_x \\ \partial_y \\ \partial_z \end{pmatrix} = \frac{1}{r\sin\theta} \begin{pmatrix} r\sin^2\theta\cos\phi & \sin\theta\cos\theta\cos\phi & -\sin\phi \\ r\sin^2\theta\sin\phi & \sin\theta\cos\theta\sin\phi & \cos\phi \\ r\sin\theta\cos\theta & -\sin^2\theta & 0 \end{pmatrix} \begin{pmatrix} \partial_r \\ \partial_\theta \\ \partial_\phi \end{pmatrix}. \qquad (8)$$

Now the orbital angular momentum operators can be written in terms of spherical coordinates,

$$\begin{aligned}
L_x &= \frac{\hbar}{i}\left(-\sin\phi\frac{\partial}{\partial\theta} - \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right), \qquad (9) \\
L_y &= \frac{\hbar}{i}\left(\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right), \qquad (10) \\
L_z &= \frac{\hbar}{i}\frac{\partial}{\partial\phi}. \qquad (11)
\end{aligned}$$

It is useful to take the combinations

$$L_\pm = \frac{\hbar}{i}e^{\pm i\phi}\left(\pm i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\phi}\right). \qquad (12)$$

Finally,

$$\vec{L}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]. \qquad (13)$$

The free-particle Hamiltonian is

$$\frac{\vec{p}^2}{2m} = \frac{-\hbar^2}{2m}(\partial_x^2 + \partial_y^2 + \partial_z^2) = \frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + \frac{\vec{L}^2}{2mr^2}. \qquad (14)$$

Looking at the expression for L_z, you can see that it is of the same form as the momentum operator of a particle on a circle, whose eigenvalues are quantized as $n\hbar$ for $n \in \mathbb{Z}$. Therefore, L_z is also quantized as $m\hbar$ for $m \in \mathbb{Z}$. An immediate consequence is that no half-odd values are allowed for L_z, and hence half-odd j cannot be obtained for orbital angular momentum. Only integer j is possible.

2 Spherical Harmonics

Now we look for eigenstates of $\vec{L}^2$ and L_z to find the Hilbert space for the orbital angular momentum.

In any spherically symmetric systems, energy eigenstates can be given by produce wave functions of the form*

$$\psi(\vec{x}) = R(r) Y_l^m(\theta, \phi). \tag{15}$$

In other words, we are parameterizing the position eigenbasis in terms of polar rather than Cartesian coordinates,

$$\langle \vec{x}| = \langle r, \theta, \phi|. \tag{16}$$

The spherical harmonics are defined as the wave functions of angular momentum eigenstates

$$Y_l^m(\theta, \phi) = \langle \theta, \phi | l, m\rangle. \tag{17}$$

Sakurai uses the notation $\langle \vec{n}|$ and call them "direction eigenkets."

Clearly, the defintions of angular momemum eigenstates

$$\begin{aligned} \vec{L}^2 |l, m\rangle &= l(l+1)\hbar^2 |l, m\rangle, & (18) \\ L_z |l, m\rangle &= m\hbar |l, m\rangle, & (19) \end{aligned}$$

translate to the differential equations

$$\begin{aligned} -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right] Y_l^m &= l(l+1)\hbar^2 Y_l^m, & (20) \\ \frac{\hbar}{i} \frac{\partial}{\partial\phi} Y_l^m &= m\hbar Y_l^m. & (21) \end{aligned}$$

The latter equation is easy to solve: the azimuth dependence of the spherical harmonics must be $e^{im\phi}$. But figuring out the polar angle dependence needs more work. The rest of the discussion here is on this issue.

Both in the case of the harmonic oscillator and the Landau levels (energy levels of a charged particle in a uniform magnetic field), it was useful to write

*This corresponds to the separation of variables in Hailton–Jacobi theory, where the action S is written as a sum of different pieces $S(r) + S(\theta, \phi)$. Because the wave function corresponds to $e^{iS/\hbar}$, it is natural for the wave function to be given by a product of different pieces.

down an equation for the ground state of the form $a|0\rangle = 0$. It was useful because it gave us a linear differential equation instead of a quadratic one (e.g., Schrödinger equation). The linear differential equations are far easier to solve. We can take the same strategy for the spherical harmonics.

2.1 Derivation of Spherical Harmonics

We know from the general representation theory of angular momenta that $L_-|l,-l\rangle = 0$ because it cannot be lowered any more. Sakurai starts with $|l,l\rangle$ instead. Of course you get the same result, but I find this way somewhat less confusing. In the position representation, we find

$$0 = \langle\theta,\phi|L_-|l,-l\rangle = \frac{\hbar}{i}e^{-i\phi}\left(-i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\phi}\right)Y_l^{-l}(\theta,\phi) = 0. \tag{22}$$

On the other hand, we know already that

$$-l\hbar Y_l^{-l} = \langle\theta,\phi|L_z|l,-l\rangle = \frac{\hbar}{i}\frac{\partial}{\partial\phi}Y_l^{-l} \tag{23}$$

and hence the azimuth dependence of Y_l^{-l} is $Y_l^{-l}(\theta,\phi) = f(\theta)e^{-il\phi}$. Therefore, Eq. (22) becomes

$$\left(-i\frac{d}{d\theta} + il\cot\theta\right)f(\theta) = 0. \tag{24}$$

This equation is solved easily, by writing it as

$$\frac{1}{f}df = l\cot\theta d\theta, \tag{25}$$

and integrating both sides to

$$\log f = l\log\sin\theta + \text{const.} \tag{26}$$

Therefore,

$$f(\theta) = c\sin^l\theta \tag{27}$$

with an overall normalization constant c.

Putting things together, we find

$$Y_l^{-l}(\theta,\phi) = c\sin^l\theta e^{-il\phi}. \tag{28}$$

The absolute value of c can be fixed by the normalization

$$1 = \int d\Omega |Y_l^l|^2 = \int_{-1}^{1} d\cos\theta \int_0^{2\pi} d\phi |c|^2 \sin^{2l}\theta. \tag{29}$$

ϕ integral trivially gives a factor of 2π. The θ integral is most conveniently done using the variable $x = \cos\theta$,

$$1 = 2\pi |c|^2 \int_{-1}^{1} dx (1-x^2)^l.. \tag{30}$$

Writing $1-x^2 = (1-x)(1+x)$, and further change the variable to $x = -1+2t$,

$$1 = 2\pi|c|^2 \int_0^1 2dt\ (2t(2-2t))^l = 2\pi|c|^2 2^{2l+1} \int_0^1 dt\ t^l (1-t)^l. \tag{31}$$

The integral is nothing but the Beta function

$$B(p,q) = \int_0^1 dt\ t^{p-1}(1-t)^{q-1} = \frac{\Gamma(p)\Gamma(q)}{\Gamma(p+q)}. \tag{32}$$

Therefore,

$$1 = 2\pi|c|^2 2^{2l+1} \frac{\Gamma(l+1)\Gamma(l+1)}{\Gamma(2l+2)} = 4\pi|c|^2 2^{2l} \frac{l!l!}{(2l+1)!}. \tag{33}$$

We find

$$|c| = \frac{1}{2^l l!}\sqrt{\frac{(2l+1)!}{4\pi}}. \tag{34}$$

The phase of c is fixed by picking a convention. The commonly used convention (the same as Sakurai's) is not to have an additional phase factor

$$Y_l^{-l}(\theta,\phi) = \frac{1}{2^l l!}\sqrt{\frac{(2l+1)!}{4\pi}}\ \sin^l\theta e^{-il\phi}. \tag{35}$$

Now that we know Y_l^{-l}, we can keep acting L_+ on it to obtain all Y_l^m. Recall that the general discussion of angular momentum taught us that

$$L_+|l,m\rangle = \sqrt{l(l+1)-m(m+1)}|l,m+1\rangle = \sqrt{(l-m)(l+m+1)}|l,m+1\rangle. \tag{36}$$

Then we find

$$Y_l^m(\theta,\phi) = \frac{1}{\hbar\sqrt{(l+m)(l-m+1)}}\frac{1}{\hbar\sqrt{(l+m-1)(l-m+2)}}$$
$$\cdots\frac{1}{\hbar\sqrt{(2)(l+l-1)}}\frac{1}{\hbar\sqrt{(1)(l+l)}}\left[\frac{\hbar}{i}e^{i\phi}\left(i\frac{\partial}{\partial\theta}-\cot\theta\frac{\partial}{\partial\phi}\right)\right]^{l+m}Y_l^{-l}(\theta,\phi)$$
$$= \sqrt{\frac{(l-m)!}{(2l)!(l+m)!}}\left[e^{i\phi}\left(\frac{\partial}{\partial\theta}+i\cot\theta\frac{\partial}{\partial\phi}\right)\right]^{l+m}Y_l^{-l}(\theta,\phi) \tag{37}$$

Now the question is to bring it to a more usable form.

The ϕ derivatives always give eigenvalues. But each time L_+ acts, there is a factor of $e^{+i\phi}$ and makes the eigenvalue of $-i\partial/\partial\phi$ increase one by one. Therefore,

$$\begin{aligned}Y_l^m(\theta,\phi) &= \frac{1}{2^l l!}\sqrt{\frac{(2l+1)!}{4\pi}}\sqrt{\frac{(l-m)!}{(2l)!(l+m)!}}e^{im\phi}\left(\frac{d}{d\theta}-(m-1)\cot\theta\right)\\ &\quad\left(\frac{d}{d\theta}-(m-2)\cot\theta\right)\cdots\left(\frac{d}{d\theta}+(l-1)\cot\theta\right)\left(\frac{d}{d\theta}+l\cot\theta\right)\sin^l\theta.\\ &= \frac{1}{2^l l!}\sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}e^{im\phi}\left(\frac{d}{d\theta}-(m-1)\cot\theta\right)\\ &\quad\left(\frac{d}{d\theta}-(m-2)\cot\theta\right)\cdots\left(\frac{d}{d\theta}+(l-1)\cot\theta\right)\left(\frac{d}{d\theta}+l\cot\theta\right)\sin^l\theta.\end{aligned} \tag{38}$$

Here we have cancelled factors of $\hbar$ and i. The next trick we need is to write

$$\left(\frac{d}{d\theta}+k\cot\theta\right) = \frac{1}{\sin^k\theta}\frac{d}{d\theta}\sin^k\theta \tag{39}$$

Then

$$\begin{aligned}Y_l^m(\theta,\phi) &= \frac{1}{2^l l!}\sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}e^{im\phi}\left(\frac{1}{\sin^{-(m-1)}\theta}\frac{d}{d\theta}\sin^{-(m-1)}\theta\right)\\ &\quad\left(\frac{1}{\sin^{-(m-2)}\theta}\frac{d}{d\theta}\sin^{-(m-2)}\theta\right)\cdots\left(\frac{1}{\sin^{l-1}\theta}\frac{d}{d\theta}\sin^{l-1}\theta\right)\left(\frac{1}{\sin^l\theta}\frac{d}{d\theta}\sin^l\theta\right)\sin^l\theta\end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{2^l l!}\sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} e^{im\phi}\sin^m\theta\left(\frac{1}{\sin\theta}\frac{d}{d\theta}\right)^{l+m}\sin^{2l}\theta \\
&= \frac{1}{2^l l!}\sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} e^{im\phi}\sin^m\theta\left(-\frac{d}{d\cos\theta}\right)^{l+m}\sin^{2l}\theta \\
&= \frac{(-1)^{l+m}}{2^l l!}\sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} e^{im\phi}(1-x^2)^{m/2}\frac{d^{l+m}}{dx^{l+m}}(1-x^2)^{2l}. \qquad (40)
\end{aligned}
$$

In the last line, we used the variable $x = \cos\theta$.

2.2 Legendre Polynomials

Here are a few new notations. Legendre polynomials are defined by

$$
\begin{aligned}
P_l(x) &= \frac{(-1)^l}{2^l l!}\frac{d^l}{dx^l}(1-x^2)^l \qquad (41) \\
P_l^m(x) &= (1-x^2)^{m/2}\frac{d^m}{dx^m}P_l(x). \qquad (42)
\end{aligned}
$$

The definition Eq. (42) works only for $m > 0$. Another way to write P_l^m is just putting them together,

$$
P_l^m(x) = \frac{(-1)^l}{2^l l!}(1-x^2)^{m/2}\frac{d^{l+m}}{dx^{l+m}}(1-x^2)^l. \qquad (43)
$$

This expression allows you to pick $m < 0$.

P_l^m is called associated Legendre polynomials, and $P_l^m(x) = P_l(x)$. The definitions look complicated, but they are just polynomials! P_l is a polynomial of order l. P_l^m has this funny factor $(1-x^2)^{m/2}$ with a fractional power, but we will set $x = \cos\theta$ in the end, and $(1-x^2)^{m/2} = \sin^m\theta$. Remember θ is the polar angle, and we only consider $0 \leq \theta \leq \pi$ so that $\sin\theta \geq 0$. Therefore, P_l^m is a polynomial of order m in $\sin\theta$ and $l-m$ in $\cos\theta$.

Now let us prove a surprising identity

$$
P_l^{-m}(x) = (-1)^m\frac{(l-m)!}{(l+m)!}P_l^m(x). \qquad (44)
$$

Let us start with $\frac{d^{l+m}}{dx^{l+m}}(1-x^2)^l$ for $m > 0$ which appears in $P_l^m(x)$. We expand it out and see how it can be related to $\frac{d^{l-m}}{dx^{l-m}}(1-x^2)^l$

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

$$= \sum_{r=0}^{l+m} {}_{l+m}C_r \left(\frac{d^r}{dx^r}(1-x)^l \right) \left(\frac{d^{l+m-r}}{dx^{l+m-r}}(1+x)^l \right). \quad (45)$$

Even though the sum extends for $0 \le r \le l+m$, the term in the first parentheses vanishes for $r > l$ while the second for $l+m-r > l$. Therefore, the sum is taken only for $m \le r \le l$. Then

$$\begin{aligned} &\frac{d^{l+m}}{dx^{l+m}}(1-x^2)^l \\ &= \sum_{r=m}^{l} {}_{l+m}C_r \frac{(-1)^r l!}{(l-r)!}(1-x)^{l-r} \frac{l!}{(r-m)!}(1+x)^{r-m} \\ &= \sum_{s=0}^{l-m} {}_{l+m}C_{m+s} \frac{(-1)^{m+s} l!}{(l-m-s)!}(1-x)^{l-m-s} \frac{l!}{s!}(1+x)^s. \end{aligned} \quad (46)$$

In the last line, I rewrote it with $r = m+s$. Now I multiply it by $(1-x^2)^m$ and divide by it,

$$\begin{aligned} &\frac{d^{l+m}}{dx^{l+m}}(1-x^2)^l \\ &= \frac{1}{(1-x^2)^m} \sum_{s=0}^{l-m} {}_{l+m}C_{s+s} \frac{(-1)^{m+s} l!}{(l-m-s)!}(1-x)^{l-s} \frac{l!}{s!}(1+x)^{m+s} \\ &= \frac{1}{(1-x^2)^m} \sum_{s=0}^{l-m} \frac{(l+m)!}{(m+s)!(l-s)!} \frac{(-1)^{m+s} l!}{(l-m-s)!}(1-x)^{l-s} \frac{l!}{s!}(1+x)^{m+s} \\ &= \frac{1}{(1-x^2)^m} \sum_{s=0}^{l-m} \frac{(l+m)!}{s!(l-m-s)!} \frac{(-1)^{m+s} l!}{(l-s)!}(1-x)^{l-s} \frac{l!}{(m+s)!}(1+x)^{m+s} \\ &= \frac{(l+m)!}{(l-m)!} \frac{1}{(1-x^2)^m} \sum_{s=0}^{l-m} \frac{(l-m)!}{s!(l-m-s)!}(-1)^{m+s} \\ &\qquad \left((-1)^s \frac{d^s}{dx^s}(1-x)^{l-s} \right) \left(\frac{d^{l-m-s}}{dx^{l-m-s}}(1+x)^{m+s} \right) \\ &= \frac{(l+m)!}{(l-m)!} \frac{(-1)^m}{(1-x^2)^m} \sum_{s=0}^{l-m} {}_{l-m}C_s \left(\frac{d^s}{dx^s}(1-x)^{l-s} \right) \left(\frac{d^{l-m-s}}{dx^{l-m-s}}(1+x)^{m+s} \right) \\ &= \frac{(l+m)!}{(l-m)!} \frac{(-1)^m}{(1-x^2)^m} \frac{d^{l-m}}{dx^{l-m}}(1-x^2)^l. \end{aligned} \quad (47)$$

Multiplying both sides of the equation by $\frac{(-1)^l}{2^l l!}(1-x^2)^{m/2}$, we find

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

$$= \frac{(l+m)!}{(l-m)!}(-1)^m \frac{(-1)^l}{2^l l!} \frac{1}{(1-x^2)^{m/2}} \frac{d^{l-m}}{dx^{l-m}}(1-x^2)^l$$
$$= \frac{(l+m)!}{(l-m)!}(-1)^m P_l^{-m}(x). \tag{48}$$

This is indeed Eq. (44).

The orthogonality relation among Legendre polynomials is important:

$$\int_{-1}^{1} dx P_n^m(x) P_l^m(x) = \frac{2}{2l+1} \frac{(l+m)!}{(l-m)!} \delta_{n,l}. \tag{49}$$

Note that both polynomials share the same m.

It can be shown as follows. In this discussion, we assume $m \geq 0$. But $m \leq 0$ case follows from Eq. (44). We substitute in the explicit expression,

$$\int_{-1}^{1} dx P_n^m(x) P_l^m(x)$$
$$= \int_{-1}^{1} dx \left(\frac{(-1)^n}{2^n n!}(1-x^2)^{m/2} \frac{d^{n+m}}{dx^{n+m}}(1-x^2)^n \right)$$
$$\left(\frac{(-1)^l}{2^l l!}(1-x^2)^{m/2} \frac{d^{l+m}}{dx^{l+m}}(1-x^2)^l \right)$$
$$= \frac{(-1)^{n+l}}{2^{n+l} n! l!} \int_{-1}^{1} dx (1-x^2)^m \left(\frac{d^{n+m}}{dx^{n+m}}(1-x^2)^n \right) \left(\frac{d^{l+m}}{dx^{l+m}}(1-x^2)^l \right). \tag{50}$$

To show the orthogonality when $n \neq l$, let us assume $n > l$ without a loss of generality. The point is to keep doing integration by parts so that $d^{n+m}/dx^{n+m}4$ acting on $(1-x^2)^{n+m}$ acts on the rest of the integrand. But the rest is a polynomial of order $2m + 2l - (l+m) = l + m < n + m$, and its $(n+m)$-th derivative vanishes. At each integration by parts, the surface term also vanishes. For the first m-times, the surfact term vanishes because of $(1-x^2)^m$ factor. For the remaining n-times, it vanishes because of the $(1-x^2)^n$ factor. This proves the orthogonality. When $n = l$, we again go through the same procedure and only the top power in x contributes,

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

$$
\begin{aligned}
&= \frac{(-1)^{l+l}}{2^{l+l}l!l!}(-1)^{l+m}\int_{-1}^{1} dx(1-x^2)^l \left(\frac{d^{l+m}}{dx^{l+m}}(-1)^m(x^2)^m\frac{d^{l+m}}{dx^{l+m}}(-1)^l(x^2)^l\right) \\
&= \frac{1}{2^{2l}l!l!}\int_{-1}^{1} dx(1-x^2)^l \left(\frac{d^{l+m}}{dx^{l+m}}(x^2)^m\frac{(2l)!}{(l-m)!}x^{l-m}\right) \\
&= \frac{1}{2^{2l}l!l!}\int_{-1}^{1} dx(1-x^2)^l(l+m)!\frac{(2l)!}{(l-m)!}. \qquad (51)
\end{aligned}
$$

Change the variable to $x = -1 + 2t$,

$$
\begin{aligned}
\int_{-1}^{1} dx P_l^m(x)P_l^m(x) &= \frac{1}{2^{2l}l!l!}\frac{(2l)!(l+m)!}{(l-m)!}\int_0^1 2dt(2t(2-2t))^l \\
&= \frac{2}{l!l!}\frac{(2l)!(l+m)!}{(l-m)!}\int_0^1 dt t^l(1-t)^l \\
&= \frac{2}{l!l!}\frac{(2l)!(l+m)!}{(l-m)!}\frac{\Gamma(l+1)\Gamma(l+1)}{\Gamma(2l+2)} \\
&= \frac{2}{(2l+1)!}\frac{(2l)!(l+m)!}{(l-m)!} \\
&= \frac{2}{2l+1}\frac{(l+m)!}{(l-m)!} \qquad (52)
\end{aligned}
$$

2.3 More Conventional Expression

Compared to Eq. (40), we see that P_l^m gives Y_l^m,

$$
Y_l^m = (-1)^m\sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}e^{im\phi}P_l^m(\cos\theta). \qquad (53)
$$

A special case of this is

$$
Y_l^0 = \sqrt{\frac{(2l+1)}{4\pi}}P_l(\cos\theta). \qquad (54)
$$

When $m < 0$, an alternative expression is obtained by using the identity Eq. (44),

$$
Y_l^m = \sqrt{\frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!}}e^{im\phi}P_l^{|m|}(\cos\theta). \qquad (55)
$$

In particular, this expression shows a relation

$$
Y_l^m = (-1)^m(Y_l^{-m})^*. \qquad (56)
$$

2.4 Orthonormality and Completeness

You can verify the orthonormality of spherical harmonics explicitly. Here and below, Ω refers to the polar coordinates θ, ϕ, and the integration volume is $d\Omega = d\cos\theta d\phi$.

$$\begin{aligned}
&\int d\Omega Y_l^m(\Omega)(Y_{l'}^{m'}(\Omega))^* \\
&= (-1)^{m+m'}\sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}\sqrt{\frac{(2l'+1)(l'-m')!}{4\pi(l'+m')!}} \\
&\qquad \int_{-1}^{1} d\cos\theta \int_0^{2\pi} d\phi P_l^m(\cos\theta)P_{l'}^{m'}(\cos\theta)e^{im\phi}e^{-im'\phi}. \qquad (57)
\end{aligned}$$

Because ϕ integral vanishes unless $m = m'$,

$$\begin{aligned}
&= 2\pi\delta_{m,m'}\sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}\sqrt{\frac{(2l'+1)(l'-m)!}{4\pi(l'+m)!}}\int_{-1}^{1} dx P_l^m(x)P_{l'}^m(x) \\
&= 2\pi\delta_{m,m'}\sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}\sqrt{\frac{(2l'+1)(l'-m)!}{4\pi(l'+m)!}}\frac{2}{2l+1}\frac{(l+m)!}{(l-m)!}\delta_{l,l'} \\
&= 2\pi\delta_{m,m'}\delta_{l,l'}\frac{(2l+1)(l-m)!}{4\pi(l+m)!}\frac{2}{2l+1}\frac{(l+m)!}{(l-m)!}\delta_{l,l'} \\
&= \delta_{m,m'}\delta_{l,l'}. \qquad (58)
\end{aligned}$$

This is an explicit verification of the expected orthonormality

$$\delta_{m,m'}\delta_{l,l'} = \langle l', m'|l, m\rangle = \int d\Omega\langle l', m'|\theta, \phi\rangle\langle\theta, \phi|l, m\rangle = \int d\Omega(Y_{l'}^{m'})^* Y_l^m. \qquad (59)$$

The completeness relation is

$$\begin{aligned}
\delta^2(\Omega - \Omega') &= \langle\theta, \phi|\theta'\phi'\rangle \\
&= \sum_{l,m}\langle\theta, \phi|l, m\rangle\langle l, m|\theta'\phi'\rangle \\
&= \sum_{l,m} Y_l^m(\theta, \phi)(Y_l^m(\theta', \phi'))^*. \qquad (60)
\end{aligned}$$

Here,

$$\delta^2(\Omega - \Omega') = \delta(\cos\theta - \cos\theta')\delta(\phi - \phi') = \frac{\delta(\theta - \theta')}{\sin\theta}\delta(\phi - \phi'). \qquad (61)$$

2.5 Examples

It is useful to look at a few examples:

$$Y_0^0 = \frac{1}{\sqrt{4\pi}}, \tag{62}$$

$$Y_1^{\pm 1} = \mp\sqrt{\frac{3}{8\pi}} \sin\theta e^{\pm i\phi}, \tag{63}$$

$$Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos\theta, \tag{64}$$

$$Y_2^{\pm 2} = \sqrt{\frac{15}{32\pi}} \sin^2\theta e^{\pm 2i\phi}, \tag{65}$$

$$Y_2^{\pm 1} = \mp\sqrt{\frac{15}{8\pi}} \sin\theta\cos\theta e^{\pm i\phi}, \tag{66}$$

$$Y_2^0 = \sqrt{\frac{5}{16\pi}} (3\cos^2\theta - 1). \tag{67}$$

In spectroscopic symbols, $l = 0, 1, 2, 3, 4, \cdots$ correspond to $s, p, d, f, g, \cdots$ orbitals.†

In chemistry and solid-state physics, you see symbols like p_x, $d_{x^2-y^2}$. They refer to certain linear combinations of spherical harmonics. The general rule is to first multiply the spherical harmonics by r^l, and you find

$$Y_0^0 = \frac{1}{\sqrt{4\pi}}, \tag{68}$$

$$rY_1^{\pm 1} = \mp\sqrt{\frac{3}{8\pi}} (x \pm iy), \tag{69}$$

$$rY_1^0 = \sqrt{\frac{3}{4\pi}} z, \tag{70}$$

$$r^2Y_2^{\pm 2} = \sqrt{\frac{15}{32\pi}} (x \pm iy)^2, \tag{71}$$

$$r^2Y_2^{\pm 1} = \mp\sqrt{\frac{15}{8\pi}} (x \pm iy)z, \tag{72}$$

$$r^2Y_2^0 = \sqrt{\frac{5}{16\pi}} (3z^2 - r^2). \tag{73}$$

† s for sharp, p for principal, d for diffuse, f for fundamental, and the rest is just alphabetical.

Then you look at x, y, z dependences to identify a particular orbital. Note that the dependence on r should not be taken seriously; it is supposed to be multiplied by a radial wave function anyway. We multiplied spherical harmonics by r^l just to make to expressions become polynomials in x, y, z. From these expressions, it is clear that the p_z orbital corresponds to Y_1^0, while p_x to $(Y_1^1 + Y_1^{-1})/\sqrt{2}$ and p_y to $(Y_1^1 - Y_1^{-1})/i\sqrt{2}$. $d_{x^2-y^2}$ corresponds to $(Y_2^2 + Y_2^{-2})/\sqrt{2}$, d_{yz} to $(Y_2^1 - Y_2^{-1})/i\sqrt{2}$.

I'm sure you have seen "shapes" of spherical harmonics in textbooks. It is important to understand what they actually are. In many cases, what is shown is a surface given by points

$$r = |Y_l^m(\theta, \phi)|^2. \tag{74}$$

In other words, the distance of the surface from the origin along a direction is determined by the probability of finding the particle along that direction. They actually do not represent the "shapes" of the wave function. They just show along which direction the probability is big or small.

In certain cases, though, these plots do represent the "shapes" of the actual wave function. Remember that the actual wave function has the radial wave function on top of the spherical harmonics. Suppose the radial wave function is a smoothly decaying function, say, e^{-r/a_0}. Now you try to draw a surface of constant probability density in three dimensions. Then along the directions where $|Y_l^m|^2$ is larger, the constant probability is attained even at higher r; but along the directions with small $|Y_l^m|^2$, you need to go closer to the origin to get the same probability density. Then the plot mentioned above can approximate the "shape" of the actual wave function. But if you want to interpret the plots in this manner, it obviously depends on the details of the radial wave function, and what value you chose for the surface of constant probability density. Just presenting the "shapes" of, say, p_z orbitals independent of n (the principal quantum number) is therefore misleading.

2.6 Mathematica

It is useful to know that Mathematica has built-in commands for the spherical harmonics `SphericalHarmonicY[l,m,θ,φ]` for $Y_l^m(\theta, \phi)$, the Legendre polynomials `LegendreP[n,x]` for $P_n(x)$, and the associated Legendre polynomials `LegendreP[n,m,x]` for $P_n^m(x)$.