Phys 506 lecture 8: Spherical Harmonics the Algebraic Way

1 Introduction to spherical harmonics

Recall from last time that we worked out that the ket pointing in the θ and ϕ direction is given by the rotation of the state from the north-pole state via

$$|\theta, \phi\rangle = e^{-i\phi\frac{\hat{L}_z}{\hbar}} e^{-i\theta\frac{\hat{L}_y}{\hbar}} |\theta{=}0, \phi{=}0\rangle \, .$$

The spherical harmonic is then defined to be the overlap of this angular position state $\langle\theta, \phi|$ with the angular momentum state that has definite total and z-component of angular momentum $|lm\rangle$. We have,

$$\begin{aligned} Y_{lm}(\theta, \phi) = & \ \langle\theta, \phi|lm\rangle \\ & = \langle\theta{=}0, \phi{=}0|e^{i\theta\frac{\hat{L}_y}{\hbar}} e^{i\phi\frac{\hat{L}_z}{\hbar}}|lm\rangle. \end{aligned}$$

But $\hat{L}_z |lm\rangle = m\hbar |lm\rangle$, so

$$Y_{lm}(\theta, \phi) = \langle\theta{=}0, \phi{=}0|e^{i\theta\frac{\hat{L}_y}{\hbar}} e^{im\phi}|lm\rangle.$$

Inserting the identity operator within the angular momentum multiplet with total angular momentum l just to the right of $\langle\theta{=}0, \phi{=}0|$ gives us

$$Y_{lm}(\theta, \phi) = e^{im\phi} \sum_{m'} \langle\theta{=}0, \phi{=}0\big|lm'\rangle \, \langle lm'|e^{i\theta\frac{\hat{L}_y}{\hbar}}|lm\rangle.$$

The matrix element $d^{(l)}_{mm'} \equiv \langle lm'|e^{i\theta\frac{\hat{L}_y}{\hbar}}|lm\rangle$ is called the *rotation matrix*. It is a continuous matrix representation of the rotation group with $(2l+1)\times(2l+1)$ matrices. Note that we computed $d^{(\frac{1}{2})}_{mm'}$ when we worked with the Pauli matrices in **Lecture 1**.

Fortunately, we do not need the whole matrix.

2 Simplification due to the north-pole state

Note that $\langle\theta{=}0, \phi| = \langle\theta{=}0, \phi{=}0|\, e^{i\phi\frac{\hat{L}_z}{\hbar}} = \langle\theta{=}0, \phi{=}0|$. Think about what this is physically: It is a state pointing along the north pole. If I rotate about the north pole, I do nothing to the state.

In other words, the state for $\theta = 0$ is the same for all ϕ. But, we already saw that

$$\begin{aligned}\langle \theta{=}0, \phi | lm \rangle &= \langle \theta{=}0, \phi{=}0 | e^{i\phi \frac{\hat{L}_z}{\hbar}} | lm \rangle \\ &= e^{im\phi} \langle \theta{=}0, \phi{=}0 | lm \rangle .\end{aligned}$$

Hence,

$$\langle \theta{=}0, \phi{=}0 | lm \rangle = \begin{cases} 0 & m \neq 0 \\ \langle \theta{=}0, \phi{=}0 | l, m{=}0 \rangle & m{=}0 \end{cases} .$$

Note that this also implies that l is an integer since $m{=}0$ only occurs when $l \in \mathbb{Z}$. Hence, we have

$$Y_{lm}(\theta, \phi) = e^{im\phi} \langle \theta{=}0, \phi{=}0 | l, m{=}0 \rangle \langle l, m{=}0 | e^{i\theta \frac{\hat{L}_y}{\hbar}} | lm \rangle,$$

that is, only the $m{=}0$ term survives in the summation.

3 Calculating the $m{=}0$ matrix element of the y-rotation

To calculate $\langle l, m{=}0 | e^{i\theta \frac{\hat{L}_y}{\hbar}} | lm \rangle$, we use exponential disentangling. We have

$$\langle l, m{=}0 | e^{i\theta \frac{\hat{L}_y}{\hbar}} | lm \rangle = \langle l, m{=}0 | e^{-\tan\left(\frac{\theta}{2}\right) \frac{\hat{L}_-}{\hbar}} e^{\ln \cos^2\left(\frac{\theta}{2}\right) \frac{\hat{L}_z}{\hbar}} e^{\tan\left(\frac{\theta}{2}\right) \frac{\hat{L}_+}{\hbar}} | lm \rangle.$$

Now, recall that

$$\begin{aligned}\frac{\hat{L}_+}{\hbar} | lm \rangle &= \sqrt{(l-m)(l+m+1)} \, | l, m+1 \rangle \\ \frac{\hat{L}_-}{\hbar} | lm \rangle &= \sqrt{(l+m)(l-m+1)} \, | l, m-1 \rangle .\end{aligned}$$

We can expand each exponential factor in a power series.

$$e^{\tan \frac{\theta}{2} \frac{\hat{L}_+}{\hbar}} = \sum_{n=0}^{\infty} \frac{(\tan \frac{\theta}{2})^n}{n!} \left(\frac{\hat{L}_+}{\hbar} \right)^n .$$

So we have that

$$e^{\tan \frac{\theta}{2} \frac{\hat{L}_+}{\hbar}} | lm \rangle = \sum_{n=0}^{\infty} \frac{(\tan \frac{\theta}{2})^n}{n!} \left(\frac{\hat{L}_+}{\hbar} \right)^n | lm \rangle .$$

But $(\hat{L}_+)^n | lm \rangle = 0$ if $n > l - m$ since $\hat{L}_+ | l, m = l \rangle = 0$. So, the summation truncates after a finite number of terms, and we have

$$\begin{aligned}e^{\tan\left(\frac{\theta}{2}\right) \frac{\hat{L}_+}{\hbar}} | lm \rangle &= \sum_{n=0}^{l-m} \frac{(\tan \frac{\theta}{2})^n}{n!} \left(\frac{\hat{L}_+}{\hbar} \right)^n | lm \rangle \\ &= \sum_{n=0}^{l-m} \frac{(\tan \frac{\theta}{2})^n}{n!} \left(\prod_{r=1}^{n} \sqrt{(l-m-r+1)(l+m+r)} \right) | l, m+n \rangle .\end{aligned}$$

Now, we operate the next factor $e^{\ln\cos^2\left(\frac{\theta}{2}\right)\frac{\hat{L}_z}{\hbar}}$ onto this. It is easy since $\frac{\hat{L}_z}{\hbar}|lm\rangle = m|lm\rangle$.

$$e^{\ln\cos^2\left(\frac{\theta}{2}\right)\frac{\hat{L}_z}{\hbar}} e^{\tan\left(\frac{\theta}{2}\right)\frac{\hat{L}_+}{\hbar}}|lm\rangle = \sum_{n=0}^{l-m}\frac{(\tan\frac{\theta}{2})^n}{n!}\left(\prod_{r=1}^{n}\sqrt{(l-m-r+1)(l+m+r)}\right)\left(\cos\frac{\theta}{2}\right)^{2m+2n}|l, m+n\rangle\,.$$

Finally, we operate

$$e^{-\tan\left(\frac{\theta}{2}\right)\frac{\hat{L}_-}{\hbar}} = \sum_{n'=0}^{\infty}\frac{(-\tan\frac{\theta}{2})^{n'}}{n'!}\left(\frac{\hat{L}_-}{\hbar}\right)^{n'}$$

onto the state. But since we multiply by $\langle l, m{=}0|$ on the left in the end, we only need to include the term where $n' = n+m$. Since $n' \geq 0$, n must be at least $-m$ for a nonzero result. So $\langle l, m{=}0|e^{i\theta\frac{\hat{L}_y}{\hbar}}|lm\rangle$ becomes

$$\sum_{n=\max(0,-m)}^{l-m} = \frac{(-\tan\frac{\theta}{2})^{m+n}}{(m+n)!}\frac{(\tan\frac{\theta}{2})^n}{n!}\left(\prod_{r=1}^{n}\sqrt{(l-m-r+1)(l+m+r)}\right)\left(\cos\frac{\theta}{2}\right)^{2m+2n}$$
$$\times\prod_{s=1}^{m+n}\sqrt{(l+m+n-s+1)(l-m-n+s)}$$

because $\langle l, m{=}0|l, m{=}0\rangle = 1$.

Now, we need to simplify. Note that

$$\begin{aligned}\left(-\tan\frac{\theta}{2}\right)^{m+n}\left(\tan\frac{\theta}{2}\right)^{n}\left(\cos\frac{\theta}{2}\right)^{2m+2n} &= (-1)^{m+n}\left(\sin\frac{\theta}{2}\right)^{2n+m}\left(\cos\frac{\theta}{2}\right)^{m}\\ &= (-1)^{m+n}\left(\frac{1}{2}\right)^{m}(\sin\theta)^m\left(\sin^2\frac{\theta}{2}\right)^{n}\\ &= \left(\frac{1}{2}\right)^{m+n}(\sin\theta)^m(1-\cos\theta)^n,\end{aligned}$$

where we made use of the half-angle identities $\sin\frac{\theta}{2}\cos\frac{\theta}{2} = \frac{\sin\theta}{2}$ and $\cos\theta = 1-2\sin^2\frac{\theta}{2}$. The two product factors become

$$\prod_{r=1}^{n}\sqrt{(l-m-r+1)(l+m+r)}\prod_{s=1}^{m+n}\sqrt{(l+m+n-s+1)(l-m-n+s)}$$
$$= \sqrt{\frac{(l-m)!}{(l-m-n)!}\frac{(l+m+n)!}{(l+m)!}\frac{(l+m+n)!}{l!}\frac{l!}{(l-m-n)!}}.$$

Simplifying, we find

$$= \frac{(l+m+n)!}{(l-m-n)!}\sqrt{\frac{(l-m)!}{(l+m)!}}.$$

4 Putting it all together

So the spherical harmonic becomes (deep breath)

$$Y_{lm}(\theta,\phi) = \langle \theta{=}0,\phi{=}0|l,m{=}0\rangle\, e^{im\phi} \sum_{n=\max(0,-m)}^{l-m} \left(\frac{1}{2}\right)^{m+n} (\sin\theta)^m (1-\cos\theta)^n \times \frac{(l+m+n)!}{(l-m-n)!}\sqrt{\frac{(l-m)!}{(l+m)!}}\frac{1}{n!}\frac{1}{(m+n)!}.$$

Pulling out the n-independent factors,

$$Y_{lm}(\theta,\phi) = \langle \theta{=}0,\phi{=}0|l,m{=}0\rangle\, e^{im\phi}(\sin\theta)^m \left(-\frac{1}{2}\right)^{m} \sqrt{\frac{(l-m)!}{(l+m)!}} \times \sum_{n=\max(0,-m)}^{l-m} \left(-\frac{1}{2}\right)^{n} (1-\cos\theta)^n \frac{(l+m+n)!}{(l-m-n)!}\frac{1}{n!(m+n)!}$$

In essence, we are finished. But it is customary to re-express this in terms of functions defined by dead French and German mathematicians. To do this, recall the *associated Legendre polynomial*, which is given by

$$P_l^m(\cos\theta) = \frac{1}{2^m}(\sin\theta)^m \sum_{n=0}^{l-m}(-1)^n \frac{(l+m+n)!}{(l-m-n)!(m+n)!n!}\left(\frac{1-\cos\theta}{2}\right)^n.$$

In spite of its name, it is not a polynomial of its argument. So, for $m \geq 0$, we have

$$\boxed{Y_{lm}(\theta,\phi) = e^{im\phi}(-1)^m \sqrt{\frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta)\, \langle \theta{=}0,\phi{=}0|l,m{=}0\rangle}$$

In my personal opinion, this is a much clearer way to find the spherical harmonics than using differential equations. It is a classic "French cooking" exercise. Every step is rather simple, but there are many of them. One needs to work carefully and cautiously to get to the right final answer.

What about $m < 0$? We use the fact that $Y_{l,-|m|}(\theta,\phi) = (-1)^{|m|}(Y_{l,|m|}(\theta,\phi))^*$ to find it. One can also compute it directly using a similar scheme to what we just did.

5 Normalization constant

We still need $\langle \theta{=}0,\phi{=}0|l,m{=}0\rangle$ which comes from normalization. One can do this most easily for $m = l$:

$$P_l^l(\cos\theta) = \frac{1}{2^l}(\sin\theta)^l \frac{(2l)!}{l!}$$

So,

$$Y_{ll}(\theta,\phi) = \langle \theta{=}0,\phi{=}0|l,m{=}0\rangle\, e^{il\phi}\left(-\frac{1}{2}\right)^l (\sin\theta)^l \frac{\sqrt{(2l)!}}{l!}.$$

Integrate to find the normalization:

$$\begin{aligned} 1 &= \int_0^\pi d\theta\, (\sin\theta)^{2l+1} \frac{1}{4^l}\frac{(2l)!}{(l!)^2} |\langle\theta{=}0,\phi{=}0|l,m{=}0\rangle|^2 \int_0^{2\pi} d\phi \\ &= \frac{2\pi}{4^l}\frac{(2l)!}{(l!)^2} |\langle\theta{=}0,\phi{=}0|l,m{=}0\rangle|^2 \int_0^\pi d\theta\, (\sin\theta)^{2l+1}. \end{aligned}$$

By Wolfram Alpha, I find

$$\int_0^\pi d\theta\, (\sin\theta)^{2l+1} = \frac{\sqrt{\pi}\,\Gamma(l+1)}{\Gamma\left(l+\frac{3}{2}\right)} = \frac{2^{2l+1}(l!)^2}{(2l+1)!}$$

Therefore,

$$1 = |\langle\theta{=}0,\phi{=}0|l,m{=}0\rangle|^2 \frac{4\pi}{l+1} \implies \langle\theta{=}0,\phi{=}0|l,m{=}0\rangle = \sqrt{\frac{2l+1}{4\pi}}.$$

So, in conclusion, for $m \geq 0$

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

and for $m < 0$,

$$\boxed{Y_{l,-|m|}(\theta,\phi) = (-1)^{|m|}Y^*_{l,|m|}(\theta,\phi)}.$$

I encourage you to think about the other way you solved this problem with differential equations and think about which method felt more concrete and clear to you about what you calculated.