Phys 506 Lecture 8
Spherical harmonics done right

Recall from last time that we worked out

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

The spherical harmonic is defined to be the overlap of $\langle\theta,\phi|$ with $|lm\rangle$. We have

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

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

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

$$\mathbb{I} = \sum_{m'}|lm'\rangle\langle l,m'|$$

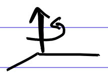
$$Y_{lm}(\theta,\phi) = e^{im\phi}\sum_{m'}\langle\theta=0,\phi=0|\,l\,m'\rangle\,\langle lm'|\,e^{i\theta\frac{\hat{L}_y}{\hbar}}|lm\rangle$$

The matrix element $d^{(l)}_{m'm}(\theta) = \langle lm'|e^{i\theta\frac{\hat{L}_y}{\hbar}}|lm\rangle$ is called the rotation matrix. It is a continuous matrix representation of the rotation group with $(2l+1)\times(2l+1)$ matrices. We already computed $d^{(\frac{1}{2})}_{m'm}(\theta,\phi)$ when we worked with Pauli matrices in lecture 1.

Fortunately, we do not need the whole matrix.

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 of what this is – it is a state pointing along the north pole. If I rotate about the north pole axis, I do <u>nothing</u>



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

$$\langle\theta=0,\phi|\,lm\rangle = \langle\theta=0,\phi=0|\,e^{i\phi\frac{\hat{L}_z}{\hbar}}|lm\rangle$$
$$= e^{im\phi}\,\langle\theta=0;\phi=0|\,lm\rangle$$

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

(Note, this implies l = integer, since $m=0$ only occurs when l = integer)

Hence, we have

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

$\uparrow$ just a number (norm const).

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

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

Now recall that

$$\frac{\hat{L}_+}{\hbar} | \ell, m \rangle = \sqrt{(\ell-m)(\ell+m+1)}\, | \ell, m+1 \rangle$$

$$\frac{\hat{L}_-}{\hbar} | \ell, m \rangle = \sqrt{(\ell+m)(\ell-m+1)}\, | \ell, m-1 \rangle$$

We expand the exponential 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 $e^{\tan\frac{\theta}{2} \frac{\hat{L}_+}{\hbar}} | \ell, m \rangle = \sum_{n=0}^{\infty} \frac{(\tan\frac{\theta}{2})^n}{n!} \left(\frac{\hat{L}_+}{\hbar}\right)^n | \ell, m \rangle$

But $(\hat{L}_+)^n | \ell, m \rangle = 0$ if $n > \ell - m$, since $\hat{L}_+ | \ell\, m=\ell \rangle = 0$

so $e^{\tan\frac{\theta}{2} \frac{\hat{L}_+}{\hbar}} | \ell, m \rangle = \sum_{n=0}^{\ell-m} \frac{(\tan\frac{\theta}{2})^n}{n!} \left(\frac{\hat{L}_+}{\hbar}\right)^n | \ell, m \rangle$

$$= \sum_{n=0}^{\ell-m} \frac{(\tan\frac{\theta}{2})^n}{n!} \left[\prod_{r=1}^{n} \sqrt{(\ell-m-r+1)(\ell+m+r)} \right] | \ell, m+n \rangle$$

operate the middle term $e^{\ln \cos^2\frac{\theta}{2} \frac{\hat{L}_z}{\hbar}}$ onto this. It is easy since $\frac{\hat{L}_z}{\hbar} | \ell, n \rangle = n | \ell, n \rangle$

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

Finally, we operate

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

onto the state. But since we multiply by $\langle \ell, m=0 |$ on the left, we need only include the term where $n' = m+n$. Since $n' \geq 0 \Rightarrow n$ must be at least $-m$

For a nonzero result,

so $\langle l\ m{=}0|\, e^{i\theta \hat{L}_y/\hbar}\, |l,m\rangle$ becomes

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

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

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

Now we need to simplify. Note that

$$\left(-\tan\frac{\theta}{2}\right)^{m+n} \left(\tan\frac{\theta}{2}\right)^{n} \left(\cos\frac{\theta}{2}\right)^{2m+2n}$$

$$= (-1)^{m+n} \left(\sin\frac{\theta}{2}\right)^{2n+m} \left(\cos\frac{\theta}{2}\right)^{m} \qquad \text{but } \sin\frac{\theta}{2}\cos\frac{\theta}{2} = \frac{\sin\theta}{2}$$

$$= (-1)^{m+n} \left(\frac{1}{2}\right)^{m} (\sin\theta)^{m} \left(\sin^2\frac{\theta}{2}\right)^{n} \qquad \text{but } \cos\theta = 1-2\sin^2\frac{\theta}{2}$$

$$= \left(-\frac{1}{2}\right)^{m+n} (\sin\theta)^{m} (1-\cos\theta)^{n}$$

The two product terms become

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

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

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

So, the spherical harmonic becomes (deep breath)

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

$$\times \frac{(l+m+n)!}{(l-m-n)!} \sqrt{\frac{(l-m)!}{(l+m)!}} \frac{1}{n!} \frac{1}{(m+n)!}$$

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

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

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, we note that the associated Legendre polynomial satisfies

$$P_\ell^m(\cos\theta) = \frac{1}{2^m}(\sin\theta)^m \sum_{n=0}^{\ell-m} (-1)^n \frac{(\ell+m+n)!}{(\ell-m-n)!\,(m+n)!\,n!}\left(\frac{1-\cos\theta}{2}\right)^n$$

So, for $m \geq 0$, we have

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

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 <u>many</u> of them. One needs to work carefully and cautiously to get the right final answer.

What about $m<0$? We use the fact that

$$Y_{\ell\,-|m|}(\theta,\phi) = (-1)^{|m|}\left[Y_{\ell|m|}(\theta,\phi)\right]^*$$

to find it. One can also compute it directly.

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

$$P_\ell^\ell(\cos\theta) = \frac{1}{2^\ell}(\sin\theta)^\ell\frac{(2\ell)!}{\ell!}$$

so $Y_{\ell\ell}(\theta,\phi) = \langle\theta=0,\phi=0,\ell,m=0\rangle e^{i\ell\phi}\left(-\frac{1}{2}\right)^\ell(\sin\theta)^\ell\frac{\sqrt{(2\ell)!}}{\ell!}$

Integrate to get the normalization:

$$1 = \int_0^\pi d\theta\,(\sin\theta)^{2\ell+1}\frac{1}{4^\ell}\frac{(2\ell)!}{(\ell!)^2}|\langle\theta=0,\phi=0|\ell,m=0\rangle|^2\int_0^{2\pi}d\phi$$

$$= \frac{2\pi\ (2\ell)!}{4^\ell(\ell!)^2}|\langle\theta=0,\phi=0|\ell,m=0\rangle|^2\int_0^\pi d\theta\,(\sin\theta)^{2\ell+1}$$

But $\int_0^\pi d\theta\,(\sin\theta)^{2\ell+1} = \frac{\sqrt{\pi}\,\Gamma(\ell+1)}{\Gamma(\ell+\frac{3}{2})}$ (Wolfram alpha)

$$= \frac{\sqrt{\pi}\,\ell!}{(\ell+\frac{1}{2})(\ell-\frac{1}{2})(\ell-\frac{3}{2})\cdots(\frac{3}{2})(\frac{1}{2})\Gamma(\frac{1}{2})}$$

$$= \frac{\sqrt{\pi}\, l!}{\frac{1}{2^{l+1}} (2l+1)!!\, \sqrt{\pi}} = \frac{2^{l+1} l!\, 2^l\, l!}{(2l+1)!}$$

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$$= \frac{2^{2l+1} (l!)^2}{(2l+1)!}$$

$$\Rightarrow \quad 1 = |\langle \theta=0, \phi=0 | l, m=0 \rangle|^2 \cdot \frac{4\pi}{(2l+1)}$$

$$\text{or} \quad \langle \theta=0, \phi=0 | l, m=0 \rangle = \sqrt{\frac{2l+1}{4\pi}}$$

So

$$\boxed{Y_{lm}(\theta,\phi) = \sqrt{\frac{(2l+1)}{4\pi} \frac{(l-m)!}{(l+m)!}}\, (-1)^m P_l^m(\cos\theta)\, e^{im\phi}} \quad \text{for } m \geq 0$$

$$\boxed{Y_{l\,-|m|}(\theta,\phi) = (-1)^{|m|}\, Y^*_{l\,|m|}(\theta,\phi) \quad \text{for } m<0}$$