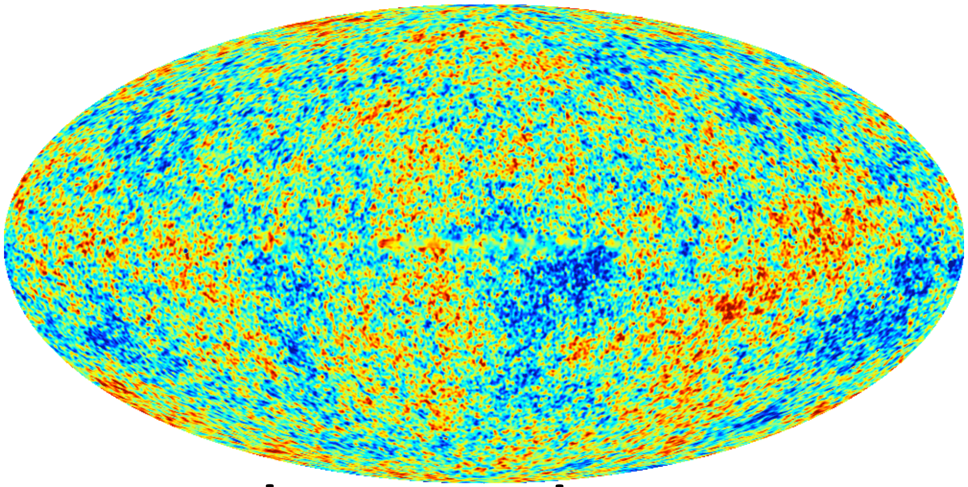
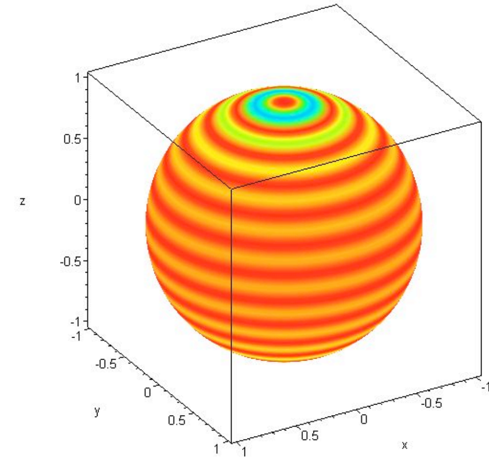
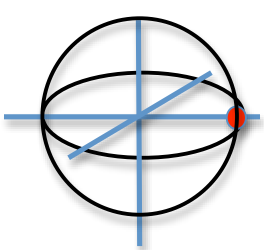
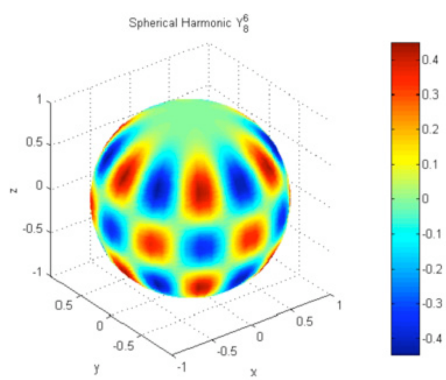


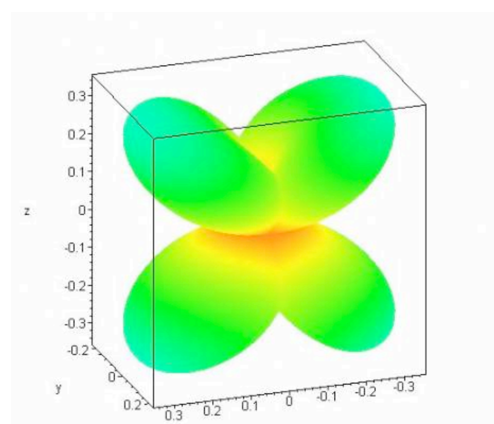


The Rigid Rotor Problem: A quantum particle confined to a sphere
Spherical Harmonics

Reading: McIntyre 7.6







Legendre's equation (m = 0)
The series must be finite!

- If the series is not finite, the polynomial blows up (check ratio for large n)

$$A = n_{\max}\left(n_{\max}+1\right)$$

$$A = \ell\left(\ell+1\right)$$ ← Anticipated this!

$$a_{n+2} = \frac{n(n+1) - A}{(n+2)(n+1)} a_n$$

- These special values of A give Legendre polynomials.

$$P_0(z) = 1$$

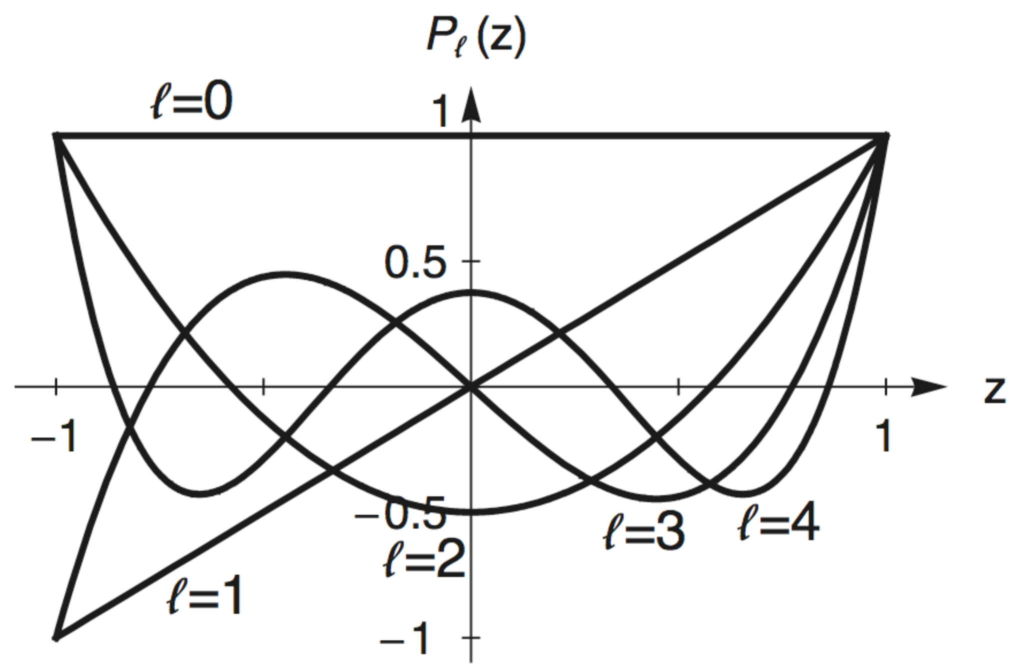
$$P_1(z) = z$$

$$P_2(z) = \frac{1}{2}(3z^2 - 1)$$

$$P_3(z) = \frac{1}{2}(5z^3 - 3z)$$

$$P_4(z) = \frac{1}{8}(35z^4 - 30z^2 + 3)$$

$$P_5(z) = \frac{1}{8}(63z^5 - 70z^3 + 15z)$$



The energy for the rigid rotor problem

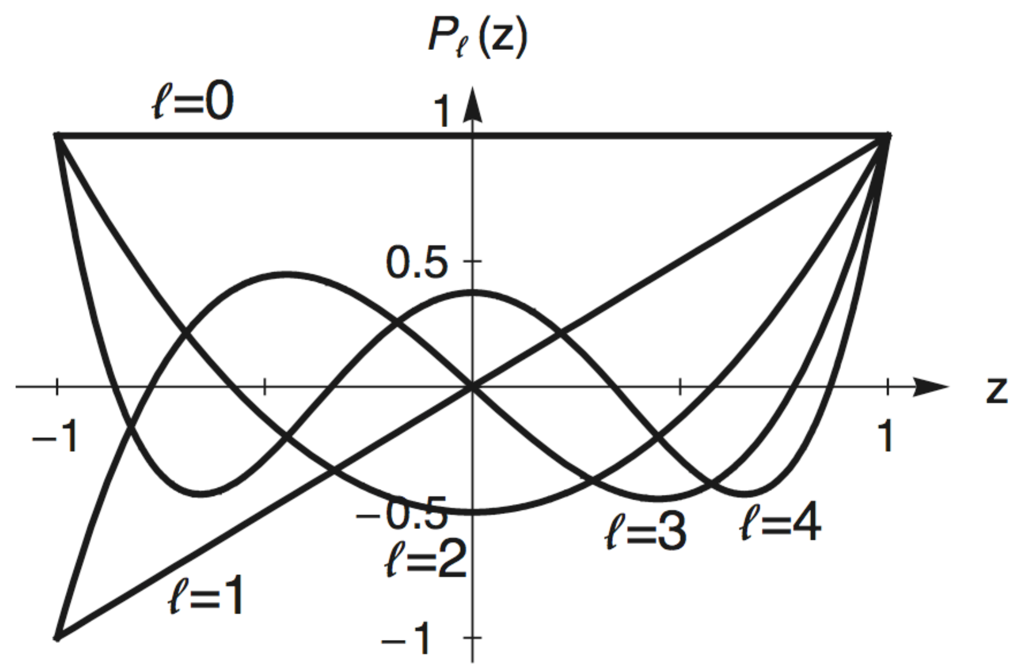
- Go back to the original statement of the rigid rotor problem to see how *A* is related to *E*.

$$A = \ell(\ell+1) \Rightarrow E_\ell = \frac{\ell(\ell+1)\hbar^2}{2I}$$

- el is an integer (energy is quantized)

Legendre polynomials

- Rodrigues' formula $$P_\ell(z) = \frac{1}{2^\ell \ell!} \frac{d^\ell}{dz^\ell} \left(z^2 - 1\right)^\ell$$
- Orthogonal (Herm op)! $$\int_{-1}^{1} P_k^*(z) P_\ell(z) dz = \frac{\delta_{k\ell}}{\ell + \frac{1}{2}}$$
- Of degree ℓ
- Either even or odd

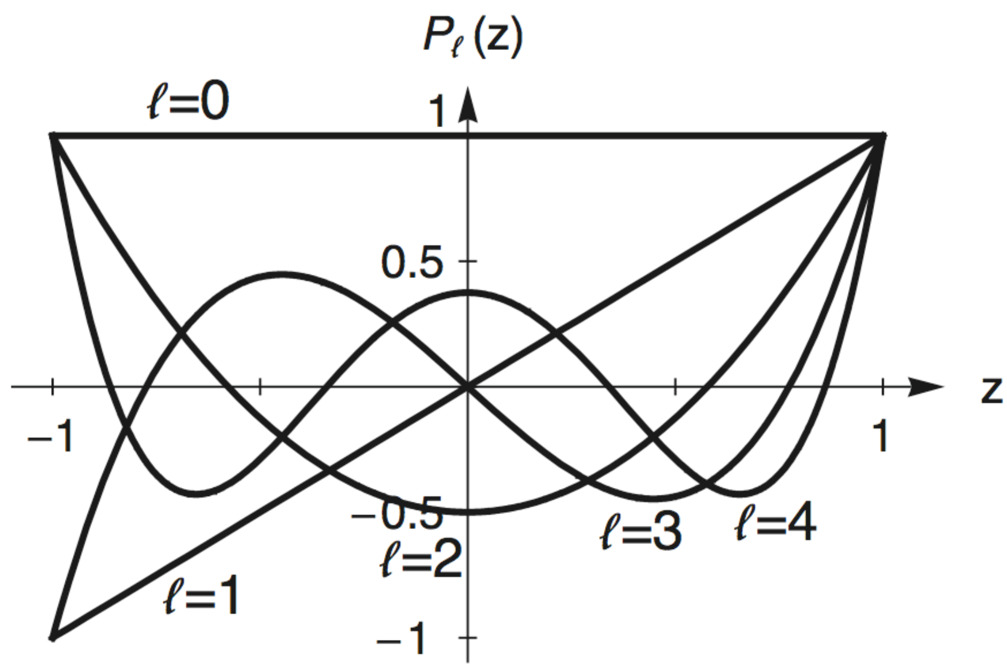


Legendre polynomials

- Orthogonal means we can express any function defined on that interval as a superposition of Legendre polynomials: HW

$$\left(\ell+\tfrac{1}{2}\right)\int_{-1}^{1} P_k^*(z)P_\ell(z)dz = \delta_{k\ell}$$

- This means we can project and find probabilities just as with sines, cosines and exp($im\phi$)



Associated Legendre polynomials

- $m \neq 0$

$$\left((1-z^2)\frac{d^2}{dz^2} - 2z\frac{d}{dz} + \ell(\ell+1) - \frac{m^2}{(1-z^2)} \right) P(z) = 0$$

$$P_\ell^m(z) = P_\ell^{-m}(z) = (1-z^2)^{m/2}\frac{d^m}{dz^m}\left(P_\ell(z)\right)$$

$$= \frac{1}{2^\ell \ell!}(1-z^2)^{m/2}\frac{d^{m+\ell}}{dz^{m+\ell}}\left((z^2-1)^\ell\right)$$

Associated Legendre polynomials

- $m \neq 0$, ℓ integer

$$P_0^0 = 1$$

$$P_1^0 = \cos\theta$$

$$P_1^1 = \sin\theta$$

$$P_2^0 = \tfrac{1}{2}(3\cos^2\theta - 1)$$

$$P_2^1 = 3\sin\theta\cos\theta$$

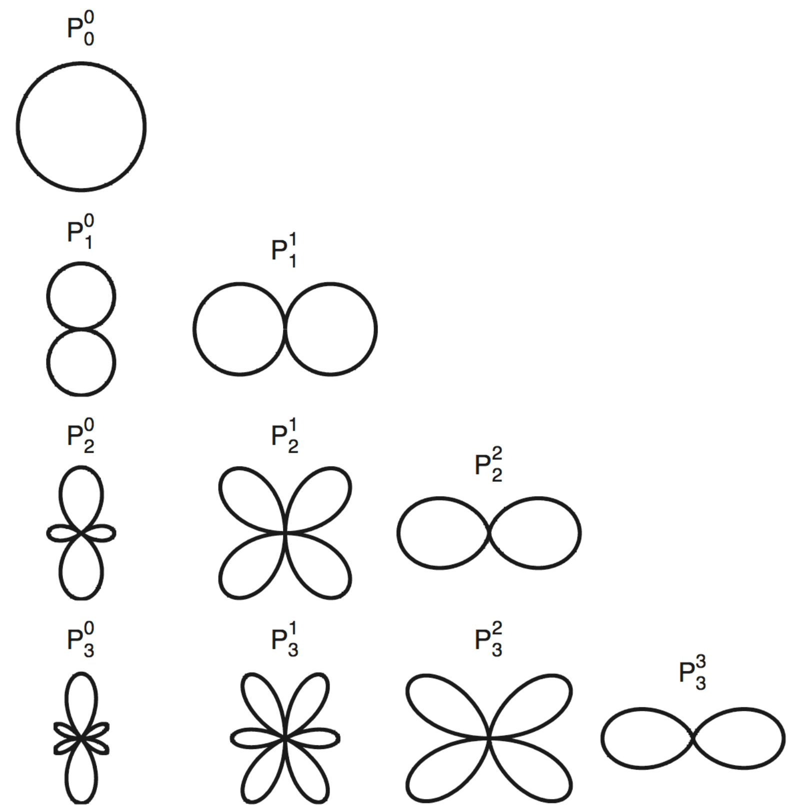
$$P_2^2 = 3\sin^2\theta$$

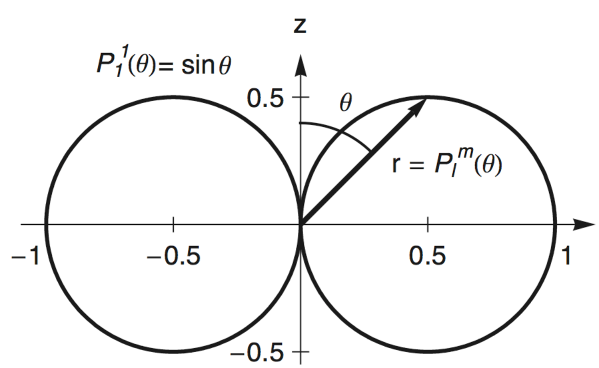
$$P_3^0 = \tfrac{1}{2}(5\cos^3\theta - 3\cos\theta)$$

$$P_3^1 = \tfrac{3}{2}\sin\theta(5\cos^2\theta - 1)$$

$$P_3^2 = 15\sin^2\theta\cos\theta$$

$$P_3^3 = 15\sin^3\theta$$

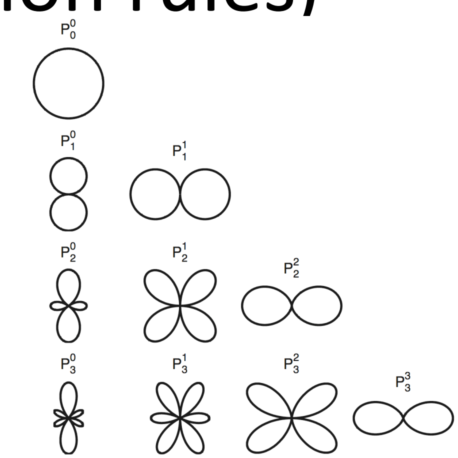




Associated Legendre polynomials

- $P_\ell^m(z) = 0 \text{ if } |m| > \ell$ restricts *m* to ± el → determines # of orbitals
- $P_\ell^{-m}(z) = P_\ell^m(z)$ opposite projections have same spatial form
- $P_\ell^m(\pm 1) = 0 \text{ for } m \neq 0$ *yz* plane is a node
- $P_\ell^m(-z) = (-1)^{\ell - m} P_\ell^m(z)$ parity (selection rules)
- Orthogonal (for given *m*)

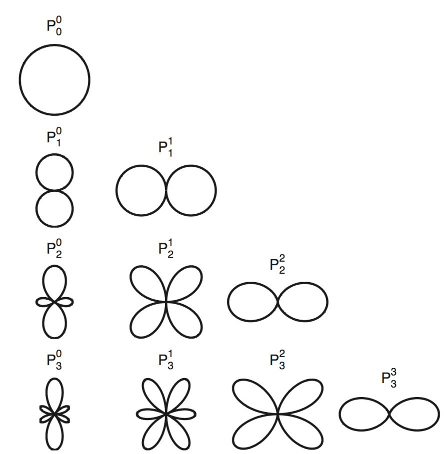
$$\int_{-1}^{1} P_\ell^m(z) P_q^m(z)\, dz = \frac{2}{(2\ell+1)} \frac{(\ell+m)!}{(\ell-m)!} \delta_{\ell q}$$



Finally …..

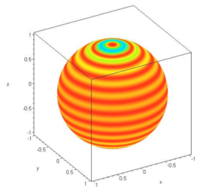
- The normalized polynomial that solves the theta equation is (typo in book Eq. 7.156) :

$$\Theta_{\ell}^{m}(\theta)=\left(-1\right)^{m}\sqrt{\frac{(2\ell+1)}{2}\frac{(\ell-|m|)!}{(\ell+|m|)!}}\;P_{\ell}^{m}(\cos\theta)$$



Summary

- The fact that the series must be finite polynomial of degree *el* is what (mathematically) leads to a maximum (and integer) value of *el*!
- The fact that the series is finite means that we can differentiate it only a finite number of times (*el*) and that number turns out to be *m*!! Thus *m* is limited to –*el* … *el*.
- Legendre functions are orthogonal on [-1,1]
- Legendre and associated Legendre functions.



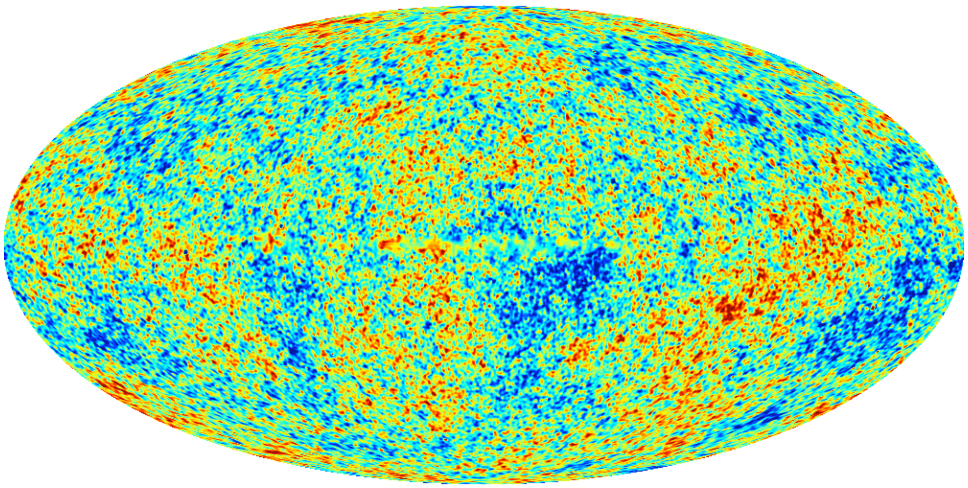
Spherical harmonics:

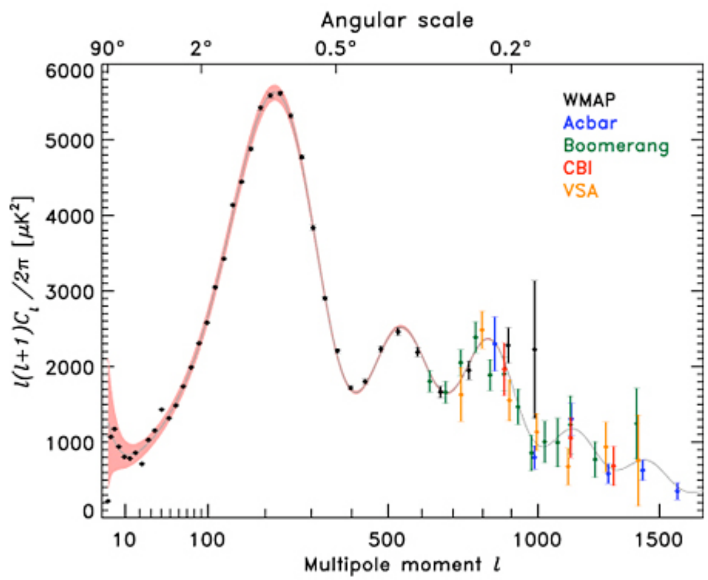
- Original problem was separated into angular and radial parts. We further separated angular parts into theta and phi.

$$Y_\ell^m(\theta,\phi) = \Theta_\ell^m(\theta)\Phi_m(\phi)$$

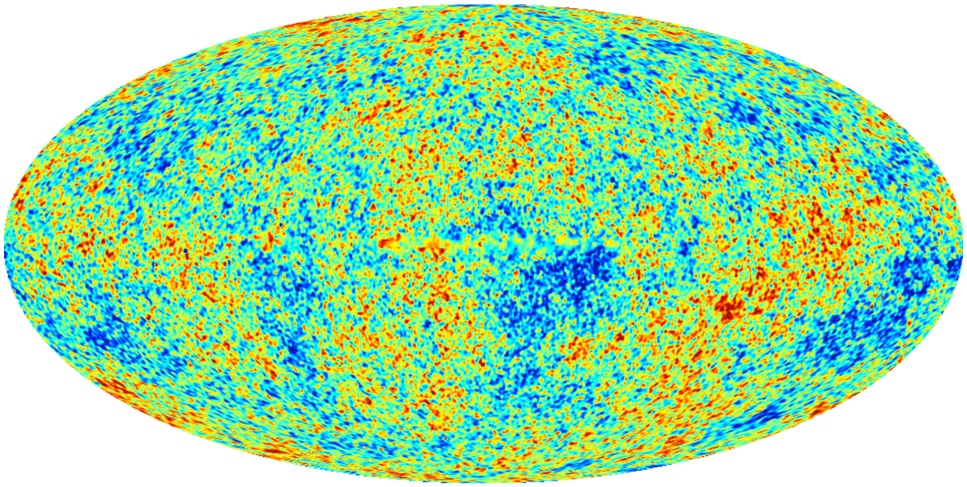
- These functions are the angular part of the solution to the hydrogen atom problem, and indeed ANY central force problem!!

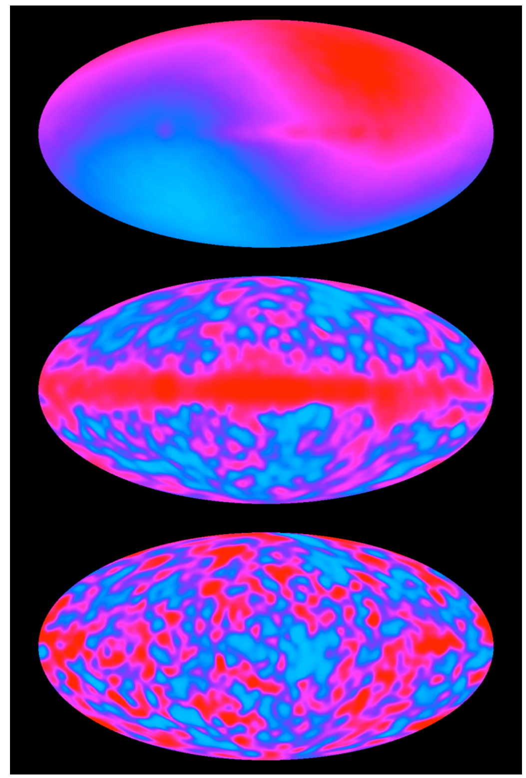
Do you know what this is?

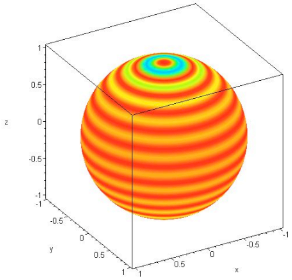




The cosmic microwave background is analyzed with spherical harmonics!



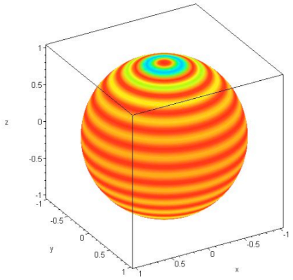




Spherical Harmonics

$$Y_\ell^m(\theta,\phi) = (-1)^{(m+|m|)/2}\sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-|m|)!}{(\ell+|m|)!}}P_\ell^m(\cos\theta)e^{im\phi}$$

ℓ	m	$Y_\ell^m(\theta,\phi)$
0	0	$Y_0^0 = \sqrt{\frac{1}{4\pi}}$
1	0	$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$
	±1	$Y_1^{\pm1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\phi}$
2	0	$Y_2^0 = \sqrt{\frac{5}{16\pi}}\left(3\cos^2\theta - 1\right)$
	±1	$Y_2^{\pm1} = \mp\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{\pm i\phi}$
	±2	$Y_2^{\pm2} = \sqrt{\frac{15}{32\pi}}\sin^2\theta e^{\pm i2\phi}$
3	0	$Y_3^0 = \sqrt{\frac{7}{16\pi}}\left(5\cos^3\theta - 3\cos\theta\right)$
	±1	$Y_3^{\pm1} = \mp\sqrt{\frac{21}{64\pi}}\sin\theta\left(5\cos^2\theta - 1\right)e^{\pm i\phi}$
	±2	$Y_3^{\pm2} = \sqrt{\frac{105}{32\pi}}\sin^2\theta\cos\theta e^{\pm i2\phi}$
	±3	$Y_3^{\pm3} = \sqrt{\frac{35}{64\pi}}\sin^3\theta e^{\pm i3\phi}$



Spherical Harmonics

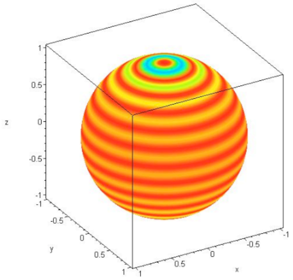
$$Y_\ell^m(\theta,\phi) = (-1)^{(m+|m|)/2}\sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-|m|)!}{(\ell+|m|)!}}P_\ell^m(\cos\theta)e^{im\phi}$$

- What is the action of these operators on the spherical harmonics?

$$L^2 Y_\ell^m(\theta,\phi) = ?$$

$$L_z Y_\ell^m(\theta,\phi) = ?$$

- Do the two operators commute?



Spherical Harmonics

$$\left|\ell m\right\rangle$$

- What is the action of these operators on the spherical harmonics?

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$$L_z\left|\ell m\right\rangle = ?$$

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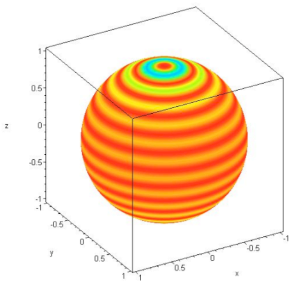


Spherical Harmonics

$$Y_\ell^m(\theta,\phi) = (-1)^{(m+|m|)/2}\sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-|m|)!}{(\ell+|m|)!}}P_\ell^m(\cos\theta)e^{im\phi}$$

- Orthonormal on the sphere

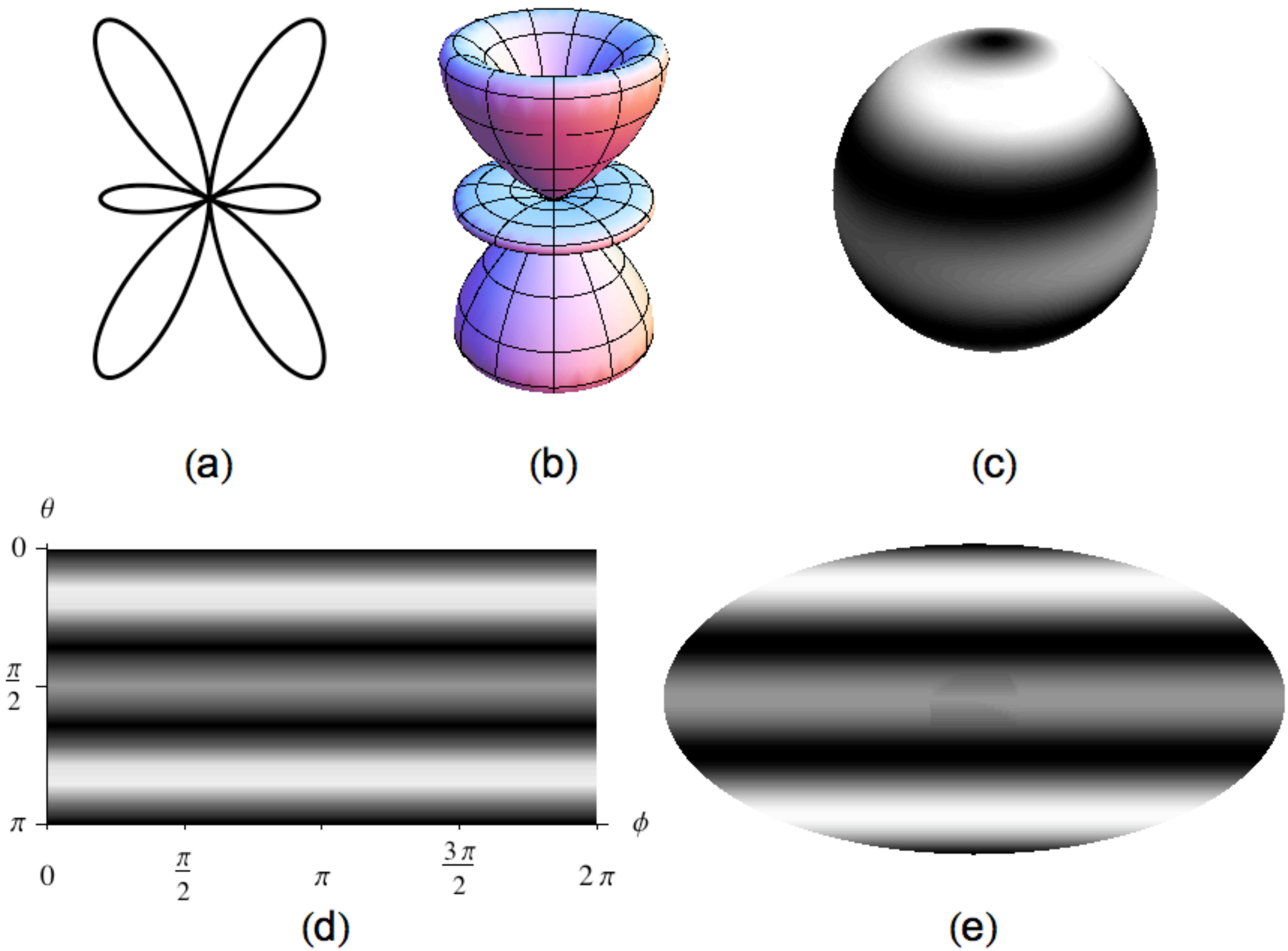
$$\left\langle \ell_1 m_1 \middle| \ell_2 m_2 \right\rangle = \delta_{\ell_1\ell_2}\delta_{m_1m_2}$$

$$\int_0^{2\pi}\int_0^{\pi}\left(Y_{\ell_1}^{m_1}(\theta,\phi)\right)^* Y_{\ell_2}^{m_2}(\theta,\phi)\underbrace{\sin\theta\, d\theta\, d\phi}_{?} = \delta_{\ell_1\ell_2}\delta_{m_1m_2}$$

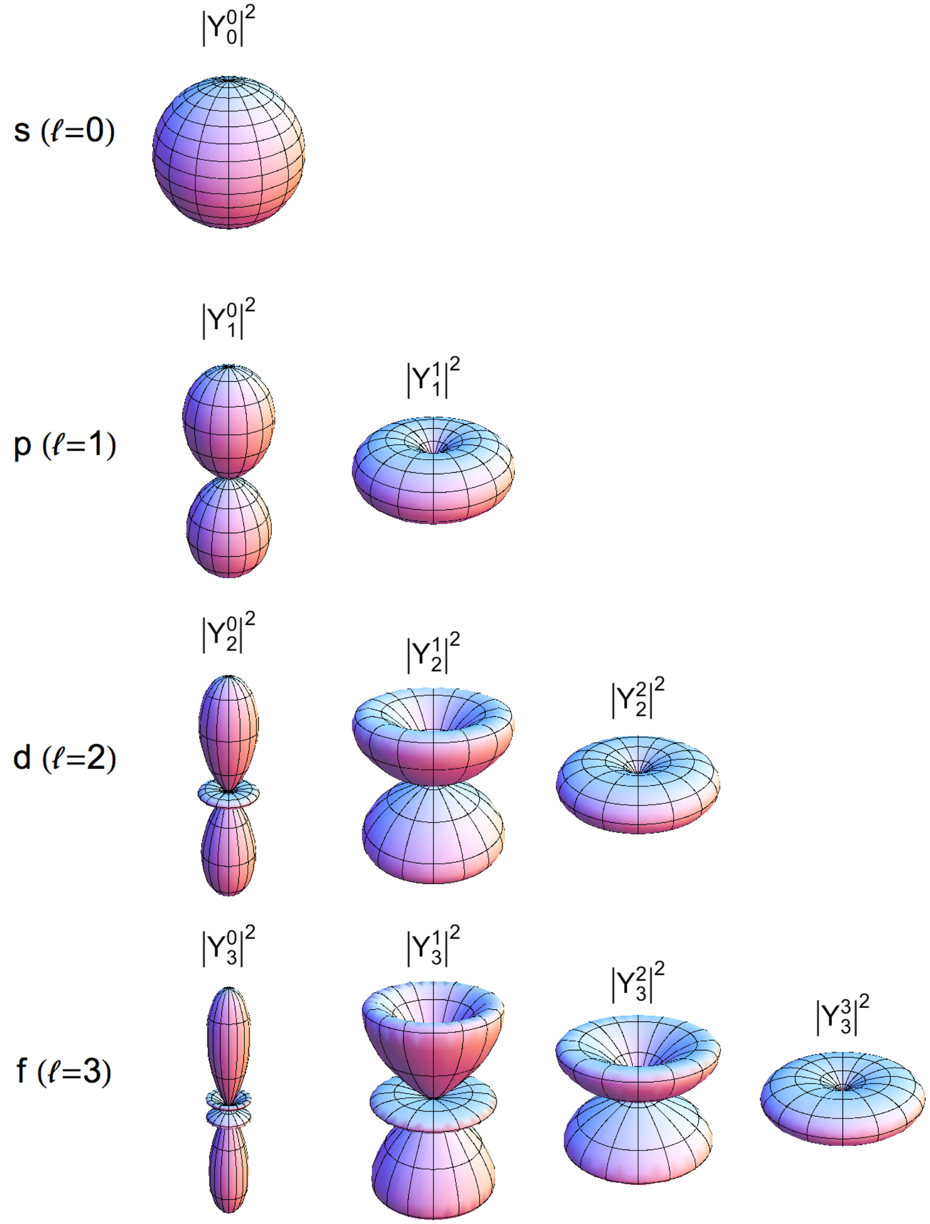
Do you remember where this comes from?

- Now we'll spend some time visualizing probability distributions of eigenstates and superpositions.

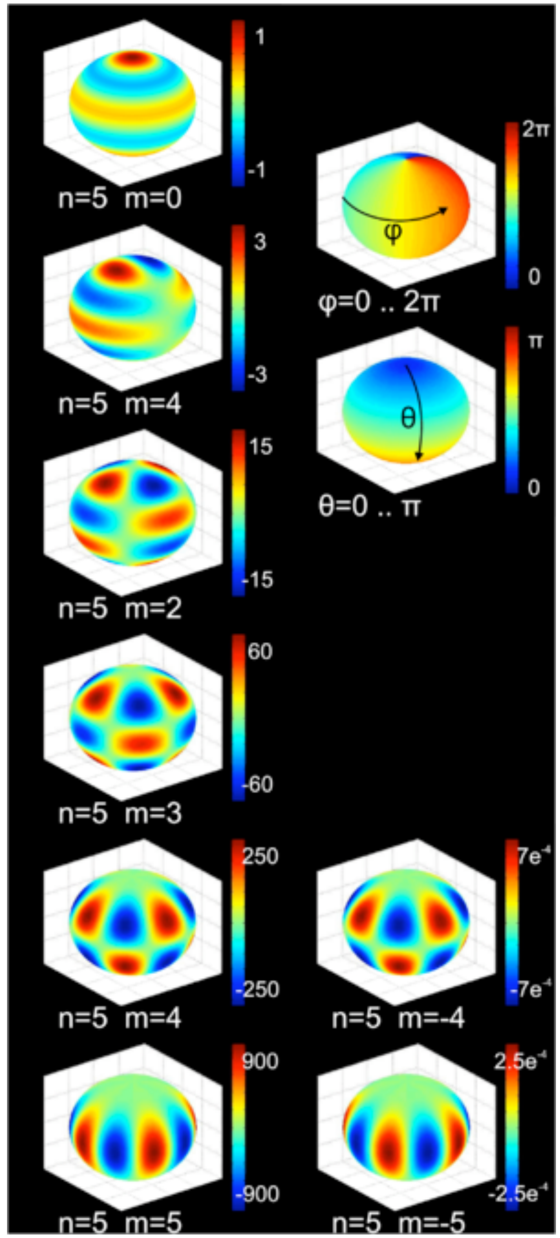
Spherical Harmonics



Spherical Harmonics



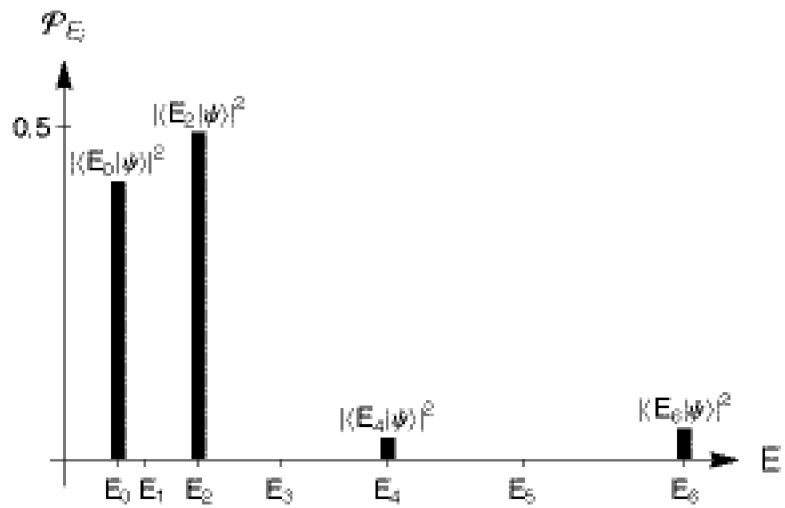
Spherical Harmonics

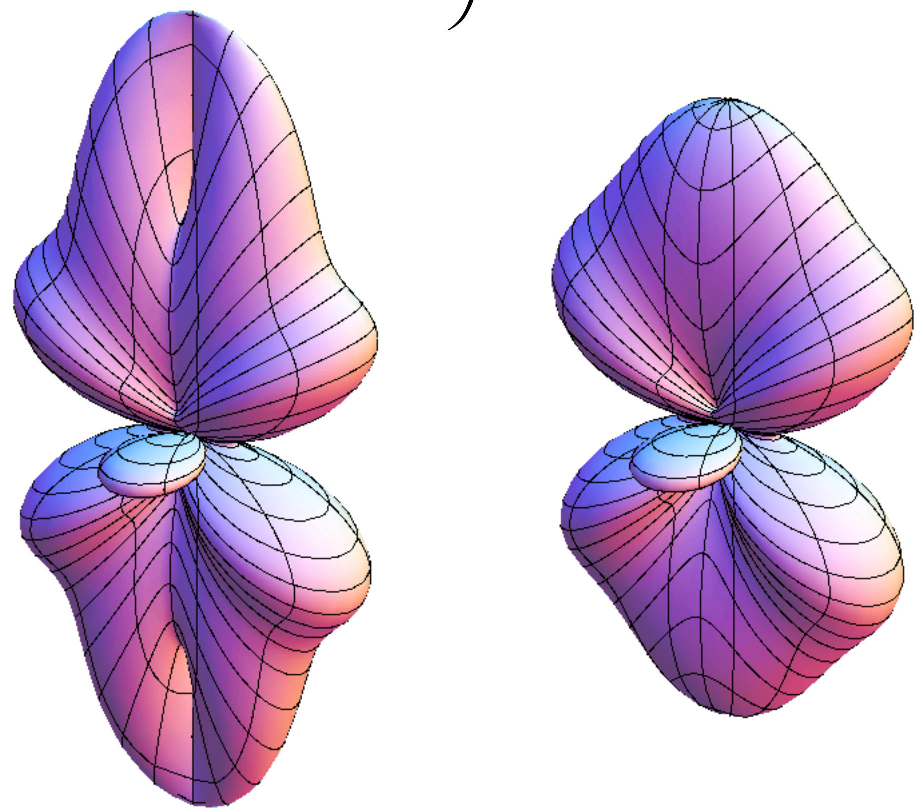


Spherical Harmonic Expansion

$$\psi(\theta,\phi) = \sqrt{\frac{60060}{139301\pi}}\left(\frac{1}{4} + \cos^3 2\theta + \sin^2\phi\right)$$

$$\mathcal{P}_{E_\ell} = \sum_{m=-\ell}^{\ell} \left|\langle \ell m | \psi \rangle\right|^2$$





(a) (b)

About the spherical harmonics

- $Y_\ell^m(\theta,\phi) = (-1)^\ell Y_\ell^m(\pi-\theta,\phi+\pi)$ parity ("even" or "odd". This will be helpful when study selection rules for transitions between states.
- opposite projections have same spatial form
- *yz* plane is a node
- Orthonormal

Spherical harmonics as a basis set

- The orthonormality of the spherical harmonics means that any function define on a sphere can be expressed as a superposition of spherical harmonics.
- Electromagnetism – multipoles of a charge distribution
- Gravitation – multipoles of a mass distribution
- The CMB example – multipoles of the temperature fluctuations of the early universe

Spherical harmonics as a basis set

- Find the coefficients of the function

$$f(\theta,\phi) = \sqrt{\frac{15}{16\pi}} \sin 2\theta \sin\phi$$

expanded as a Laplace series (series of sph. har.)

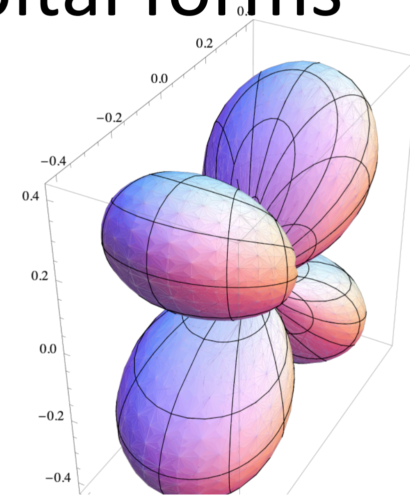
$$f(\theta,\phi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} c_{\ell m} Y_{\ell}^{m}\left(\theta,\phi\right)$$

The real (as opposed to complex) spherical harmonics

- In gravitation problems, the complex numbers in the spherical harmonics are rarely useful, so other linear combinations are used.

$$d_{yz}(\theta,\phi) \sim Y_2^1\left(\theta,\phi\right) + e^{i\delta} Y_2^{-1}\left(\theta,\phi\right)$$

- You'll recognize these as the *p, d, f* orbital forms from chemistry



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