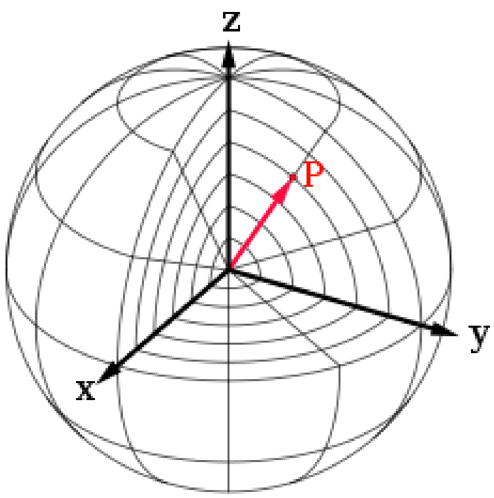
Separation of variables in spherical polar coordinates

We now consider the following class of PDEs:



$$\left(-\nabla^2 + f(r)\right)\psi = 0$$

The function $f(r)$ only depends on the distance from the origin.

Physics-y example: an electron around an atom obeys

$$-\frac{\hbar^2}{2m}\nabla^2\psi + \left[V(r) - E\right]\psi = 0$$

The general form of the PDE is

$$\left(-\nabla^2 + f(r)\right)\psi = 0$$

In spherical polar coordinates, this equation is

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2} + f(r)\psi = 0$$

Substitute a separation Ansatz:

We have found for the (r, θ) part of the equation

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)\sin^2\theta - fr^2\sin^2\theta + \frac{\sin\theta}{\Theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right) - \lambda = 0$$

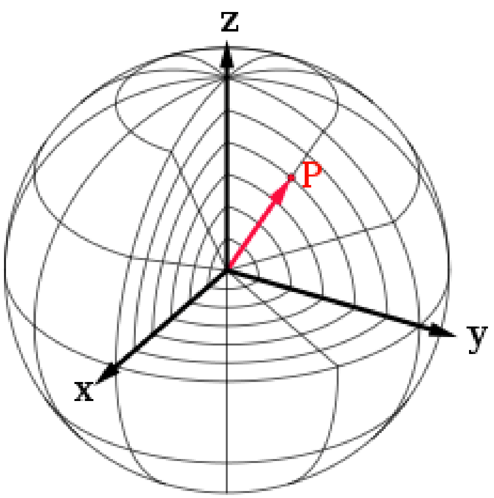
We end up with three equations:

$$\frac{1}{\Phi}\frac{\partial \Phi}{\partial \varphi} = -\lambda$$

$$\frac{1}{\Theta \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial \Theta}{\partial \theta}\right) - \frac{\lambda}{\sin^2\theta} = -\mu$$

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2 \frac{\partial R}{\partial r}\right) - f(r) r^2 = \mu$$

The problem for $\Phi(\varphi)$ is the familiar Sturm-Liouville problem:



$$\Phi'' = -\lambda\Phi$$

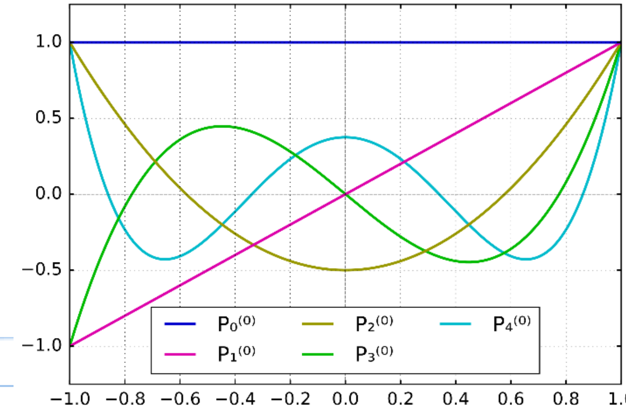
$$\Phi(0) = \Phi(2\pi),$$

$$\Phi'(0) = \Phi'(2\pi)$$

With solutions

We write the solutions to

$$\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) - \frac{m^2}{\sin^2\theta}\right]\Theta = -\mu\Theta$$



as

$$\Theta(\theta) = P_\ell^m(\cos\theta)$$

with

$$\mu = \ell(\ell+1)$$

These are (complicated) functions of $\cos\theta$, called Associated Legendre Polynomials

$$P_0^0(x) = 1$$

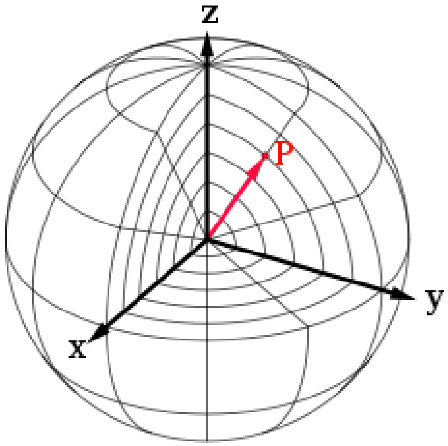
$$P_1^0(x) = x$$

$$P_2^0(x) = \frac{1}{2}(3x^2 - 1)$$

$$P_1^1(x) = -(1-x^2)^{1/2}$$

These functions are “google-able” and can be easily computed.

We have found for the φ and θ dependence that



$$\Theta(\theta) = P_\ell^m(\cos\theta)$$

$$\Phi(\varphi) = e^{im\varphi}$$

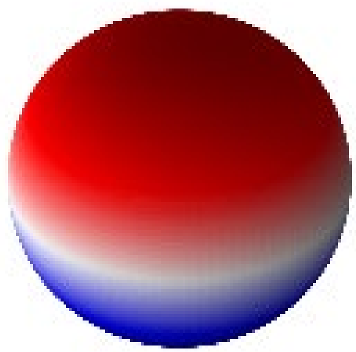
It makes sense to bundle these together into a new function, called a *spherical harmonic*

$$Y_{\ell,m}(\theta,\varphi) = P_\ell^m(\cos\theta)e^{im\varphi}$$

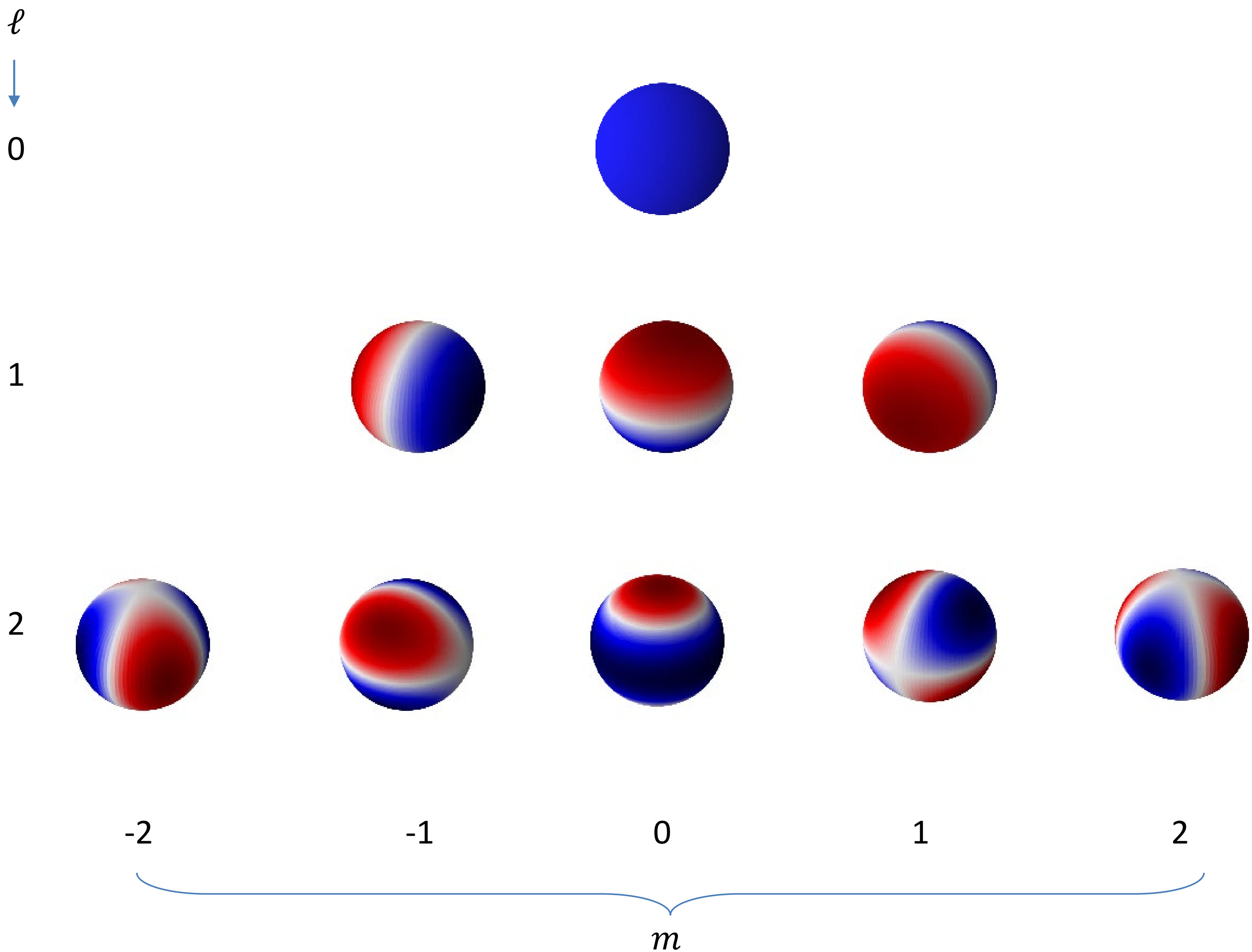
With m, ℓ integers such that

$$|m| < \ell$$

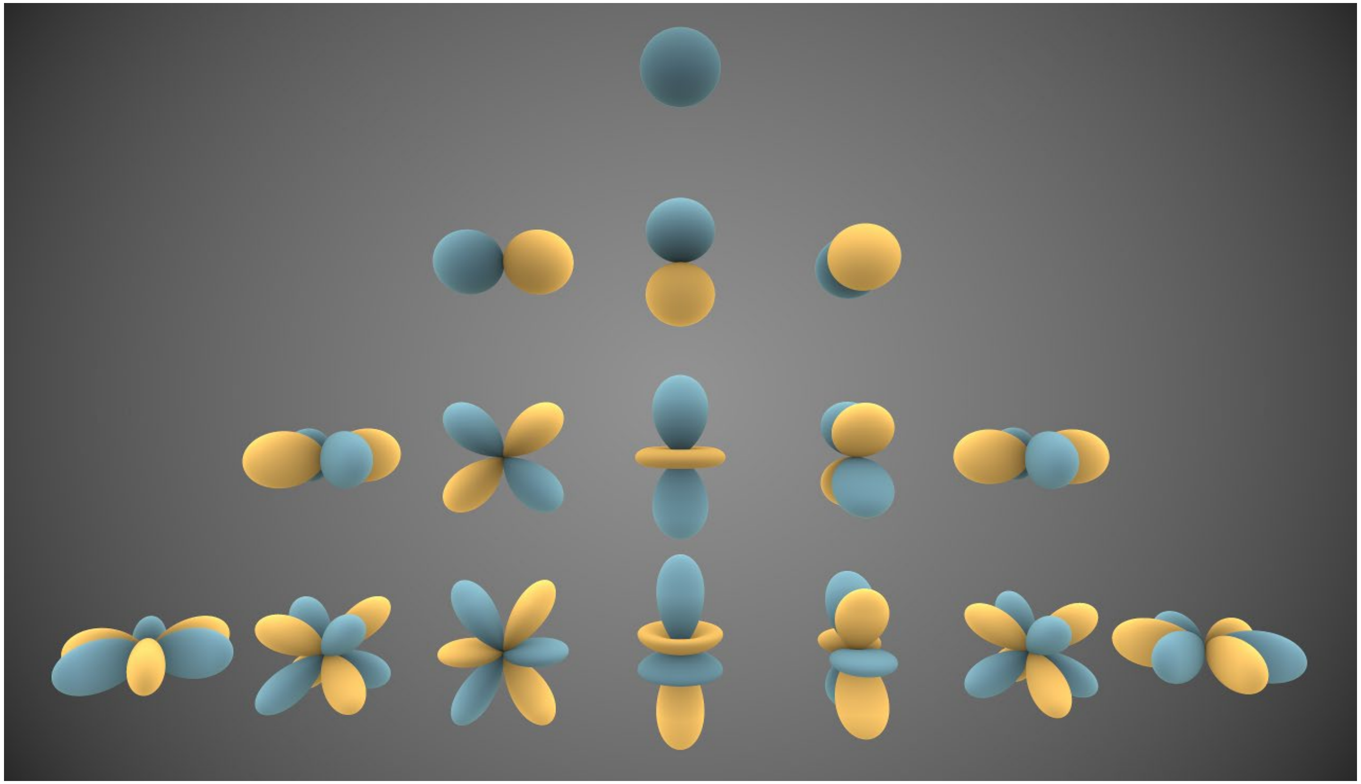
What do these look like in 3D?



$m = 0, \ell = 1$



ℓ
0
1
2
-2
-1
0
1
2
m



From Wikipedia:
“Spherical harmonics”

We end up with three equations:

$$\frac{1}{\Phi}\frac{\partial \Phi}{\partial \varphi} = -\lambda$$

$$\frac{1}{\Theta \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial \Theta}{\partial \theta}\right) - \frac{\lambda}{\sin^2\theta} = -\mu$$

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2 \frac{\partial R}{\partial r}\right) - f(r) r^2 = \mu$$

What about the problem for R? We had

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) - f(r)r^2 - \ell(\ell+1) = 0$$

The solution now depends on $f(r)$, which depends on the problem we are trying to solve.

Start with <u>Laplace's equation:</u>

Schrodinger's equation for the hydrogen atom

Separation of variables in spherical polar coordinates

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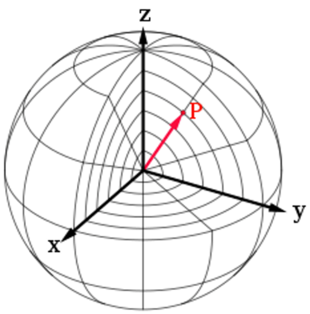
$$\left(-\nabla^2 + f(r)\right)\psi = 0$$



The function $f(r)$ only depends on the distance from the origin.

Physics-y example: an electron around an atom obeys

$$-\frac{\hbar^2}{2m}\nabla^2\psi + \left[V(r) - E\right]\psi = 0$$

$V(r)$ is the electric potential (see Week 7)

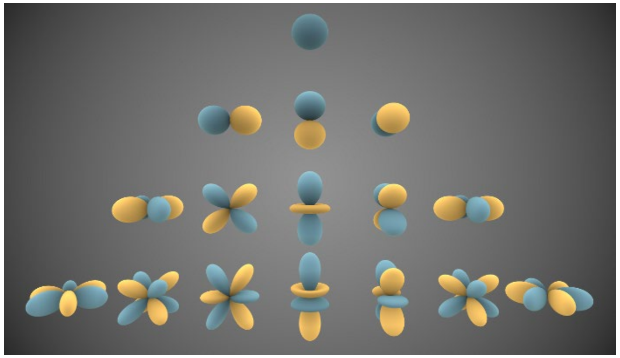
$$V(r) = -\frac{q^2}{4\pi\epsilon_0}\frac{1}{r}$$

So we want to solve

Choose the function

$$f(r) = -\frac{2m}{\hbar^2}\left(E - \frac{q^2}{4\pi\varepsilon_0 r}\right)$$

$$= -E' - \frac{k}{r}$$



and try to solve for the $\ell = 0$ case:

$$\frac{1}{r^2}\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + E' + \frac{k}{r} = 0$$