# Lecture 12: Three-dimensional systems: the spherical harmonics

We now want to find an explicit expression for the eigenfunctions of the angular momentum. In order to do so, we adopt spherical coordinates$(r, \theta, \phi)$:

$$r = \sqrt{x^2 + y^2 + z^2} \quad , \quad \theta = \tan^{-1} \frac{\sqrt{x^2 + y^2}}{z} \quad , \quad \phi = \tan^{-1} \frac{y}{x} \tag{1}$$

Assuming that the potential in the Schrödinger equation has a central symmetry: $V(\vec{r}) = V(r)$, we can separate the wavefunction into its three components:

$$\psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi) \tag{2}$$

In this new set of coordinates, the components $L_3, L_+, L_-$ read, respectively:

$$\begin{aligned} L_3 &= -i\tfrac{\partial}{\partial\phi} \\ L_+ &= e^{i\phi}\left(\tfrac{\partial}{\partial\theta} + i\cot\theta\tfrac{\partial}{\partial\phi}\right) \\ L_- &= e^{-i\phi}\left(-\tfrac{\partial}{\partial\theta} + i\cot\theta\tfrac{\partial}{\partial\phi}\right) \end{aligned} \tag{3}$$

These relations imply that:

$$L^2 = -\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \tag{4}$$

To find the eigenfunctions of $L^2$, we thus need to solve the equation:

$$-\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\Theta(\theta)\Phi(\phi) = \ell(\ell+1)\Theta(\theta)\Phi(\phi) \tag{5}$$

The solution of this equation requires a long and tedious algebraic work. We will skip it here and only provide the main results. This equation can be separated into two contributions, one for $\Theta(\theta)$ and one for $\Phi(\phi)$. The equation for $\Phi(\phi)$ is trivial and has solutions:

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}}e^{im\phi} \tag{6}$$

Using this result, the equation for $\Theta(\theta)$ will thus read:

$$\left[\frac{\mathrm{d}}{\mathrm{d}x}(1-x^2)\frac{\mathrm{d}}{\mathrm{d}x} - \frac{m^2}{1-x^2} + \ell(\ell+1)\right]\Theta_{l,m} = 0 \tag{7}$$

where $x$ is defined as $x = \cos\theta$. The first important observation is that this equation is dependent upon two quantum numbers $\ell$ and $m$. While $\ell$ is called the *orbital quantum* *number*, $m$ is usually referred to as the *azimuthal quantum number* and it can only have a value $-\ell \leq m \leq \ell$. Eq. 7 is well-known and allows polynomial solutions, known as the *associated Legendre polynomials* $P_\ell^m(x)$. These polynomials arise from the Legendre polynomials ($P_\ell(x)$), which are solution of Eq. 7 if $m = 0$. The Legendre polynomials can be calculated using the Rodrigue's formula:

$$P_\ell(x) = \frac{1}{2^\ell \ell!} \frac{\mathrm{d}^\ell}{\mathrm{d}\, x^\ell} (x^2 - 1)^\ell \tag{8}$$

Once the Legendre polynomial of order $\ell$ is calculated, the associated Legendre polynomial of orders $\ell$ and $m$ can be obtained from:

$$P_\ell^m(x) = (x^2 - 1)^{m/2} \frac{\mathrm{d}^m}{\mathrm{d}\, x^m} P_\ell(x) \tag{9}$$

The function $\Theta(\theta)$ thus reads (remember that $x = \cos\theta$):

$$\Theta(\theta) = C_\ell^m P_\ell^m(\cos\theta) \tag{10}$$

where $C_\ell^m$ is a suitable normalisation constant:

$$C_\ell^m = (-)^m i^\ell \sqrt{\frac{(2\ell + 1)(\ell - m)!}{4\pi(\ell + m)!}} \tag{11}$$

We have now all the ingredients to write the eigenfunctions for the angular momentum $Y_\ell^m$:

$$Y_\ell^m(\theta, \phi) = (-)^m i^\ell \sqrt{\frac{(2\ell + 1)(\ell - |m|)!}{4\pi(\ell + |m|)!}} P_\ell^m(\cos\theta) e^{im\phi} \tag{12}$$

These functions are called the *spherical harmonics* and they are eigenfunctions of the operator $L^2$ with eigenvalue $\ell(\ell + 1)$ and, simultaneously, of the operator $L_3$ with eigenvalue $m$:

$$\begin{aligned} L^2(Y_\ell^m(\theta, \phi)) &= \ell(\ell + 1) Y_\ell^m(\theta, \phi) \\ L_3(Y_\ell^m(\theta, \phi)) &= m Y_\ell^m(\theta, \phi) \end{aligned} \tag{13}$$