5.4: Spherical Harmonics

The rigid rotor problem was solved using the Schrödinger equation

$$-\frac{\hbar^2}{2\mu r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)\psi(\theta,\phi)=E\psi(\theta,\phi)$$

As it turns out, the solutions to this equation are very important in a number of areas in chemistry and physics. The eigenfunctions are known as the **spherical harmonics** $\left(Y_l^{m_l}(\theta,\phi)\right)$ and they appear in every problem that has spherical symmetry. The Spherical Harmonics satisfy the relationship

$$\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)Y_l^{m_l}(\theta,\phi)=\hbar^2 l(l+1)Y_l^{m_l}(\theta,\phi)$$

Each function $Y_l^{m_l}(\theta,\phi)$ has three parts: 1) a normalization constant, 2) an associated Legendre polynomial in $\cos(\theta)$, and 3) an imaginary (for $m_l \neq 0$) exponential in ϕ.

$$Y_l^{m_l}(\theta,\phi)=\left[\frac{(2l+1)\,(l-|m_l|)}{4\pi\,(l+|m_l|)}\right]^{\frac{1}{2}}P_l^{|m_l|}(\cos\theta)e^{im_l\phi}$$

The first few Spherical harmonics are shown in the table below.

I	m_I	$Y_l^{m_l}(\theta,\phi)$
0	0	$\sqrt{\frac{1}{4\pi}}$
1	0	$\sqrt{\frac{3}{4\pi}}\cos(\theta)$
	± 1	± 1
2	± 1	$\sqrt{\frac{5}{16\pi}}\left(3\cos^2(\theta)-1\right)$
	0	$\sin(\theta)\cos(\theta)e^{\pm i\phi}$
	± 2	$\sqrt{\frac{15}{32\pi}}\sin^2(\theta)e^{\pm 2i\phi}$

Notice the $(2l+1)$ degeneracy in these functions, due to the $(2l+1)$ values of m_l for each value of l. Also, it is useful to not that these functions all have l angular nodes (values of θ that cause the wavefunction to vanish.) For the $l=1$ wavefunctions, these nodes occur at $\theta=\pi/2$ for $m_l=0$ and at $\theta=0$ for $m_l=\pm 1$. The number of nodes in each wavefunction is a useful property to know when discussing how these functions related to the radial wavefunction in the Hydrogen atom.