21. Spherical Harmonics

Now that we know the eigen*values* of L^2 and L_z, it's time to figure out the corresponding eigen*functions*. They're functions of the angles θ and ϕ (but not of r), so in order to find them, we need to express each of the angular momentum operators in terms of spherical coordinates.

Again I'll refer you to Griffiths for the details. In Section 4.3.2 he starts with the vector definition of angular momentum, $\vec{L} = \vec{r} \times \vec{p}$, then writes the momentum operator as $-i\hbar\vec{\nabla}$, expresses the gradient in spherical coordinates, and works out the cross product. This gives a formula for $\vec{L}$ that's written entirely in terms of θ, ϕ, $\hat{\theta}$, and $\hat{\phi}$. But that's not what we want! We want the *Cartesian* components of $\vec{L}$ written in terms of angular functions and derivatives, so the next step is to rewrite the unit vectors $\hat{\theta}$ and $\hat{\phi}$ in terms of $\hat{\imath}$, $\hat{\jmath}$, and $\hat{k}$. I strongly suggest that you draw a picture or two to understand the relations among these unit vectors.

Having expressed $\vec{L}$ in terms of spherical coordinates but Cartesian unit vectors, Griffiths simply reads off the components L_x, L_y, and L_z. It's then straightforward to work out the ladder operators L_+ and L_-, and to plug these into a formula from a few pages back to obtain L^2. (You'll fill in a few missing algebraic steps in the homework.)

The final expressions for L^2 and L_z are

$$L^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right], \qquad L_z = -i\hbar\frac{\partial}{\partial\phi}, \tag{1}$$

and, thanks to the previous lesson, we know that these operators have a common set of eigenfunctions with eigenvalues $l(l+1)\hbar^2$ and $m\hbar$. The eigenvalue equation for L_z tells us that these eigenfunctions are proportional to $e^{im\phi}$, where m must be an integer for the functions to be single-valued. The procedure for finding the θ dependence of the eigenfunctions is analogous to what we did for the simple harmonic oscillator: Start with a function at one end of the "ladder," so operating on it with one of the ladder operators gives zero. Use the explicit representation of that ladder operator to write this fact as a differential equation, and solve that equation to obtain the formula for that eigenfunction. Then act on this function with the other ladder operator to obtain the next eigenfunction, and so on. One of your homework problems takes you through these steps.

The resulting eigenfunctions of L^2 and L_z are called *spherical harmonics*, denoted $Y_l^m(\theta,\phi)$. Griffiths, in Section 4.1, provides a table of all the spherical harmonics up to $l = 3$, and you can obtain many more with the Mathematica function `SphericalHarmonicY[`l`,`m`,`θ`,`ϕ`]`. It's a good investment to spend some time studying the formulas and looking for patterns. (The spherical harmonics can be expressed in terms of so-called *associated Legendre functions* of $\cos\theta$, but I've rarely found this fact to be useful.)