Lecture 12, February 15, 2006

Solved Homework

We are allowed to know any one component of the total angular momentum to perfect accuracy. Although historically one nearly always speaks of the z component as being the one that is knowable (i.e., for which we can find eigenfunctions), this is a completely arbitrary labeling scheme. We might as easily name it x or y and the mathematics are identical. The Heisenberg uncertainty principle simply says that we cannot know *more* than one simultaneously. So, the eigenvalues of L_x^2 are the same as those of L_y^2 are the same as those of L_z^2—but we can only measure any one of these at any given time to arbitrary accuracy. In any case, we have generically for any coordinate q

$$L_q^2 \Psi = L_q \left[L_q \Psi \right]$$
$$= L_q \left[m_l \hbar \Psi \right]$$
$$= m_l \hbar \left[L_q \Psi \right]$$
$$= m_l \hbar \left[m_l \hbar \Psi \right]$$
$$= m_l^2 \hbar^2 \Psi$$

where the quantum numbers m_l can take on integer values from $-l$ to l where l is the quantum number for the square of the total angular momentum operator.

Now, given what we just discussed above, one might think that it is impossible to obtain eigenvalues for $L_x^2 + L_y^2$, but that's not true. It's not possible to have eigenvalues for each operator in the sum simultaneously, but it's entirely OK to have an eigenvalue for the sum without knowing the two parts. To see this, note that

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

so

$$L^2 - L_z^2 = L_x^2 + L_y^2$$

and we already know that we can know both L^2 and L_z^2 simultaneously! Thus, we have

$$\left(L_x^2 + L_y^2\right)\Psi = \left(L^2 - L_z^2\right)\Psi$$

$$= \left[l(l+1)\hbar^2 - m_l^2\hbar^2\right]\Psi$$

$$= \hbar^2\left[l(l+1) - m_l^2\right]\Psi$$

One can think of these eigenvalues as being the part that needs to be added to L_z^2 in order to reach L^2, but this additional component of the angular momentum can point in any direction within the plane defined by the z component having a constant value; that is, we don't know the individual x and y components, so at best we know a circle of points around the z axis at which our angular momentum vector terminates. The angular momentum is said to "precess" about the z axis on this circle.

Angular Momentum Eigenfunctions

We've now learned a great deal about angular momentum eigenvalues without ever determining the eigenfunctions. The time has come, however, to examine those functions. First, however, it is helpful to transform our coordinate system to spherical polar coordinates, because angular momentum intrinsically involves rotational motion, so it is useful to work in a coordinate system natural to rotation.

In the spherical polar coordinate system, a point in space is defined by its distance from the origin, r, its angle from the z axis, θ, and its angle from the x axis when the coordinate vector is projected into the xz plane, ϕ. To form the various angular momentum operators in this coordinate system, we need the relation between these variables and x, y, and z, and their differential operators. This is a tedious and boring derivation and we simply list the results here

$$x = r\sin\theta\cos\phi \quad y = r\sin\theta\sin\phi \quad z = r\cos\theta$$

$$\frac{\partial}{\partial x} = \sin\theta\cos\phi\frac{\partial}{\partial r} + \frac{\cos\theta\cos\phi}{r}\frac{\partial}{\partial\theta} - \frac{\sin\phi}{r\sin\theta}\frac{\partial}{\partial\phi}$$

$$\frac{\partial}{\partial y} = \sin\theta\sin\phi\frac{\partial}{\partial r} + \frac{\cos\theta\sin\phi}{r}\frac{\partial}{\partial\theta} + \frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial\phi} \tag{12-1}$$

$$\frac{\partial}{\partial z} = \cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta}$$

From these terms, we can work out the forms of the total angular momentum operator, the component angular momentum operators, and the raising and lowering operators in spherical polar coordinates by substitution.

Let us consider the raising operator first, because it is useful in learning something about the angular momentum eigenfunctions. If we carry through the various substitutions we have

$$L_+ = \hbar(\cos\theta + i\sin\theta)\left(\frac{\partial}{\partial\theta} + i\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\phi}\right) \tag{12-2}$$

Now, recall that the effect of the raising operator operating on the angular momentum eigenfunction having the maximal value of the z component of the angular momentum is to annihilate it. That is,

$$L_+Y_{l,l}(\theta,\phi) = \hbar(\cos\theta + i\sin\theta)\left(\frac{\partial}{\partial\theta} + i\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\phi}\right)Y_{l,l}(\theta,\phi) = 0 \tag{12-3}$$

where we represent our unknown eigenfunctions as $Y(\theta,\phi)$ with two subscripts. The first subscript is the quantum number for the total angular momentum squared and the second is the subscript for the z component of the angular momentum. Because we are working with the Y that is maximal for the latter value, both subscripts are l.

Now, since h-bar$(\cos\theta + i\sin\theta)$ is never equal to zero, we can divide both sides by that quantity and obtain

$$\left(\frac{\partial}{\partial\theta} + i\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\phi}\right)Y_{l,l}(\theta,\phi) = 0 \tag{12-4}$$

If we assume that we may separate Y into a part dependent on θ and a part dependent on ϕ (in the same fashion we did previously when separating time and position in the Schrödinger equation), we have

$$\left(\frac{\partial}{\partial\theta} + i\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\phi}\right)Y_{l,l}(\theta,\phi) = \left(\frac{\partial}{\partial\theta} + i\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\phi}\right)\Theta(\theta)\Phi(\phi)$$

$$= \Phi(\phi)\frac{\partial\Theta(\theta)}{\partial\theta} + i\frac{\cos\theta}{\sin\theta}\Theta(\theta)\frac{\partial\Phi(\phi)}{\partial\phi} \tag{12-5}$$

Recalling that this is equal to zero for the special case of $Y_{l,l}$ we may rearrange eq. 12-5 to

$$\frac{\sin\theta}{\Theta(\theta)\cos\theta}\frac{\partial\Theta(\theta)}{\partial\theta} = -\frac{i}{\Phi(\phi)}\frac{\partial\Phi(\phi)}{\partial\phi} \tag{12-6}$$

Since eq. 12-6 is true for *any* choice of θ or ϕ, it must be the case that both sides are equal to the same constant. Actually, we know the particular value of that constant in this case. That is because setting the right hand side equal to a constant C gives, after rearrangement

$$-i\frac{\partial}{\partial\phi}\Phi(\phi) = C\Phi(\phi) \tag{12-7}$$

However, in spherical polar coordinates, the operator L_z is simply

$$L_z = -i\hbar \frac{\partial}{\partial \phi} \tag{12-8}$$

(it is the simplicity of this operator in spherical polar coordinates that motivates the typical choice of z as the distinguished coordinate in angular momentum). Thus, eq. 12-7 can be rewritten

$$\frac{1}{\hbar} L_z \Phi(\phi) = C\Phi(\phi) \tag{12-9}$$

We've already specified that Y is an eigenfunction of L_z with eigenvalue l times h-bar, and L_z only depends on ϕ, so the ϕ-dependent part of Y must be the part that is acted upon to generate l times h-bar, and thus the constant C must be l. Putting this into eq. 12-7 gives after rearrangement

$$-i \frac{\partial \Phi(\phi)}{\partial \phi} - l\Phi(\phi) = 0 \tag{12-10}$$

A satisfactory normalized solution to this equation (you may wish to verify this) is

$$\Phi(\phi) = \frac{1}{\sqrt{2\pi}} e^{il\phi} \tag{12-11}$$

Note that one of the requirements for a good wave function is that it be single-valued. For the coordinate ϕ, this requires that $\Phi(\phi) = \Phi(\phi + 2\pi)$, since adding 2π radians to the coordinate ϕ simply cycles us back to the same place in spherical polar coordinates. Recall that the definition of the complex exponential is

$$e^{il\omega} = \cos(l\omega) + i\sin(l\omega) \tag{12-12}$$

The cosine and sine functions are periodic with period 2π. So, in order for eq. 12-12 to be the same for ω equal to either ϕ or $\phi + 2\pi$, it must be the case that the difference between $l\phi$ and $l(\phi + 2\pi)$ is an integral multiple of 2π. That is,

$$l(\phi + 2\pi) - l\phi = \pm n(2\pi) \quad n = 0,1,2,\ldots \tag{12-13}$$

This equation requires that $l = \pm n$. *This requirement of periodicity is why we are restricted to integer values of m_l and half-integer values are not allowed, even though our work with raising and lowering operators did not establish this point.*

What about the remaining part of the wave function that depends on θ? We already know our constant is l, so the other side of eq. 12-6 may be set equal to it to generate

$$\frac{\sin\theta}{\Theta(\theta)\cos\theta}\frac{\partial\Theta(\theta)}{\partial\theta} = l \tag{12-14}$$

The solution to this differential equation is not so obvious, but a bit of playing around gives the normalized solution

$$\Theta(\theta) = \frac{1}{2^l l!}\left[\frac{(2l+1)!}{2}\right]^{1/2}\sin^l\theta \tag{12-15}$$

So, the complete eigenfunction for the state having the maximum component of the z angular momentum is

$$Y_{l,l}(\theta,\phi) = \frac{1}{2^l l!}\left[\frac{(2l+1)!}{4\pi}\right]^{1/2}\left(\sin^l\theta\right)e^{il\phi} \tag{12-16}$$

To find the remaining eigenfunctions, we need simply apply the lowering operator successively to generate the states having quantum numbers $m_l = l - 1$, then $l - 2$, etc.

The application of the lowering operator to the wave function of eq. 12-16 is not at all a pleasant undertaking, and leads to the fairly horrifying but completely general result

$$Y_{l,m_l}(\theta,\phi) = \frac{(-1)^l}{2^l l!}\left[\frac{(2l+1)(l-|m_l|)!}{4\pi(l+|m_l|)!}\right]^{1/2}\left(\sin^{m_l}\theta\right)\frac{d^{l+|m_l|}}{d(\cos\theta)^{l+|m_l|}}\left(1-\cos^2\theta\right)^l e^{im_l\phi} \tag{12-17}$$

Fortunately, for lower values of l, it is quite straightforward to write the wave functions, which are generically known as the "spherical harmonics", in a much more sensible fashion. The spherical harmonics appear in many problems in physics, and they were known long before the advent of quantum mechanics. The complex functions derived here have the property that they are simultaneously eigenfunctions of both L^2 and L_z. If we are willing to give up the property of their being eigenfunctions of the latter operator, we can take linear combinations of some of the complex functions to generate other functions that are everywhere real-valued. These are called the "real spherical harmonics". Note from eq. 12-17 that any spherical harmonic for which $m_l = 0$ is immediately real valued, since the only term involving i is the argument of the exponential function. The table below lists the first few spherical harmonics and some of their properties.

The Initial Spherical Harmonics

Complex form	Real (spherical) form	Real (cartesian) form	Nomenclature	$\langle L^2 \rangle$	$\langle L_z \rangle$
$\left(\dfrac{1}{4\pi}\right)^{1/2}$	$\left(\dfrac{1}{4\pi}\right)^{1/2}$	$\left(\dfrac{1}{4\pi}\right)^{1/2}$	$Y_{0,0}$; s_0	0	0
$\left(\dfrac{3}{8\pi}\right)^{1/2}\sin\theta\, e^{-i\phi}$			$Y_{1,-1}$; p_{-1}	$2\hbar^2$	$-\hbar$
	$\left(\dfrac{3}{4\pi}\right)^{1/2}\sin\theta\sin\phi$	$\left(\dfrac{3}{4\pi}\right)^{1/2}\dfrac{y}{r}$	$Y_{1,\sin\phi}$; p_y	$2\hbar^2$	a
$\left(\dfrac{3}{4\pi}\right)^{1/2}\cos\theta$	$\left(\dfrac{3}{4\pi}\right)^{1/2}\cos\theta$	$\left(\dfrac{3}{4\pi}\right)^{1/2}\dfrac{z}{r}$	$Y_{1,0}$; p_0; p_z	$2\hbar^2$	0
	$\left(\dfrac{3}{4\pi}\right)^{1/2}\sin\theta\cos\phi$	$\left(\dfrac{3}{4\pi}\right)^{1/2}\dfrac{x}{r}$	$Y_{1,\cos\phi}$; p_x	$2\hbar^2$	a
$\left(\dfrac{3}{8\pi}\right)^{1/2}\sin\theta\, e^{i\phi}$			$Y_{1,1}$; p_1	$2\hbar^2$	$\hbar$
$\left(\dfrac{15}{32\pi}\right)^{1/2}\sin^2\theta\, e^{-2i\phi}$			$Y_{2,-2}$; d_{-2}	$6\hbar^2$	$-2\hbar$
	$\left(\dfrac{15}{4\pi}\right)^{1/2}\sin^2\theta\sin 2\phi$	$\left(\dfrac{15}{4\pi}\right)^{1/2}\dfrac{xy}{r^2}$	$Y_{2,\sin 2\phi}$; d_{xy}	$6\hbar^2$	a
$\left(\dfrac{15}{8\pi}\right)^{1/2}\sin\theta\cos\theta\, e^{-i\phi}$			$Y_{2,-1}$; d_{-1}	$6\hbar^2$	$-\hbar$

	$\left(\dfrac{15}{4\pi}\right)^{1/2}\sin\theta\cos\theta\sin\phi$	$\left(\dfrac{15}{4\pi}\right)^{1/2}\dfrac{yz}{r^2}$	$Y_{2,\sin\phi};\ d_{yz}$	$6\hbar^2$	a
$\left(\dfrac{5}{16\pi}\right)^{1/2}\left(3\cos^2\theta-1\right)$	$\left(\dfrac{5}{16\pi}\right)^{1/2}\left(3\cos^2\theta-1\right)$	$\left(\dfrac{5}{16\pi}\right)^{1/2}\left(3\dfrac{z^2}{r^2}-1\right)$	$Y_{2,0};\ d_0;\ d_{z2}$	$6\hbar^2$	0
	$\left(\dfrac{15}{4\pi}\right)^{1/2}\sin\theta\cos\theta\cos\phi$	$\left(\dfrac{15}{4\pi}\right)^{1/2}\dfrac{xz}{r^2}$	$Y_{2,\cos\phi};\ d_{xz}$	$6\hbar^2$	a
$\left(\dfrac{15}{8\pi}\right)^{1/2}\sin\theta\cos\theta\,e^{i\phi}$			$Y_{2,1};\ d_1$	$6\hbar^2$	$\hbar$
	$\left(\dfrac{15}{4\pi}\right)^{1/2}\sin^2\theta\cos2\phi$	$\left(\dfrac{15}{16\pi}\right)^{1/2}\dfrac{x^2-y^2}{r^2}$	$Y_{2,\cos2\phi};\ d_{x2-y2}$	$6\hbar^2$	a
$\left(\dfrac{15}{32\pi}\right)^{1/2}\sin^2\theta\,e^{2i\phi}$			$Y_{2,2};\ d_2$	$6\hbar^2$	$2\hbar$

[a] This real spherical harmonic is not an eigenfunction of L_z and thus its expectation value is not tabulated.

The spherical harmonics continue through f, g, h, i, and higher functions (can you guess why e is skipped?), but those are not tabulated above. Very nice pictures of the square moduli of the complex spherical harmonics through f, as well as individual pictures of their real and complex components, can be found at http://mathworld.wolfram.com/SphericalHarmonic.html. Stunning pictures of the square moduli of the real spherical harmonics through f (although following a slightly different naming convention then that in the table) can be found at http://www.uniovi.es/qcg/harmonics/harmonics.html. Both links are on the class webpage.

Homework

To be solved in class: Demonstrate explicitly that the eigenfunctions of L_z, i.e., the $\Phi_{m_l}(\phi)$, are orthogonal.

To be turned in for possible grading Feb. 17: Nothing! Relax, catch up, take a deep breath — whatever applies.