Angular Momentum

Lecture 23

Physics 342
Quantum Mechanics I

Monday, March 31st, 2008

We know how to obtain the energy of Hydrogen using the Hamiltonian operator – but given a particular E_n, there is degeneracy – many $\psi_{n\ell m}(r,\theta,\phi)$ have the same energy. What we would like is a set of operators that allow us to determine ℓ and m. The angular momentum operator $\hat{\mathbf{L}}$, and in particular the combination L^2 and L_z provide precisely the additional Hermitian observables we need.

23.1 Classical Description

Going back to our Hamiltonian for a central potential, we have

$$H = \frac{\mathbf{p}\cdot\mathbf{p}}{2\,m} + U(r). \tag{23.1}$$

It is clear from the dependence of U on the radial distance only, that angular momentum should be conserved in this setting. Remember the definition:

$$\mathbf{L} = \mathbf{r}\times\mathbf{p}, \tag{23.2}$$

and we can write this in indexed notation which is slightly easier to work with using the Levi-Civita symbol, defined as (in three dimensions)

$$\epsilon_{ijk} = \begin{cases} 1 & \text{for } (ijk) \text{ an even permutation of } (123). \\ -1 & \text{for an odd permutation} \\ 0 & \text{otherwise} \end{cases} \tag{23.3}$$

Then we can write

$$L_i = \sum_{j=1}^{3}\sum_{k=1}^{3} \epsilon_{ijk}\,r_j\,p_k = \epsilon_{ijk}\,r_j\,p_k \tag{23.4}$$

where the sum over j and k is implied in the second equality (this is Einstein summation notation). There are three numbers here, L_i for $i = 1, 2, 3$, we associate with L_x, L_y, and L_z, the individual components of angular momentum about the three spatial axes.

To see that this is a conserved vector of quantities, we calculate the classical Poisson bracket:

$$[H, L_i] = \frac{\partial H}{\partial r_j}\frac{\partial L_i}{\partial p_j} - \frac{\partial H}{\partial p_j}\frac{\partial L_i}{\partial r_j} \quad = \frac{dU}{dr}\frac{\partial r}{\partial r_j}\,\epsilon_{ikj}\,r_k - \frac{p_j}{2\,m}\,\epsilon_{ijk}\,p_k \tag{23.5}$$

and $p_j\,p_k\,\epsilon_{ijk} = 0$[1]. Noting that $\frac{\partial r}{\partial r_j} = \frac{r_j}{r}$, we have the first term in the bracket above proportional to $\epsilon_{ijk}\,r_j\,r_k$, and this is zero as well. So we learn that along the dynamical trajectory, $\frac{dL_i}{dt} = 0$.

The vanishing of the classical Poisson bracket suggests that we take a look at the quantum commutator of the operator form $\hat{\mathbf{L}}$ and the Hamiltonian operator $\hat{H}$. If these did commute, then we know that the eigenvectors of $\hat{\mathbf{L}}$ can be shared by $\hat{H}$.

23.2 Quantum Commutators

Consider the quantum operator:

$$\hat{\mathbf{L}} = \mathbf{r} \times \left(\frac{\hbar}{i}\,\nabla\right) \tag{23.7}$$

which, again, we can write in indexed form:

$$\hat{L}_i = \epsilon_{ijk}\,r_j\,\frac{\hbar}{i}\,\partial_k. \tag{23.8}$$

We have seen that the replacement $[\ ,\ ]_{PB} \longrightarrow \frac{[\ ,\ ]}{i\,\hbar}$ leads from the Poisson bracket to the commutator, and so it is reasonable to ask how $\hat{L}_i$ commutes with $\hat{H}$ – we expect, from the classical consideration, that $[\hat{H}, \hat{L}_i] = 0$ for $i = 1, 2, 3$. To see that this is indeed the case, let's use a test function $f(r_n)$ (shorthand for $f(x, y, z)$), and consider the commutator directly:

$$[\hat{H}, \hat{L}_i]\,f(r_n) = \hat{H}\,\hat{L}_i\,f(r_n) - \hat{L}_i\,\hat{H}\,f(r_n). \tag{23.9}$$

[1] the object $p_j\,p_k$ is unchanged under $j \leftrightarrow k$, while ϵ_{ijk} flips sign

$$\epsilon_{ijk}\,p_j\,p_k = \epsilon_{ijk}\,p_k\,p_j = \epsilon_{ikj}\,p_k\,p_j = -\epsilon_{ijk}\,p_k\,p_j = -\epsilon_{ijk}\,p_j\,p_k, \tag{23.6}$$

and then we must have $\epsilon_{ijk}\,p_j\,p_k = 0$ since it is equal to its own negative.

The first term, written out, is

$$\begin{aligned}\frac{i}{\hbar}\,\hat{H}\,\hat{L}_i\,f(r_n) &= \left(-\frac{\hbar^2}{2\,m}\,\partial_q\,\partial_q + U(r)\right)(\epsilon_{ijk}\,r_j\,\partial_k\,f(r_n)) \\ &= -\frac{\hbar^2}{2\,m}\,\partial_q\,(\epsilon_{ijk}\,\delta_{jq}\,\partial_k\,f(r_n) + \epsilon_{ijk}\,r_j\,\partial_q\,\partial_k\,f(r_n)) + U(r)\,(\epsilon_{ijk}\,r_j\,\partial_k\,f(r_n)) \\ &= -\frac{\hbar^2}{2\,m}\,(\epsilon_{iqk}\,\partial_q\,\partial_k\,f(r_n) + \epsilon_{ijk}\,\delta_{jq}\,\partial_q\,\partial_k\,(f(r_n)) + \epsilon_{ijk}\,r_j\,\partial_q\,\partial_q\,\partial_k\,f(r_n)) \\ &\quad + U(r)\,(\epsilon_{ijk}\,r_j\,\partial_k\,f(r_n))\end{aligned} \tag{23.10}$$

and note that the first two terms involving second derivatives are automatically zero. Then, in vector notation, we can write:

$$\hat{H}\,\hat{\mathbf{L}}\,f(r_n) = \frac{\hbar}{i}\left[-\frac{\hbar^2}{2\,m}\,\mathbf{r}\times\nabla\,(\nabla^2\,f) + U(r)\,\mathbf{r}\times\nabla\,f\right]. \tag{23.11}$$

Now consider the other direction,

$$\begin{aligned}\frac{i}{\hbar}\,\hat{L}_i\,\hat{H}\,f(r_n) &= \epsilon_{ijk}\,r_j\,\partial_k\left(-\frac{\hbar^2}{2\,m}\,\partial_q\,\partial_q\,f(r_n) + U(r)\,f(r_n)\right) \\ &= -\frac{\hbar^2}{2\,m}\,\epsilon_{ijk}\,r_j\,\partial_k\,\partial_q\,\partial_q\,f(r_n) + \epsilon_{ijk}\,r_j\left(\frac{\partial U}{\partial r}\,\frac{\partial r}{\partial r_k}\,f(r_n) + U(r)\,\partial_k\,f(r_n)\right)\end{aligned} \tag{23.12}$$

where, once again, $\frac{\partial r}{\partial r_k} \sim r_k$ so the term involving the derivative of U will vanish, leaving us with

$$\hat{\mathbf{L}}\,\hat{H}\,f(r_n) = \frac{\hbar}{i}\left[-\frac{\hbar^2}{2\,m}\,\mathbf{r}\times\nabla\,(\nabla^2\,f) + U(r)\,\mathbf{r}\times\nabla\,f\right]. \tag{23.13}$$

So it is, indeed, the case that $[\hat{H}, \hat{L}_i] = 0$.

23.2.1 $\hat{L}_i$ Commutators

Before exploring the implications of the shared eigenfunctions of $\hat{H}$ and $\hat{L}_i$, let's calculate the commutators of the components of $\hat{L}_i$ with themselves. Consider, for example

$$\begin{aligned}-\frac{1}{\hbar^2}\,\hat{L}_i\,\hat{L}_j\,f(r_n) &= \epsilon_{ipq}\,r_p\,\partial_q\,(\epsilon_{juv}\,r_u\,\partial_v\,f(r_n)) \\ &= \epsilon_{ipq}\,r_p\,\epsilon_{jqv}\,\partial_v\,f(r_n) + \epsilon_{ipq}\,r_p\,\epsilon_{juv}\,r_u\,\partial_q\,\partial_v\,f(r_n)\end{aligned} \tag{23.14}$$

and the other direction, obtained by interchanging $i \leftrightarrow j$:

$$-\frac{1}{\hbar^2}\,\hat{L}_j\,\hat{L}_i\,f(r_n) = \epsilon_{jpq}\,r_p\,\epsilon_{iqv}\,\partial_v\,f(r_n) + \epsilon_{jpq}\,r_p\,\epsilon_{iuv}\,r_u\,\partial_q\,\partial_v\,f(r_n), \quad (23.15)$$

then the commutator is

$$-\frac{1}{\hbar^2}\,[\hat{L}_i,\hat{L}_j]\,f(r_n) = \epsilon_{ipq}\,r_p\,\epsilon_{jqv}\,\partial_v\,f(r_n) - \epsilon_{jpq}\,r_p\,\epsilon_{iqv}\,\partial_v\,f(r_n). \quad (23.16)$$

Using the identity $\epsilon_{qip}\,\epsilon_{qjv} = \delta_{ij}\,\delta_{pv} - \delta_{iv}\,\delta_{pj}$, we can rearrange

$$\begin{aligned}
-\frac{1}{\hbar^2}\,[\hat{L}_i,\hat{L}_j]\,f(r_n) &= (\delta_{iv}\,\delta_{pj} - \delta_{jv}\,\delta_{pi})]\,r_p\,\partial_v\,f(r_n) \\
&= -(\delta_{ip}\,\delta_{jv} - \delta_{iv}\,\delta_{jp})\;\partial_v\,f(r_n) \\
&= -\epsilon_{\ell ij}\,\epsilon_{\ell pv}\,r_p\,\partial_v\,f(r_n) \\
&= -\frac{i}{\hbar}\,\epsilon_{\ell ij}\,\hat{L}_\ell,
\end{aligned} \quad (23.17)$$

or, finally

$$[\hat{L}_i,\hat{L}_j] = i\,\hbar\,\epsilon_{\ell ij}\,\hat{L}_\ell. \quad (23.18)$$

We learn that, for example, $[\hat{L}_x,\hat{L}_y] = i\,\hbar\,L_z$. This tells us that it is impossible to find eigenfunctions of L_x that are simultaneously eigenfunctions of L_y and/or L_z.

So returning to the issue of $[\hat{H},\hat{L}_i] = 0$, we can, evidently, choose any *one* of the angular momentum operators, and have shared eigenfunctions of $\hat{H}$ and $\hat{L}_i$, but we cannot *also* have these eigenfunctions for $\hat{L}_j$. That may seem strange – after all, if a vector is an eigenvector of $\hat{H}$ and $\hat{L}_x$, and we can also make an eigenvector that is shared between $\hat{H}$ and $\hat{L}_z$, then surely there is an eigenvector shared by all three? The above says that this is not true, and we shall see some explicit examples next time.

For now, let's look for *combinations* of angular momentum operators that simultaneously commute with $\hat{H}$ and $\hat{L}_z$, for example (we are preferentially treating $\hat{L}_z$ as *the* operator that shares its eigenstates with $\hat{H}$, but this is purely a matter of choice). The most obvious potential operator is $\hat{L}^2$:

$$\begin{aligned}
[\hat{L}^2,\hat{L}_z] &= [(L_x^2 + L_y^2 + L_z^2), L_z] = L_x\,[L_x,L_z] - i\,\hbar\,L_y\,L_x + L_y\,[L_y,L_z] + i\,\hbar\,L_x\,L_y + 0 \\
&= L_x\,(-i\,\hbar L_y) + L_y\,(i\,\hbar\,L_x) - i\,\hbar\,L_y\,L_x + i\,\hbar\,L_x\,L_y \\
&= 0
\end{aligned} \quad (23.19)$$

and the same is true for $[\hat{L}^2,\hat{L}_x]$ and $[\hat{L}^2,\hat{L}_y]$. In addition, it is the case that $[\hat{L}^2,\hat{H}] = 0$, clearly, since the individual operators do.

23.3 Raising and Lowering Operators

We can make a particular algebraic combination of $\hat{L}_x$ and $\hat{L}_y$ that plays a role similar to the $a_\pm$ operators from the harmonic oscillator example. Take

$$L_\pm \equiv L_x \pm i\, L_y, \tag{23.20}$$

then the commutator of these with L_z is

$$\begin{aligned}[L_\pm, L_z] &= [L_x, L_z] \pm i\,[L_y, L_z] = -i\,\hbar\, L_y \mp \hbar L_x = \mp\hbar\,(L_x \pm i\, L_y) \\ &= \mp\hbar\, L_\pm.\end{aligned} \tag{23.21}$$

For an eigenfunction of L_z, call it f such that $L_z\, f = \alpha\, f$, the operator L_+ acting on f is also an eigenfunction, but with eigenvalue:

$$L_z\,(L_\pm f) = (L_\pm L_z \pm \hbar\, L_\pm)\, f = (\alpha \pm \hbar)\,(L_\pm\, f) \tag{23.22}$$

so acting on f with $L_\pm$ increases (or decreases) the eigenvalue by $\hbar$.

Similarly, if we take the function f to be simultaneously an eigenfunction of L^2 (which we know can be done), the $L_\pm f$ is still an eigenfunction, with[2]

$$L^2\,(L_\pm\, f) = L_\pm\, L^2\, f = \beta\, L_\pm\, f \tag{23.23}$$

for eigenvalue β – in other words, $L_\pm f$ is an eigenfunction of L^2 with the same eigenvalue as f itself. The last observation we need is that there must be a minimal and maximal state for the $L_\pm$ operators – since the state $L_\pm f$ has the same L^2 eigenvalue as f does, while its eigenvalue w.r.t. L_z is going up or down, there will be a point at which the eigenvalue (result of measurement) of L_z is greater than the total magnitude of the eigenvalue w.r.t. L^2 (the result of a measurement of total angular momentum) – so we demand the existence of a "top" $L_+ f_t = 0$ and, for the same reasons, a "bottom" $L_- f_b = 0$

So what? So remember that for the harmonic oscillator, we wrote H in terms of the products $a_\pm a_\mp$, and that allowed us to build a lowest energy state from which we could define $|0\rangle$ as a wavefunction. The same type of game applies here, we will write L^2 in terms of $L_\pm\, L_\mp$:

$$L_\pm\, L_\mp = (L_x^2 \underbrace{\mp i\, L_x\, L_y \pm i\, L_y\, L_x}_{=\mp i\,[L_x, L_y]} + L_y^2) = L_x^2 + L_y^2 \pm \hbar\, L_z \tag{23.24}$$

[2]I'm going to do a commutator down here – too many in the main portion gets boring. Since $[L^2, L_i] = 0$, we have $[L^2, L_x \pm i L_y] = 0$.

so that we can write

$$L^2 = L_\pm \, L_\mp + L_z^2 \mp \hbar \, L_z. \tag{23.25}$$

Our first goal is to relate the spectrum of L^2 to that of L_z – consider the top state f_t with eigenvalue $L_z \, f_t = \hbar \, \ell \, f_t$ (the $\hbar$ is in there just to make the eigenvalue under lowering a bit nicer), and $L^2 \, f_t = \alpha \, f_t$. Now from the above factorization of L^2 (23.25), we have

$$L^2 \, f_t = (L_- L_+ + L_z^2 + \hbar \, L_z) \, f = (0 + \hbar^2 \, \ell^2 + \hbar^2 \, \ell) \, f = \alpha \, f \tag{23.26}$$

so the maximum eigenvalue for L_z is related to the eigenvalue α via $\alpha = \hbar^2 \, \ell \, (\ell + 1)$. Similarly, if we take the minimum eigenvalue for L_z corresponding to the state f_b: $L_z \, f_b = \hbar \, \bar{\ell} \, f_b$, then we use the other factorization and get $\alpha = \hbar \, \ell \, (\ell - 1)$, which tells us that $\bar{\ell} = -\ell$.

So L_+ takes us from f_b with eigenvalue $-\ell$ to f_t with eigenvalue ℓ – it does so in integer steps, since $L_z \, (L_+ \, f_b) = \hbar \, (\ell + 1) \, L_+ \, f_b$, so ℓ itself must either be an integer, or, potentially, a half-integer.

We have described the eigenstates of L^2 and L_z, then, in terms of two numbers: $\ell = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$ and m which, for each ℓ takes integer values $m \in [-\ell, \ell]$. The states can be labelled f_ℓ^m, and, if we are lucky, these will be the simultaneous eigenstates of H. . .

23.4 Eigenstates of L^2

To find the eigenstates of L^2, let's first work out, carefully, the classical value – then we will attempt to make scalar operators which will be easy to write down in spherical coordinates:

$$\begin{aligned} L^2 &= (\epsilon_{ijk} \, r_j \, p_k) \, (\epsilon_{imn} \, r_m \, p_n) = (\delta_{jm} \, \delta_{kn} - \delta_{jn} \, \delta_{km}) \, r_j \, p_k \, r_m \, p_n \\ &= r_j \, p_k \, r_j \, p_k - r_j \, p_k \, r_k \, p_j. \end{aligned} \tag{23.27}$$

There are some obvious simplifications here, but remember that while it is true, classically, that $r_j \, p_k = r_k \, p_j$, this is not true when we move to operators, so let's keep the ordering as above, and input $p_k \longrightarrow \frac{\hbar}{i} \partial_k$ etc. We will introduce the test function f to keep track:

$$\begin{aligned} L^2 \, f &= -\hbar^2 \, \left[(r_j \, \partial_k) \, (r_j \, \partial_k \, f) - (r_j \, \partial_k) \, (r_k \, \partial_j \, f) \right] \\ &= -\hbar^2 \, \left[r_j \, \delta_{jk} \, \partial_k \, f + r_j \, r_j \, \partial_k \, \partial_k \, f - (r_j \, \partial_k) \, (\partial_j \, (r_k \, f) - \delta_{jk} \, f) \right] \\ &= -\hbar^2 \, \left[\mathbf{r} \cdot \nabla \, f + r^2 \, \nabla^2 \, f - (r_j \, \partial_j \, \partial_k \, (r_k \, f) - r_k \, \partial_k \, f) \right] \\ &= -\hbar^2 \, \left[\mathbf{r} \cdot \nabla \, f + r^2 \, \nabla^2 \, f - (\mathbf{r} \cdot \nabla \, (3 \, f + \mathbf{r} \cdot \nabla \, f) - \mathbf{r} \cdot \nabla \, f) \right], \end{aligned} \tag{23.28}$$

and combining terms, the final scalar form can be written:

$$L^2\, f = -\hbar^2\, \left[r^2\, \nabla^2\, f - \mathbf{r} \cdot \nabla\, f - (\mathbf{r} \cdot \nabla)\, (\mathbf{r} \cdot \nabla\, f) \right]. \tag{23.29}$$

Now, think of the operator $\mathbf{r} \cdot \nabla\, f$ in spherical coordinates, that's just $r\, \frac{\partial f}{\partial r}$ and we know the ∇^2 operator, so in spherical coordinates, we can write the above trivially:

$$\begin{aligned} L^2\, f &= -\hbar^2 \left[\frac{\partial}{\partial r} \left(r^2\, \frac{\partial f}{\partial r} \right) + \frac{1}{\sin\theta}\, \frac{\partial}{\partial \theta} \left(\sin\theta\, \frac{\partial f}{\partial \theta} \right) + \frac{1}{\sin^2\theta}\, \frac{\partial^2 f}{\partial \phi^2} - r\, \frac{\partial f}{\partial r} - r\, \frac{\partial}{\partial r} \left(r\, \frac{\partial f}{\partial r} \right) \right] \\ &= -\hbar^2\, \left[\frac{1}{\sin\theta}\, \frac{\partial}{\partial \theta} \left(\sin\theta\, \frac{\partial f}{\partial \theta} \right) + \frac{1}{\sin^2\theta}\, \frac{\partial^2 f}{\partial \phi^2} \right]. \end{aligned} \tag{23.30}$$

But this is precisely the angular portion of the Laplacian itself – and we know the solutions to this that have "separation constant" $\ell\, (\ell + 1)$, they are precisely the spherical harmonics, conveniently indexed appropriately. We have

$$L^2\, Y_\ell^m = \hbar^2\, \ell\, (\ell + 1)\, Y_\ell^m. \tag{23.31}$$

23.5 Eigenstates of L_z

The fastest route to the operator expression for L_z comes from the observation that classically, if we had a constant angular momentum pointing along the $\hat{\mathbf{z}}$ axis, then we have counter-clockwise rotation in the $x - y$ plane. If we use cylindrical coordinates (with $x = s\, \cos\phi$, $y = s\, \sin\phi$), then the only "motion" is in the $\hat{\boldsymbol{\phi}}$ direction. We might mimic this on the operator side by considering a test function that depends on ϕ only. Then

$$L_z\, f(\phi) \doteq (r_x\, p_y - r_y\, p_x)\, f(\phi) = \frac{\hbar}{i}\, \left[r\, \cos\phi\, \frac{\partial f}{\partial \phi}\, \frac{\partial \phi}{\partial x} - r\, \sin\phi\, \frac{\partial f}{\partial \phi}\, \frac{\partial \phi}{\partial y} \right] \tag{23.32}$$

and from $\phi = \tan^{-1}(y/x)$, we have $\frac{\partial \phi}{\partial x} = -\frac{\sin\phi}{r}$ and $\frac{\partial \phi}{\partial y} = \frac{\cos\phi}{r}$, then

$$L_z\, f(\phi) = \frac{\hbar}{i}\, \left(\cos^2\phi + \sin^2\phi \right)\, \frac{\partial f}{\partial \phi} \tag{23.33}$$

or, to be blunt,

$$L_z = \frac{\hbar}{i}\, \frac{\partial}{\partial \phi}. \tag{23.34}$$

The eigenstates of L_z are defined by $L_z\, f = \hbar\, m\, f$ for integer m (now m is an integer aside from any periodicity concerns, it comes to us as an integer from the algebraic approach). The solution is $f = e^{i\, m\, \phi}$, and of course, this is the ϕ-dependent portion of the spherical harmonics,

$$L_z Y_\ell^m = \frac{\hbar}{i} \frac{\partial}{\partial \phi} \left(A_\ell^m\, P_\ell^m(\cos\theta)\, e^{i\, m\, \phi} \right) = m\, \hbar\, Y_\ell^m \tag{23.35}$$

where we have written the ugly normalization as A_ℓ^m.

In the end, the $Y_\ell^m(\theta, \phi)$ are eigenstates of both the L^2 and L_z operators. In addition, to the extent that they form the angular part of the full Hamiltonian, $\psi_{n\ell m} \sim R_n(r)\, Y_\ell^m(\theta, \phi)$ is an eigenstate of H: $H\psi_{n\ell m} = E_n\, \psi_{n\ell m}$, and of course, the angular momentum operators do not see the radial function at all (there being no radial derivatives in L^2 or L_z), so

$$L^2\, \psi_{n\ell m} = \hbar^2\, \ell(\ell+1)\, \psi \qquad L_z\, \psi_{n\ell m} = \hbar\, m\, \psi_{n\ell m}, \tag{23.36}$$

and these separated wavefunctions (spherical infinite well, Hydrogen, etc.) are eigenstates of all three H, L^2 and L_z.

Homework

Reading: Griffiths, pp. 160–170.

Problem 23.1

Using only the commutator for position and momentum: $[r_j, p_k] = i\, \hbar\, \delta_{jk}$ and the definition of angular momentum in terms of the Levi-Civita symbol: $L_i = \epsilon_{ijk}\, r_j\, p_k$:

a. Show that

$$[L_i, L_j] = i\, \hbar\, \epsilon_{kij} L_k \tag{23.37}$$

b. Show that the components of $\mathbf{L}$ commute with L^2:

$$[L_i, L^2] = 0 \tag{23.38}$$

for $i = 1, 2, 3$.

Problem 23.2

Griffiths 4.20. Here you will explore the classical correspondence of torque and angular momentum.