Discussion 12

1 Introduction

Continuing from last week, let's now consider the part of 3d quantum mechanics that is not "painless": angular momentum. But you know what they say: no pain no gain. There is an immense amount to gain from studying angular momentum, once you get past the (admittedly rather large) amount of formalism. I would say it the second most important and useful topic in this class, after the harmonic oscillator.

Suppose we have a spherically symmetric system, which is to say we have a particle moving under the influence of a potential $V(|\mathbf{r}|)$ which depends only on the distance to the origin. Then we found in class that the time-independant Schrodinger equation could be simplified by making a separation of variables

$$\psi(r,\theta,\phi) = R(r)Y(\theta,\phi)$$

into radial and angular coordinates. The time-independent Schrodinger equation separates into a radial piece:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V_{eff}(r)\right]R(r) = ER(r)$$

with so-called *effective potential* given by

$$V_{eff}(r) = \frac{\ell(\ell+1)\hbar^2}{2mr^2} + V(r)$$

where $V(r)$ is the potential governing the system. The other half is the angular equation, which I won't write down here (see lecture notes 22). This equation does *not* involve the potential $V(r)$, which means if we solve it once, we've solved it for all time. The solutions are the *spherical harmonics* $Y_\ell^m(\theta,\phi)$, labelled by two numbers $\ell = 0,1,2,3,...$, and $m = -\ell,...,0,...,+\ell$, sometimes called (rather unhelpfully) the azimuthal quantum number, and the magnetic quantum number, respectively. I prefer to call them the total angular momentum quantum number, and the z-angular momentum quantum number.

The first few spherical harmonics are:

$$Y_0^0(\theta,\varphi) = \sqrt{\frac{1}{4\pi}} \quad Y_1^{\pm1}(\theta,\varphi) = \mp\sqrt{\frac{3}{8\pi}}e^{\pm i\phi}\sin\theta \quad Y_2^{\pm2}(\theta,\varphi) = \sqrt{\frac{15}{32\pi}}e^{\pm 2i\varphi}\sin^2\theta$$

$$Y_1^0(\theta,\varphi) = \sqrt{\frac{3}{4\pi}}\cos\theta \quad Y_2^{\pm1}(\theta,\varphi) = \mp\sqrt{\frac{15}{8\pi}}e^{\varphi}\sin\theta\cos\theta$$

$$Y_2^0(\theta,\varphi) = \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1)$$

We also have the angular momentum operators

$$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y$$
$$\hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z$$
$$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$$

which act on states $|\phi\rangle$ in the Hilbert space of 3d wavefunctions. They are Hermitian operators, each possessing a complete orthonormal eigenbasis. They can be conveniently packaged into a vector of operators, $\hat{\mathbf{L}} = (\hat{L}_x, \hat{L}_y, \hat{L}_z)$, in which case we can write $\hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$, just like in classical mechanics. Just using the commutators of the position and momentum operators, we can verify that

$$[\hat{L}_z, \hat{p}^2] = 0$$
$$[\hat{L}_z, \hat{r}^2] = 0$$

which together imply that $\hat{L_z}$ commutes with a spherically symmetric Hamiltonian $\hat{H}$. Of course there is nothing special about $\hat{L}_z$, so we also have $[\hat{L}_x, \hat{H}] = 0$ and $[\hat{L}_y, \hat{H}] = 0$. Together these tell us that the system is invariant under arbitrary rotations, and that angular momentum is conserved.

In addition, we can also show that $[\hat{L}^2, \hat{H}] = 0$, and $[\hat{L}^2, \hat{L}_z] = 0$ so the operator $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$ (called the total angular momentum operator) is also conserved, and $\hat{L}^2$ and $\hat{L}_z$ are compatible observable. We can therefore have states $|E, \ell, m\rangle$ which are simultaneous eigenstates of the operators $\hat{H}$, $\hat{L^2}$, and any one of the angular momentum operators, conventionally chosen to be $\hat{L}_z$. We cannot pick more than one of them at a time, because they are mutually incompatible with each other, like $\hat{x}$ and $\hat{p}_x$. These operators have spectra

$$\hat{H}\,|E, \ell, m\rangle = E\,|E, \ell, m\rangle$$
$$\hat{L}^2\,|E, \ell, m\rangle = \ell(\ell+1)\hbar^2\,|E, \ell, m\rangle$$
$$\hat{L}_z\,|E, \ell, m\rangle = m\hbar\,|E, \ell, m\rangle$$

where the energies E are determined by the radial equation, $\ell = 0, 1, 2, 3, ...$ is a non-negative integer, and m is an integer between $-\ell$ and $+\ell$.

The position-space representations of the angular momentum operators are:

$$\hat{L}_x \to -i\hbar\left(\hat{y}\frac{\partial}{\partial z} - \hat{z}\frac{\partial}{\partial y}\right)$$
$$\hat{L}_y \to -i\hbar\left(\hat{z}\frac{\partial}{\partial x} - \hat{x}\frac{\partial}{\partial z}\right)$$
$$\hat{L}_z \to -i\hbar\left(\hat{x}\frac{\partial}{\partial y} - \hat{y}\frac{\partial}{\partial x}\right)$$

or, in spherical coordinates:

$$\begin{aligned}
\hat{L}_x &\to -i\hbar\left(-\sin\varphi\frac{\partial}{\partial\theta} - \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}\right)\\
\hat{L}_y &\to -i\hbar\left(\cos\varphi\frac{\partial}{\partial\theta} - \cot\theta\sin\varphi\frac{\partial}{\partial\varphi}\right)\\
\hat{L}_z &\to -i\hbar\frac{\partial}{\partial\varphi}\\
\hat{L}^2 &\to -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]
\end{aligned}$$

Thankfully, it's not really necessary to use the formulas. Finally, we have the lovely fact tying together the operator viewpoint and differential equation viewpoint, that the spherical harmonics are nothing but the position-space wavefunctions of the states $|\ell, m\rangle$:

$$\langle\theta,\varphi|\ell,m\rangle = Y_\ell^m(\theta,\varphi)$$

As such, they obey:

$$\begin{aligned}
\langle\theta,\varphi|\, L_z \,|\ell,m\rangle &= -i\hbar\frac{\partial}{\partial\varphi}Y_\ell^m(\theta,\phi) = m\hbar Y_\ell^m(\theta,\varphi)\\
\langle\theta,\varphi|\, \hat{L}^2 \,|\ell,m\rangle &= L^2 Y_\ell^m(\theta,\phi) = \ell(\ell+1)\hbar^2 Y_\ell^m(\theta,\phi)
\end{aligned}$$

Commutators

1. The *canonical commutation relations* between the position operators x, y, z and the momentum operators p_x, p_y, p_z are $[x, p_x] = i\hbar$, $[y, p_y] = i\hbar$, and $[z, p_z] = i\hbar$. All other commutators are zero, for example $[x, z] = 0$ and $[p_x, y] = 0$. Starting with these, work out the following:

$$\begin{aligned}
[L_z, x] = i\hbar y \quad &, \quad [L_z, y] = -i\hbar x \quad , \quad [L_z, z] = 0\\
[L_z, p_x] = i\hbar p_y \quad &, \quad [L_z, p_y] = -i\hbar p_x \quad , \quad [L_z, p_z] = 0
\end{aligned}$$

2. * Use the answers to the above to evaluate $[L_z, L_x] = i\hbar L_y$ directly.

3. Evaluate $[L_z, r^2]$ and $[L_z, p^2]$ (where $r^2 = x^2 + y^2 + z^2$ and $p^2 = p_x^2 + p_y^2 + p_z^2$).

4. Using (5), argue that the Hamiltonian $H = (p^2/2m) + V(\vec{r})$ commutes with all three components of $\vec{L}$, provided that $V(\vec{r})$ depends only on $r = |\vec{r}|$. As a result, in this case H, L^2, and L_z are all mutually compatible observables.

Discussion 12

Orbital Angular Momentum

5. * A particle is known to be in a state $\psi(r, \theta, \varphi)$ with a total angular momentum quantum number $\ell = 3$.
   (a) A measurement of the total angular momentum $\hat{L}^2$ is made. What are the possible results?
   (b) A measurement of $\hat{L}_z$ is made. What are the possible results?
   (c) After having measured $\hat{L}_z$, does measuring $\hat{L}^2$ now give different results than it used to?

6. * Just as p_x has position-space representation $-i\hbar\partial/\partial x$, the operator L_z has position space representation $-i\hbar\partial/\partial\varphi$, where φ is the azimuthal angle in spherical coordinates. Suppose a wave function $\psi(r, \theta, \varphi)$ satisfies

$$L_z\psi = -i\hbar\frac{\partial}{\partial\varphi}\psi(r, \theta, \varphi) = m\hbar\psi(r, \theta, \varphi)$$

   and is therefore an eigenfunction of the L_z operator. By separating variables in spherical coordinates $\psi(r, \theta, \varphi) = R(r)\Phi(\varphi)\Theta(\theta)$, derive an equation satisfied by $\Phi(\varphi)$ and solve it. What are the possible values of m?

7. * Suppose we are told that a particle has wavefunction $\psi(r, \theta, \varphi) = f(r)\cos\varphi + g(r)e^{3i\varphi}$, where $f(r)$ and $g(r)$ are just some functions of r. If a measurement of L_z is made, what are the possible outcomes?

8. Suppose we are told that a particle has wavefunction $\psi(r, \theta, \varphi) = (x + y + z)f(r)$, where $f(r)$ is some function of r. If a measurement of $\hat{L}^2$ is made, what are the possible results? If a measurement of $\hat{L}_z$ is made, what are the possible results? What are the probabilities of recieving the outcomes just mentioned?

9. A *rigid rotor* is a system with Hamiltonian $\hat{H} = \hat{L}^2/2I$, where I is the moment of inertia of the system. You can think of it as a particle attached to the origin by a rigid rod of a fixed length, in which the $I = ma^2$, where m is the mass of the particle and a is the length of the rod. Notice that this is just the time independent Schrodinger equation with $\frac{d^2}{dr^2} = 0$ and $V(r) = 0$, leaving just the "effective potential".
   (a) What are the allowed energies of this system?
   (b) This is a rotationally invariant system, so we can simultaneously label the states by $|E, \ell, m\rangle$. Explain why the E label is redundant.
   (c) At time $t = 0$, the rigid rotor is put in a state

$$\langle\theta, \varphi|\psi(0)\rangle = \sqrt{\frac{3}{4\pi}}\sin\theta\sin\varphi$$

What is the state at a later time? (Suggestion: write this as a linear combination of spherical harmonics).

(d) What values of L_z can be obtained in a measurement, and with what probabilities will they occur?

(e) What is $\langle L_x \rangle$ for this state as a function of time?

Solutions

1. $[L_z, x] = [xp_y - yp_x, x]$

$= [xp_y, x] - [yp_x, x]$

This is zero because x commutes with both x and p_y

$= -y[p_x, x]$

$$\boxed{[L_z, x] = i\hbar y}$$

Similarly,

$$[L_z, y] = [xp_y - yp_x, y] = [xp_y, y] - \cancel{[yp_x, y]}^{\,0}$$

$$= \boxed{-i\hbar x}$$

$$[L_z, z] = [xp_y - yp_x, z] = \boxed{0}$$

because z commutes with all of x, y, p_x, p_y.

Next,

$$[L_z, p_x] = [xp_y - yp_x, p_x] = [xp_y, p_x] - \cancel{[yp_x, p_x]}^{\,0}$$

$$= \boxed{p_y i\hbar}$$

$$[L_z, p_y] = [xp_y - yp_x, p_y] = \cancel{[xp_y, p_y]}^{\,0} - [yp_x, p_y]$$

$$= \boxed{-p_x i\hbar}$$

$$[L_z, p_z] = [xp_y - yp_x, p_z] = \boxed{0}$$

because p_z commutes with all of x, y, p_x, p_y.

2 $[L_z, L_x] = [L_z, yP_z - zP_y]$

$$= [L_z, yP_z] - [L_z, zP_y] \qquad [L_z, P_z] = 0$$

$$= P_z[L_z, y] - z[L_z, P_y] \qquad [L_z, z] = 0$$

$$= P_z(-i\hbar x) - z(-i\hbar P_x)$$

$$= i\hbar(zP_x - xP_z)$$

$$= i\hbar L_y$$

3 $[L_z, r^2] = [L_z, x^2] + [L_z, y^2] + \cancel{[L_z, z^2]}^{\,0}$

L_z commutes with z.

Use $[A, BC] = B[A, C] + [A, B]C$.

$$\Rightarrow [L_z, r^2] = x[L_z, x] + [L_z, x]x + y[L_z, y] + [L_z, y]y$$

$$= x(i\hbar y) + (i\hbar y)x + y(-i\hbar x) + (-i\hbar x)y$$

$= 0$ (all terms cancel).

$$\Rightarrow \boxed{[L_z, r^2] = 0}$$

Similarly,

$$[L_z, P^2] = [L_z, P_x^2] + [L_z, P_y^2] + \underbrace{[L_z, P_z^2]}_{=0}$$

$$= P_x[L_z, P_x] + [L_z, P_x]P_x + P_y[L_z, P_y] + [L_z, P_y]P_y$$

$$= P_x(i\hbar P_y) + (i\hbar P_y)P_x + P_y(-i\hbar P_x) + (-i\hbar P_x)P_y = 0$$

$$\Rightarrow \boxed{[L_z, P^2] = 0}$$

$\boxed{4}$ If $V(\vec{r}) = V(|\vec{r}|)$ is a central potential, then

$$[L_z, V(\vec{r})] = 0$$

because $V(|\vec{r}|)$ can be written as a function of $\hat{r}^2$. Then since the kinetic energy is $\hat{\vec{p}}^2/2m$,

$$[\hat{L}_z, \hat{H}] = 0$$

using $[\hat{\vec{p}}^2, \hat{L}_z] = 0$.

$\boxed{5}$ (b) With $\ell = 3$, in principle any of

$m = -3$, $m = -2$, $m = -1$, $m = 0$, $m = 1$, $m = 2$, $m = 3$

are possible, so that a measurement of L_z could yield $-3\hbar$, $-2\hbar$, $\hbar$, 0, $\hbar$, $2\hbar$, or $3\hbar$.

(a) A measurement of $\hat{L}^2$ yields $\ell(\ell+1)\hbar^2 = 3(3+1)\hbar^2 = 12\hbar^2$ with 100% certainty.

(c) No. L^2 and L_z are mutually compatible, so measuring one does not affect the other.

$\boxed{6}$ Let's solve $L_z\psi = m\hbar\psi$. Use the seperation of variables

$$\psi = R(r)\,\Theta(\theta)\,\Phi(\varphi).$$

Then:

$$L_z\psi = -i\hbar\frac{\partial}{\partial\varphi}R\Theta\Phi = m\hbar R\Theta\Phi$$

$$\Rightarrow -i\hbar R\Theta\Phi' = m\hbar R\Theta\Phi$$

Divide through by $R(r)\,\Theta(\theta)$ $\longrightarrow$

$$\Rightarrow -i\hbar \frac{d\Phi}{d\varphi} = m\hbar\,\Phi(\varphi)$$

$$\Rightarrow \frac{d\Phi}{d\varphi} = im\,\Phi(\varphi)$$

This ODE has solution $\Phi(\varphi) = A e^{im\varphi}$ naively for any values of A and φ. However, we must remember that φ is a cyclic coordinate, so that $\varphi + 2\pi$ is really the same as φ.

Then:

$$\Phi(\varphi) = \Phi(\varphi + 2\pi)$$

$$\Rightarrow e^{im\varphi} = e^{im(\varphi+2\pi)} = e^{im\varphi} e^{i2\pi m}$$

this equation can only be true if $e^{2\pi i m} = 1$, which means m must be an integer:

$$m = 0, \pm 1, \pm 2, \pm 3, \ldots$$

$\boxed{7}$ The state $\psi(r,\theta,\varphi) = f(r)\cos\varphi + g(r)\,e^{3i\varphi}$ can be written as:

$$\psi(r,\theta,\varphi) = f(r)\frac{1}{2}e^{i\varphi} + f(r)\frac{1}{2}e^{-i\varphi} + g(r)e^{3i\varphi}$$

This is a linear combination of the $m = +1, -1, +3$ eigenfunctions, so the possible outcomes ~~are~~ of measuring L_z are $-\hbar$, $+\hbar$, and $+3\hbar$.

$\boxed{8}$ The state $\psi(r,\theta,\varphi) = (x+y+z)\,f(r)$ can be written with a linear combination of spherical harmonics if we recall that:

$$Y_1^0(\theta,\varphi) = \sqrt{\frac{3}{4\pi}}\cos\theta = \sqrt{\frac{3}{4\pi}}\frac{z}{r}$$

Although slightly less obvious, we also have:

$$\frac{1}{\sqrt{2}}\left(Y_1^{-1} - Y_1^1\right) = \sqrt{\frac{3}{4\pi}}\frac{x}{r}, \qquad \frac{i}{\sqrt{2}}\left(Y_1^1 + Y_1^{-1}\right) = \sqrt{\frac{3}{4\pi}}\frac{y}{r}$$

we can therefore write

$$z = \sqrt{\frac{4\pi}{3}}\, r\, Y_1^0(\theta,\varphi)$$

$$x = \sqrt{\frac{4\pi}{3}}\, r\, \frac{1}{\sqrt{2}}\left(Y_1^{-1} - Y_1^1\right)$$

$$y = \sqrt{\frac{4\pi}{3}}\, r\, \frac{i}{\sqrt{2}}\left(Y_1^{-1} + Y_1^1\right)$$

so that

$$x+y+z = r\sqrt{\frac{4\pi}{3}}\left[Y_1^0 + \frac{1+i}{\sqrt{2}}Y_1^{-1} + \frac{-1+i}{\sqrt{2}}Y_1^1\right]$$

and finally:

$$\psi(r,\theta,\varphi) = \left[Y_1^0 + \frac{1+i}{\sqrt{2}}Y_1^{-1} + \frac{-1+i}{\sqrt{2}}Y_1^1\right]\sqrt{\frac{4\pi}{3}}\, r f(r)$$

Now we can just read off the answer:

- A measurement of L^2 results in $\ell = 1$ or $1(1+1)\hbar^2 = 2\hbar^2$ with 100% certainty.
- A measurement of L_z results in

  $-\hbar,\ 0,\ +\hbar$

  all with equal probability (1/3)

9) The Hamiltonian is $\hat{L}^2/2I$.

(a) Since the possible eigenvalues of $\hat{L}^2$ are $\ell(\ell+1)\hbar^2$ for $\ell = 0,1,2,3,\ldots$ the possible energies are

$$\frac{\ell(\ell+1)\hbar^2}{2I} \qquad \ell = 0,1,2,\ldots$$

(b) The energies are already labelled by ℓ.

(c) $\psi^{(t=0)}(\varphi,\theta) = \sqrt{\frac{3}{4\pi}}\sin\theta\sin\varphi$

This can be written as:

$$\sqrt{\frac{3}{4\pi}}\sin\theta\sin\varphi = \sqrt{\frac{3}{4\pi}}\,\frac{y}{r} = \frac{i}{\sqrt{2}}\left(Y_1^1 + Y_1^{-1}\right)$$

Both parts of this have $l=1$, so this is an energy eigenstate with energy $2\hbar^2/2I$.

$$\Rightarrow \Psi(\theta,\varphi,t) = e^{-i\hbar t/I}\sqrt{\frac{3}{4\pi}}\sin\theta\sin\varphi$$

(d) The possible values of L_z are $+1\hbar$ and $-\hbar$, with equal probability.

(e) Since $[L_x, L^2]=0$, $[L_x, H]=0$, so $\langle L_x\rangle$ is conserved (does not change with time).

At $t=0$,

$$\hat{L}_x\Psi = \frac{\hbar}{i}\left(-\sin\varphi\frac{\partial}{\partial\theta} - \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}\right)\sqrt{\frac{3}{4\pi}}\sin\theta\sin\varphi$$

$$= \sqrt{\frac{3}{4\pi}}\,\frac{\hbar}{i}\left(\cos\theta\sin^2\varphi - \cos\theta\cos^2\varphi\right)$$

$$= \sqrt{\frac{3}{4\pi}}\,\frac{\hbar}{i}\cos\theta\left(\sin^2\varphi - \cos^2\varphi\right)$$

Then

$$\langle L_x\rangle = \langle\psi(0)|L_x|\psi(0)\rangle$$

$$= \int_0^\pi d\theta\int_0^{2\pi}d\varphi\,\sin\theta\,\frac{3}{4\pi}\sin\theta\sin\varphi\,\frac{\hbar}{i}\cos\theta\left(\sin^2\varphi-\cos^2\varphi\right)$$

The integral over φ is zero, so

$$\langle L_x\rangle = 0$$

for all time. Not the most enlightening calculation maybe...