

5 Three Dimensional Mathematical Tools

2/17: 1. Consider a three-dimensional box, such that the potential is given by

$$V(x, y, z) = V_1\theta(|x| - a) + V_2\theta(|y| - b) + V_3\theta(|z| - c) \quad (5.1)$$

where the function θ is such that

$$\theta(u) = \begin{cases} 1 & u \geq 0 \\ 0 & u < 0 \end{cases} \quad (5.2)$$

This means that the potential is zero inside the box that extends from $x = -a$ to $x = a$ in the x -direction, $y = -b$ to $y = b$ in the y -direction, and $z = -c$ to $z = c$ in the z -direction and increases in steps otherwise.

- a) Analyze first the case wherein all of $V_1, V_2, V_3 \rightarrow \infty$. This is the infinite square well in three dimensions. What is the general solution for $\psi(x, y, z)$? *Hint:* Use the method of separation of variables and write $\psi(x, y, z) = X(x)Y(y)Z(z)$.

Answer. The Schrödinger equation for this case is

$$-\frac{\hbar^2}{2m} \vec{\nabla}^2 \psi = E\psi$$

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) = E\psi$$

along with the boundary conditions

$$\psi(\pm a, y, z) = 0 \quad \psi(x, \pm b, z) = 0 \quad \psi(x, y, \pm c) = 0$$

Taking the hint and writing $\psi = XYZ$, we can rearrange the above equation into the form

$$\frac{1}{X} \left[-\frac{\hbar^2}{2m} \frac{d^2 X}{dx^2} \right] + \frac{1}{Y} \left[-\frac{\hbar^2}{2m} \frac{d^2 Y}{dy^2} \right] + \frac{1}{Z} \left[-\frac{\hbar^2}{2m} \frac{d^2 Z}{dz^2} \right] = E$$

Note that we switch from partial to total derivatives here because now each function is only a function of one variable (e.g., $X(x)$ depends only on x).

Moving on, since the sum of these three independent terms is constant, each term must be equal to a constant, too. Thus, we can split the above equation into the following three.

$$-\frac{\hbar^2}{2m} \frac{d^2 X}{dx^2} = E_{n_1} X \quad -\frac{\hbar^2}{2m} \frac{d^2 Y}{dy^2} = E_{n_2} Y \quad -\frac{\hbar^2}{2m} \frac{d^2 Z}{dz^2} = E_{n_3} Z$$

As to the boundary conditions, the rewrite in the hint gives us, for example,

$$0 = \psi(\pm a, y, z) = X(\pm a)Y(y)Z(z)$$

Since Y, Z may both be nonzero for some y, z , the zero product property tells us that we must have

$$X(\pm a) = 0$$

Doing the same for the other two boundary conditions, we obtain the following three new boundary conditions.

$$X(\pm a) = 0 \quad Y(\pm b) = 0 \quad Z(\pm c) = 0$$

We will now solve the three independent boundary-value problems. Since they are all directly analogous, we will concentrate on the X -case and know that the other solutions may be observed from there via a change of variables.

To begin, it will be useful to define

$$u(x) := x + a \qquad L := 2a$$

Observe that under this definition, $du/dx = 1$. Changing variables in the ODE, we get

$$\begin{aligned} -\frac{\hbar^2}{2m} \frac{d}{dx} \left[\frac{d}{dx} [X(u(x))] \right] &= E_{n_1} X(u(x)) \\ -\frac{\hbar^2}{2m} \frac{d}{dx} \left[\frac{d}{du} [X(u)] \cdot \frac{du}{dx} \right] &= E_{n_1} X(u) \\ -\frac{\hbar^2}{2m} \frac{d}{du} \left[\frac{d}{du} [X(u)] \cdot 1 \right] \cdot \frac{du}{dx} &= E_{n_1} X(u) \\ -\frac{\hbar^2}{2m} \frac{d^2}{du^2} [X(u)] &= E_{n_1} X(u) \end{aligned}$$

Additionally, since $u(-a) = 0$ and $u(a) = 2a = L$, the relevant boundary condition with respect to u is

$$X(u = 0) = X(u = L) = 0$$

Altogether, the first ODE and boundary condition in terms of u become

$$-\frac{\hbar^2}{2m} \frac{d^2 X}{du^2} = E_{n_1} X \qquad X(0) = X(L) = 0$$

which is entirely analogous to the infinite square well ODE we solved in class on 1/17. Thus, the solutions are

$$X_{n_1}(u) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi n_1 u}{L}\right)$$

Returning the u -substitution to obtain the solutions in terms of x , we get

$$X_{n_1}(x) = \sqrt{\frac{1}{a}} \sin\left[\frac{\pi n_1 (x + a)}{2a}\right]$$

As mentioned above, we can do something analogous in the other two directions. Therefore, the general solution is

$$\boxed{\psi_{n_1 n_2 n_3}(x, y, z) = \sqrt{\frac{1}{abc}} \sin\left[\frac{\pi n_1 (x + a)}{2a}\right] \sin\left[\frac{\pi n_2 (y + b)}{2b}\right] \sin\left[\frac{\pi n_3 (z + c)}{2c}\right]}$$

□

- b) Give an expression for the total energy of the system in terms of the energies associated with the propagation in the three space directions.

Answer. Return to the step in part (a) at which we had finally obtained an ODE fully analogous to the one solved in class on 1/17. We did not state it in part (a) because it was not relevant, but just as we obtained $X_{n_1}(u)$, our work in class on 1/17 gives us the corresponding energy expression

$$E_{n_1} = \frac{\hbar^2 \pi^2 n_1^2}{2mL^2} = \frac{\hbar^2 \pi^2 n_1^2}{8ma^2}$$

Analogous results exist in the other two directions. Additionally, as in class on 2/12, setting all of our ODEs equal to constants in the separation of variables step *also* gives us the equation

$$E = E_{n_1} + E_{n_2} + E_{n_3}$$

Thus, the expression for the total energy of the system in terms of the energies associated with the propagation in the three space directions is

$$\boxed{E_{n_1 n_2 n_3} = \frac{\hbar^2 \pi^2}{8m} \left(\frac{n_1^2}{a^2} + \frac{n_2^2}{b^2} + \frac{n_3^2}{c^2} \right)}$$

□

- c) What happens when one of the three V_i 's becomes finite, and we are in a bounded state such that $E < V_i$? What would be the possible energies in such a case?

Answer. Suppose WLOG that V_1 becomes finite. The Schrödinger equation for this case is

$$-\frac{\hbar^2}{2m} \vec{\nabla}^2 \psi + V(x, y, z) \psi = E \psi$$

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) + V_1 \theta(|x| - a) \psi = E \psi$$

along with the boundary conditions

$$\psi(x, \pm b, c) = 0 \qquad \psi(x, y, \pm c) = 0$$

Writing $\psi = XYZ$, we can rearrange the above equation into the form

$$\frac{1}{X} \left[-\frac{\hbar^2}{2m} \frac{d^2 X}{dx^2} + V_1 \theta(|x| - a) X \right] + \frac{1}{Y} \left[-\frac{\hbar^2}{2m} \frac{d^2 Y}{dy^2} \right] + \frac{1}{Z} \left[-\frac{\hbar^2}{2m} \frac{d^2 Z}{dz^2} \right] = E$$

Separating variables, we obtain two ODEs familiar from part (a) and one new one. We will focus on the new one from here on out. If we let Region I span $(-\infty, -a)$, Region II span $[-a, a]$, and Region III span (a, ∞) , then this new ODE can be written as

$$-\frac{\hbar^2}{2m} \frac{d^2 X_I}{dx^2} + V_1 X_I = E_{n_1} X_I$$

$$-\frac{\hbar^2}{2m} \frac{d^2 X_{II}}{dx^2} = E_{n_1} X_{II}$$

$$-\frac{\hbar^2}{2m} \frac{d^2 X_{III}}{dx^2} + V_1 X_{III} = E_{n_1} X_{III}$$

along with the four boundary conditions

$$X_I(-a) = X_{II}(-a) \qquad X_{II}(a) = X_{III}(a)$$

$$X'_I(-a) = X'_{II}(-a) \qquad X'_{II}(a) = X'_{III}(a)$$

Define

$$k_I = \frac{\sqrt{2m(E_{n_1} - V_1)}}{\hbar} \qquad k_{II} = \frac{\sqrt{2mE_{n_1}}}{\hbar}$$

Given that $E_{n_1} < V_1$, then per PSet 2, Q2b, the solutions will be

$$X_I(x) = Ae^{\kappa_I x} + Be^{-\kappa_I x}$$

$$X_{II}(x) = S_{II} \sin(k_{II} x) + C_{II} \cos(k_{II} x)$$

$$X_{III}(x) = Fe^{\kappa_I x} + Ge^{-\kappa_I x}$$

where $i\kappa_I = k_I$. Now just like in PSet 2, Q2c, some of the exponential terms diverge. In particular, $Be^{-\kappa_I x}$ diverges as $x \rightarrow -\infty$ and $Fe^{\kappa_I x}$ diverges as $x \rightarrow \infty$. Thus, to keep the solution from blowing up, we must set

$$B = F = 0$$

to get

$$X_I(x) = Ae^{\kappa_I x}$$

$$X_{II}(x) = S_{II} \sin(k_{II} x) + C_{II} \cos(k_{II} x)$$

$$X_{III}(x) = Ge^{-\kappa_I x}$$

Before we apply the boundary conditions, there is one more thing we can do to simplify the above solutions. Let $X_{n_1}(x)$ be a full, piecewise eigenstate of the relevant Schrödinger equation. Then since this potential is symmetric about the origin — that is, $V(x) = V(-x)$ — $X_{n_1}(-x)$ will also be an eigenstate of the relevant Schrödinger equation:

$$\begin{aligned} -\frac{\hbar^2}{2m} \frac{d^2 X_I(-x)}{dx^2} + V(x) X_I(-x) &= -\frac{\hbar^2}{2m} (-1)^2 \frac{d^2 X_I(-x)}{d(-x)^2} + V(-x) X_I(-x) \\ &= -\frac{\hbar^2}{2m} \frac{d^2 X_I(-x)}{d(-x)^2} + V(-x) X_I(-x) \\ &= E_{n_1} X_I(-x) \end{aligned}$$

It follows by the linearity of the Schrödinger equation that $X_{n_1}(x) + X_{n_1}(-x)$ and $X_{n_1}(x) - X_{n_1}(-x)$ are also eigenstates of with energy E_{n_1} . Essentially, this means that we can always choose our eigenstates to be even or odd functions of x . Going back to our solutions X_I, X_{II}, X_{III} , this means that we need not consider X_{II} in full generality but can rather divide the solutions up into those with $S_{II} = 0$ (even) and those with $C_{II} = 0$ (odd). For the even solutions, the boundary conditions tell us that

$$\begin{aligned} Ae^{-\kappa_I a} &= C_{II} \cos(k_{II} a) \\ \kappa_I Ae^{-\kappa_I a} &= k_{II} C_{II} \sin(k_{II} a) \\ C_{II} \cos(k_{II} a) &= Ge^{-\kappa_I a} \\ -k_{II} C_{II} \sin(k_{II} a) &= -\kappa_I Ge^{-\kappa_I a} \end{aligned}$$

From here, we may obtain the important result that

$$\kappa_I = k_{II} \tan(k_{II} a)$$

$$\boxed{\frac{\sqrt{2m(V_1 - E_{n_1})}}{\hbar} = \frac{\sqrt{2mE_{n_1}}}{\hbar} \tan\left(\frac{\sqrt{2mE_{n_1}}}{\hbar} a\right)}$$

Similarly, for the odd solutions, we may obtain that

$$\boxed{\frac{\sqrt{2m(V_1 - E_{n_1})}}{\hbar} = -\frac{\sqrt{2mE_{n_1}}}{\hbar} \cot\left(\frac{\sqrt{2mE_{n_1}}}{\hbar} a\right)}$$

Energies may be obtained by solving either of these equations. This energy may then be added onto the other two as in part (b). \square

d) What happens when the three V_i 's become finite?

Answer. We will obtain three energies of the form in part (c), all of which may be added together as in part (b). \square

2. In the presence of a central force, the potential depends only on the radial distance and not on the direction, i.e.,

$$V(\vec{r}) = V(\sqrt{x^2 + y^2 + z^2}) \quad (5.3)$$

a) Show that in such a potential, the momentum is not conserved (that is, its mean value is not independent of time), but the angular momentum $\vec{L} = \vec{r} \times \vec{p}$ is conserved. *Hint:* Use commutation relations with \hat{H} . Test this for each component of \vec{L} separately.

Answer. We first show that the momentum is not conserved. To do this, first note that $\hat{\vec{p}}$ is time-independent. Additionally, since $\hat{\vec{p}}$ naturally commutes with any power of itself, the commutator $[\hat{H}, \hat{\vec{p}}]$ reduces as follows.

$$[\hat{H}, \hat{\vec{p}}] = [\hat{V}, \hat{\vec{p}}]$$

But by the result from class on 1/12, we have that

$$[\hat{V}, \hat{p}] = -i\hbar \vec{\nabla} V$$

Therefore, by transitivity, $[\hat{H}, \hat{p}]$ is nonzero and hence, momentum is not conserved.

We now show that the angular momentum is conserved. Taking the hint, recall from the 1/29 lecture that

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

Additionally, recall that

$$\hat{H} = \frac{\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2}{2m} + \hat{V}(r)$$

Thus, we have that

$$\begin{aligned} [\hat{H}, \hat{L}_x] &= \left[\frac{\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2}{2m} + \hat{V}(r), \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \right] \\ &= \left[\frac{\hat{p}_x^2}{2m}, \hat{y}\hat{p}_z \right] + \left[\frac{\hat{p}_y^2}{2m}, \hat{y}\hat{p}_z \right] + \left[\frac{\hat{p}_z^2}{2m}, \hat{y}\hat{p}_z \right] \\ &\quad + \left[\frac{\hat{p}_x^2}{2m}, -\hat{z}\hat{p}_y \right] + \left[\frac{\hat{p}_y^2}{2m}, -\hat{z}\hat{p}_y \right] + \left[\frac{\hat{p}_z^2}{2m}, -\hat{z}\hat{p}_y \right] \\ &\quad + [\hat{V}(r), \hat{y}\hat{p}_z] + [\hat{V}(r), -\hat{z}\hat{p}_y] \\ &= \left[\frac{\hat{p}_y^2}{2m}, \hat{y}\hat{p}_z \right] + \left[\frac{\hat{p}_z^2}{2m}, -\hat{z}\hat{p}_y \right] + i\hbar \left(\hat{y} \frac{\partial V}{\partial z} - \hat{z} \frac{\partial V}{\partial y} \right) \\ &= -\frac{i\hbar \hat{p}_y \hat{p}_z}{m} + \frac{i\hbar \hat{p}_y \hat{p}_z}{m} + i\hbar \frac{\partial V}{\partial r} \left(y \frac{\partial r}{\partial z} - z \frac{\partial r}{\partial y} \right) \\ &= 0 \end{aligned}$$

Now let's investigate some of the above substitutions a bit more closely. From line 1 to line 2, we split the commutator into $4 \cdot 2 = 8$ terms using its bilinearity. From line 2 to line 3, we eliminated all commutators that go to zero among the first six, and evaluated the last two commutators using a combination of Rule 3 and properties mentioned at the beginning of the lecture.

Notice that the only two of the first six commutators that did *not* go to zero were those for which the variable in the squared momentum operator matched the position operator, i.e., in

$$\left[\frac{\hat{p}_y^2}{2m}, \hat{y}\hat{p}_z \right]$$

we may observe that \hat{p}_y^2 and \hat{y} both concern y . Example evaluation:

$$\begin{aligned} \left[\frac{\hat{p}_x^2}{2m}, \hat{y}\hat{p}_z \right] &= \frac{1}{2m} [\hat{p}_x^2, \hat{y}\hat{p}_z] \\ &= \frac{1}{2m} (\hat{p}_x [\hat{p}_x, \hat{y}\hat{p}_z] + [\hat{p}_x, \hat{y}\hat{p}_z] \hat{p}_x) \\ &= \frac{1}{2m} (\hat{p}_x (\underbrace{\hat{y} [\hat{p}_x, \hat{p}_z]}_0) + \underbrace{[\hat{p}_x, \hat{y}]}_0 \hat{p}_z) + (\underbrace{\hat{y} [\hat{p}_x, \hat{p}_z]}_0 + \underbrace{[\hat{p}_x, \hat{y}]}_0 \hat{p}_z) \hat{p}_x \\ &= 0 \end{aligned}$$

Example evaluation:

$$\begin{aligned}
 \left[\frac{\hat{p}_y^2}{2m}, \hat{y}\hat{p}_z \right] &= \frac{1}{2m} [\hat{p}_y^2, \hat{y}\hat{p}_z] \\
 &= \frac{1}{2m} (\hat{p}_y [\hat{p}_y, \hat{y}\hat{p}_z] + [\hat{p}_y, \hat{y}\hat{p}_z] \hat{p}_y) \\
 &= \frac{1}{2m} (\hat{p}_y (\hat{y} \underbrace{[\hat{p}_y, \hat{p}_z]}_0 + \underbrace{[\hat{p}_y, \hat{y}]}_{-i\hbar} \hat{p}_z) + (\hat{y} \underbrace{[\hat{p}_y, \hat{p}_z]}_0 + \underbrace{[\hat{p}_y, \hat{y}]}_{-i\hbar} \hat{p}_z) \hat{p}_y) \\
 &= \frac{1}{2m} (\hat{p}_y (-i\hbar \hat{p}_z) + (-i\hbar \hat{p}_z) \hat{p}_y) \\
 &= -\frac{i\hbar}{2m} (\hat{p}_y \hat{p}_z + \hat{p}_z \hat{p}_y) \\
 &= -\frac{i\hbar}{2m} (\hat{p}_y \hat{p}_z + \hat{p}_y \hat{p}_z) \\
 &= -\frac{i\hbar \hat{p}_y \hat{p}_z}{m}
 \end{aligned}$$

Note that $\hat{p}_z \hat{p}_y = \hat{p}_y \hat{p}_z$ because $[\hat{p}_y, \hat{p}_z] = 0$.

Example evaluation:

$$\begin{aligned}
 [\hat{V}(r), \hat{y}\hat{p}_z] &= \hat{y} \underbrace{[\hat{V}(r), \hat{p}_z]}_{i\hbar \partial V / \partial z} + \underbrace{[\hat{V}(r), \hat{y}]}_0 \hat{p}_z \\
 &= i\hbar \hat{y} \frac{\partial V}{\partial z}
 \end{aligned}$$

Returning to the original set of equations, from line 3 to line 4, we evaluated the last two commutators and applied the chain rule. From line 4 to line 5, we algebraically expanded and cancelled everything (using $r = \sqrt{x^2 + y^2 + z^2}$ for the partial derivatives).

Moving on, similar to the above, we obtain that

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

Thus, by bilinearity once more,

$$[\hat{H}, \hat{\vec{L}}] = [\hat{H}, \hat{L}_x + \hat{L}_y + \hat{L}_z] = 0$$

□

- b) What happens if the system has a translational invariance in the z -direction and

$$V(\vec{r}) = V(\sqrt{x^2 + y^2}) \quad (5.4)$$

for all z ? Is any component of the momentum or angular momentum preserved?

Answer. First, observe that

$$[\hat{V}(\sqrt{x^2 + y^2}), \hat{x}] = V(\sqrt{x^2 + y^2})x - xV(\sqrt{x^2 + y^2}) = V(\sqrt{x^2 + y^2})x - V(\sqrt{x^2 + y^2})x = 0$$

and

$$[\hat{V}(\sqrt{x^2 + y^2}), \hat{p}_y] f = -i\hbar V(\sqrt{x^2 + y^2}) \frac{\partial f}{\partial y} + i\hbar \frac{\partial}{\partial y} (V(\sqrt{x^2 + y^2}) f) = i\hbar \frac{\partial}{\partial y} [V(\sqrt{x^2 + y^2})] f$$

Therefore,

$$\begin{aligned}
 [\hat{H}, \hat{L}_z] &= \left[\frac{\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2}{2m} + \hat{V}(\sqrt{x^2 + y^2}), \hat{x}\hat{p}_y - \hat{y}\hat{p}_x \right] \\
 &= \left[\frac{\hat{p}_x^2}{2m}, \hat{x}\hat{p}_y \right] + \left[\frac{\hat{p}_y^2}{2m}, -\hat{y}\hat{p}_x \right] + [\hat{V}(\sqrt{x^2 + y^2}), \hat{x}\hat{p}_y] + [\hat{V}(\sqrt{x^2 + y^2}), -\hat{y}\hat{p}_x] \\
 &= -\frac{i\hbar\hat{p}_x\hat{p}_y}{m} + \frac{i\hbar\hat{p}_x\hat{p}_y}{m} + i\hbar\frac{dV(u)}{du} \left[x\frac{\partial}{\partial y}(\sqrt{x^2 + y^2}) - y\frac{\partial}{\partial x}(\sqrt{x^2 + y^2}) \right] \\
 &= 0
 \end{aligned}$$

so \hat{L}_z is conserved. None of the other angular momentum directions are conserved because we need the cross partial derivatives to cancel as they do above, and that doesn't occur anywhere else.

Additionally, observe that

$$[\hat{V}(\sqrt{x^2 + y^2}), \hat{p}_z] f = -i\hbar V(\sqrt{x^2 + y^2}) \frac{\partial f}{\partial z} + i\hbar \frac{\partial}{\partial z} (V(\sqrt{x^2 + y^2}) f) = 0$$

Therefore,

$$\begin{aligned}
 [\hat{H}, \hat{p}_z] &= \left[\frac{\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2}{2m} + \hat{V}(\sqrt{x^2 + y^2}), \hat{p}_z \right] \\
 &= \left[\frac{\hat{p}_z^2}{2m}, \hat{p}_z \right] + [\hat{V}(\sqrt{x^2 + y^2}), \hat{p}_z] \\
 &= 0
 \end{aligned}$$

so \hat{p}_z is conserved. None of the other momentum directions are conserved either because we need the right commutator in line 2 to cancel as proven above, and it does not in any other case as proven above with the representative example of \hat{p}_y . \square

- c) For part (b), what would be the mean value $\langle \hat{z} \rangle(t)$ of the z -coordinate if the mean value $\langle \hat{p}_z \rangle$ of the momentum in the z -direction is constant at p_0 while $\langle \hat{z} \rangle = 0$ at time $t = 0$?

Answer. Since momentum is conserved in the z -direction under this paradigm by part (b), we have that

$$p_0 = \langle \hat{p}_z \rangle = m \frac{d}{dt} [\langle \hat{z} \rangle(t)]$$

It follows by integrating both sides and algebraically rearranging that

$$\langle \hat{z} \rangle(t) = \frac{p_0 t}{m}$$

\square

3. Imagine I have a potential such that I can find simultaneous eigenstates of \hat{L}^2 , \hat{L}_z , and \hat{H} with respective eigenvalues $\hbar^2\ell(\ell+1)$, $\hbar m$, and $E_{n\ell}$. Suppose that $[\hat{L}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{L}_k$, $[\hat{L}^2, \hat{L}_i] = [\hat{H}, \hat{L}_i] = 0$, and $\hat{L}_{\pm} = \hat{L}_x \pm i\hat{L}_y$.

- a) Show that $[\hat{L}_{\pm}, \hat{L}_z] = \mp\hbar\hat{L}_{\pm}$.

Answer. We have by the the commutator relations among the \hat{L}_i that

$$[\hat{L}_{\pm}, \hat{L}_z] = [\hat{L}_x \pm i\hat{L}_y, \hat{L}_z] = -i\hbar\hat{L}_y \pm i(i\hbar\hat{L}_x) = -i\hbar\hat{L}_y \mp \hbar\hat{L}_x = \mp\hbar(\hat{L}_x \pm i\hat{L}_y) = \mp\hbar\hat{L}_{\pm}$$

as desired. \square

- b) Show also that this implies that, given an eigenfunction $Y_{\ell m}$ of \hat{L}^2 and \hat{L}_z ,

$$\hat{L}_{\pm} Y_{\ell m} \propto Y_{\ell(m \pm 1)} \quad (5.5)$$

Answer. Let $Y_{\ell m}$ be an eigenstate of \hat{L}^2, \hat{L}_z . Then we have the following by hypothesis.

$$\hat{L}^2 Y_{\ell m} = \hbar^2 \ell(\ell + 1) Y_{\ell m} \quad \hat{L}_z Y_{\ell m} = \hbar m Y_{\ell m}$$

When we apply \hat{L}_z to $\hat{L}_+ Y_{\ell m}$, we get

$$\begin{aligned} \hat{L}_z (\hat{L}_+ Y_{\ell m}) &= [\hat{L}_+ \hat{L}_z - (\hat{L}_+ \hat{L}_z - \hat{L}_z \hat{L}_+)] Y_{\ell m} \\ &= \hat{L}_+ \hbar m Y_{\ell m} + \hbar \hat{L}_+ Y_{\ell m} \\ &= \hbar(m + 1)(\hat{L}_+ Y_{\ell m}) \end{aligned}$$

Thus,

$$\hat{L}_+ Y_{\ell m} \propto Y_{\ell(m+1)}$$

We can prove in a similar fashion that

$$\hat{L}_- Y_{\ell m} \propto Y_{\ell(m-1)}$$

□

- c) Show that $\hat{L}^2 = \hat{L}_- \hat{L}_+ + \hbar \hat{L}_z + \hat{L}_z^2$.

Answer. We have that

$$\begin{aligned} \hat{L}_- \hat{L}_+ &= (\hat{L}_x - i\hat{L}_y)(\hat{L}_x + i\hat{L}_y) \\ &= \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 - i[\hat{L}_y, \hat{L}_x] - \hat{L}_z^2 \\ &= \hat{L}^2 - \hat{L}_z^2 - \hbar \hat{L}_z \\ \hat{L}^2 &= \hat{L}_- \hat{L}_+ + \hbar \hat{L}_z + \hat{L}_z^2 \end{aligned}$$

□

- d) With the above information, use the ladder operators \hat{L}_{\pm} to compute the mean value of $\hat{L}_x, \hat{L}_y, \hat{L}_x^2$, and \hat{L}_y^2 in an eigenstate of \hat{L}^2 and \hat{L}_z .

Answer. We have that

$$\langle n\ell m | \hat{L}_x | n\ell m \rangle = \langle n\ell m | \frac{1}{2}(\hat{L}_+ + \hat{L}_-) | n\ell m \rangle$$

$$\boxed{\langle n\ell m | \hat{L}_x | n\ell m \rangle = 0}$$

Similarly,

$$\boxed{\langle n\ell m | \hat{L}_y | n\ell m \rangle = 0}$$

Additionally, we have that

$$\langle n\ell m | (\hat{L}_x^2 + \hat{L}_y^2) | n\ell m \rangle = \langle n\ell m | (\hat{L}^2 - \hat{L}_z^2) | n\ell m \rangle = \hbar^2 [\ell(\ell + 1) - m^2]$$

Since the above eigenvalue must be greater than or equal to zero, $|m| \leq \ell$. Recall that \hat{L}_x, \hat{L}_y are incompatible with \hat{L}_z . This is why we have an uncertainty associated with the quantity $\hbar^2 [\ell(\ell + 1) - m^2]$. This is also why we have

$$\langle n\ell m | (\hat{L}_x^2 + \hat{L}_y^2) | n\ell m \rangle = 2 \langle n\ell m | \hat{L}_x^2 | n\ell m \rangle = 2 \langle n\ell m | \hat{L}_y^2 | n\ell m \rangle$$

so

$$\boxed{\langle n\ell m | \hat{L}_x^2 | n\ell m \rangle = \langle n\ell m | \hat{L}_y^2 | n\ell m \rangle = \frac{\hbar^2}{2} [\ell(\ell + 1) - m^2]}$$

□

- e) Discuss the uncertainty principle for the incompatible variables \hat{L}_x and \hat{L}_y . In which way does this differ from the case of \hat{x} and \hat{p}_x ?

Answer. Using the generalized uncertainty principle, we have that

$$\sigma_{\hat{L}_x} \cdot \sigma_{\hat{L}_y} = \frac{1}{2} |\langle [\hat{L}_x, \hat{L}_y] \rangle|$$

$$\sigma_{\hat{L}_x} \sigma_{\hat{L}_y} = \frac{\hbar}{2} |\langle \hat{L}_z \rangle|$$

Thus, unlike for x -position and momentum, we see that this uncertainty relation is a state-dependent statement. If we are in a state with vanishing average angular momentum in the z -direction, the product of the uncertainties in \hat{L}_x and \hat{L}_y is 0. The analysis can be generalized by cyclicly permuting x, y, z . In doing so, we can see that the uncertainty in angular momentum in one direction can be 0 if and only if the average angular momenta in each of the other two directions are 0.

This fact can be seen in the previous part. In part (d), we were considering a state where \hat{L}_z is known precisely. In such a state, $\langle \hat{L}_x \rangle$ and $\langle \hat{L}_y \rangle$ will always be 0. \square