Review: Free particle in 3D

$$\hat{H}\psi = E\psi$$

$$\frac{\hat{p}^2}{2m}\psi = E\psi$$

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

$$-\frac{\hbar^2}{2m}\left(\frac{1}{X}\frac{\partial^2 X}{\partial x^2} + \frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} + \frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}\right) = E$$

$$-\frac{\hbar^2}{2m}\left(-k_x^2 - k_y^2 - k_z^2\right) = E$$

$$\left.\begin{aligned} \frac{\partial^2 X}{\partial x^2} = -k_x^2 X \quad \Rightarrow \quad X &= A_x e^{ik_x x} \\ Y &= A_y e^{ik_y y} \\ Z &= A_z e^{ik_z z} \end{aligned}\right\} \psi = Ae^{i\vec{k}\cdot\vec{x}}$$

No boundary conditions.

Highly degenerate! $k_x^2 + k_y^2 + k_z^2 = \frac{2mE}{\hbar^2}$ Knowing only eigenv. of $\hat{H}$ (E) won't give k_x, k_y, k_z

Consider: $[\hat{H}, \hat{p}_x] = [\hat{H}, \hat{p}_y] = [\hat{p}_x, \hat{p}_y] = 0$

$$\hat{p}_x\psi = -i\hbar\frac{\partial\psi}{\partial x} = \hbar k_x A e^{i\vec{k}\cdot\vec{x}} = \hbar k_x \psi$$

$$\hat{p}_y\psi = \hbar k_y \psi$$

So knowing eigenvalues of $(\hat{H}, \hat{p}_x, \hat{p}_y)$ "maximally commuting set" fully specifies the state (gives all separation constants).

Note: Other sets are possible! Doesn't work for ∞-cube!

Hydrogen: We know $\hat{H}$ is degenerate w.r.t. l, and l is deg. w.r.t. m, so we need to know all of n, l, m to specify state.

$$\begin{array}{ccc} n, & l, & m \\ \uparrow & \uparrow & \nwarrow \\ \hat{H} & ? & ? \end{array}$$

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\sqrt{\hat{x}^2+\hat{y}^2+\hat{z}^2})$$

we know $\hat{p}_x, \hat{p}_y, \hat{p}_z$ won't work!

Need 3 since 3 sep. constants!

Q. What hermitian operators commute w/ hydrogen $\hat{H}$?

This is a rotationally symmetric problem, so you may expect $\vec{L}$ to play a role.

So let's look at $\vec{L}$ and determine what commutes and what doesn't.

Note: More complicated than $\vec{p}$ where $[\hat{p}_i, \hat{p}_j] = 0$

Angular Momentum $\quad \vec{L} = \vec{r} \times \vec{p}$

$$\left.\begin{aligned} L_x &= y p_z - z p_y \\ L_y &= z p_x - x p_z \\ L_z &= x p_y - y p_x \end{aligned}\right\} \text{"classical orbital ang. mom."}$$

Does $[\hat{L}_x, \hat{L}_y] \stackrel{?}{=} 0$ (like $[\hat{p}_x, \hat{p}_y] = 0$)

I am going to drop hats to save time.

$[x, p_x] = [y, p_y] = [z, p_z] = i\hbar$

Recall: ~~$[x,y] = [y,z] = [x,z] = 0$~~ all others $= 0$

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

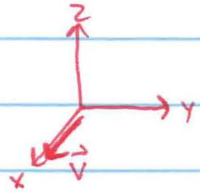
$$= (y p_z - z p_y)(z p_x - x p_z) - (z p_x - x p_z)(y p_z - z p_y)$$

$$= y p_z z p_x - \cancel{y p_z x p_z} - \cancel{z p_y z p_x} + z p_y x p_z - z p_x y p_z + \cancel{z p_x z p_y} + \cancel{x p_z y p_z} - x p_z z p_y$$

$$= y p_x (\underbrace{p_z z - z p_z}_{-i\hbar}) + x p_y (\underbrace{z p_z - p_z z}_{i\hbar})$$

$$= i\hbar (x p_y - y p_x)$$

$$\left.\begin{aligned} [L_x, L_y] &= i\hbar L_z \\ [L_y, L_z] &= i\hbar L_x \\ [L_z, L_x] &= i\hbar L_y \end{aligned}\right\}$$ This actually stems in part from classical noncommutativity of rotations:



$$(R_x^{90} R_y^{90} - R_y^{90} R_x^{90})\vec{V}$$

$$R_x^{90} \downarrow - R_y^{90} \swarrow$$

$$\longrightarrow - \downarrow \neq 0$$

This means we can't have a simultaneous basis from $\hat{L}_x$, $\hat{L}_y$, and $\hat{L}_z$.

You will prove in the HW that $[\hat{H}, \hat{L}_i] = 0$ so we can make use of one component, but at most one since $[\hat{L}_i, \hat{L}_j] \neq 0$.

Conventional choice is $\hat{L}_z$.

What else satisfies $[\hat{H}, \hat{Q}] = [\hat{L}_z, \hat{Q}] = 0$?

Consider $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$

$$[L^2, L_z] = [L_x^2, L_z] + [L_y^2, L_z] + \cancelto{0}{[L_z^2, L_z]}$$

$$= L_xL_xL_z - L_zL_xL_x + L_yL_yL_z - L_zL_yL_y$$

$L_xL_z = L_zL_x - i\hbar L_y$ $\quad$ $L_yL_z - L_zL_y = i\hbar L_x$

$$= \cancel{L_xL_zL_x} - \cancel{i\hbar L_xL_y} - \cancel{L_xL_zL_x} - \cancel{i\hbar L_yL_x}$$
$$+ \cancel{L_yL_zL_y} + \cancel{i\hbar L_yL_x} - \cancel{L_yL_zL_y} + \cancel{i\hbar L_xL_y}$$
$$= 0$$

In HW you will prove $[\hat{H}, \hat{L}^2] = 0$.

Okay, so we have $[\hat{H}, \hat{L}_z] = [\hat{H}, \hat{L}^2] = [\hat{L}_z, \hat{L}^2] = 0$
but do these give rise to sep. constants?

Need eigenvalues of $\hat{L}^2$ and $\hat{L}_z$.

Recall SHO: $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \Rightarrow$
$$\underbrace{\left.\begin{array}{l}[\hat{H}, \hat{p}_x] \neq 0 \\ [\hat{H}, \hat{x}] \neq 0\end{array}\right\} \hat{a}_\pm \equiv \frac{1}{\sqrt{2\hbar m\omega}}(m\omega\hat{x} \mp i\hat{p})}_{\substack{\hat{a}_+ \text{ raised eigenvalue of } \hat{H},\ \hat{a}_+\psi_n \to \psi_{n+1} \\ \hat{a}_- \text{ lowered eigenvalue of } \hat{H},\ \hat{a}_-\psi_n \to \psi_{n-1}}}$$

For angular momentum:
$$\underbrace{\left.\begin{array}{l}[\hat{L}_z, \hat{L}_x] \neq 0 \\ [\hat{L}_z, \hat{L}_y] \neq 0\end{array}\right\} \hat{L}_\pm \equiv \hat{L}_x \pm i\hat{L}_y}_{\substack{\text{expect } \hat{L}_+ \text{ to raise eigenvalue of } \hat{L}_z \\ \hat{L}_- \text{ to lower eigenvalue of } \hat{L}_z}}$$

Note: For SHO $\hat{a}_-$ had lower bound, i.e. $\hat{a}_-\psi_0 = 0$. For $\hat{L}_z$ we need upper and lower.