Lecture 15

1 Return to 3D

3D is where lots, but not all, of the cool stuff is.

$$i\hbar\partial_t\psi(\vec{r},t) = [-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r})]\psi(\vec{r},t) \tag{1}$$

1.1 An aside on coordinates

- Cartesian (free, harmonic oscillator, etc) (x, y, z)

$$\nabla^2 = \partial_x^2 + \partial_y^2 + \partial_z^2 \tag{2}$$

- Spherical (central potential) (r, θ, ϕ)

$$\vec{\nabla}^2 = \partial_r^2 + \frac{2}{r}\,\partial_r + \frac{1}{r^2}\,(\partial_\theta^2 + (\cot\theta)\partial_\theta) + \frac{1}{r^2\sin^2\theta}\,\partial_\phi^2 \tag{3}$$

  where

$$x = r\cos\theta\cos\phi, y = r\cos\theta\sin\phi, z = r\sin\theta \tag{4}$$

- Cylindrical (LHC beam) (ρ, ϕ, z)

$$\vec{\nabla}^2 = \partial_z^2 + \partial_\rho^2 + \frac{1}{\rho}\partial_\rho + \frac{1}{\rho^2}\partial_\phi^2 \tag{5}$$

  where

$$x = \rho\cos\phi, y = \rho\sin\phi \tag{6}$$

Example 1: Free Particle in Cartesian Coordinates

$$V(x,y,z) = 0 \tag{7}$$

$$E\psi(x,y,z) = (-\frac{\hbar^2}{2m})[\partial_x^2 + \partial_y^2 + \partial_z^2]\psi(x,y,z) \tag{8}$$

We use separation of variables. Suppose

$$\psi(x,y,z) = \psi_x(x) + \psi_y(y) + \psi_z(z) \tag{9}$$

then

$$E\psi_x\psi_y\psi_z = (-\frac{\hbar^2}{2m})[\psi_x''\psi_y\psi_z + \psi_x\psi_y''\psi_z + \psi_x\psi_y\psi_z''] \tag{10}$$

Divide by $\psi = \psi_x\psi_y\psi_z$:

$$-\frac{2m}{\hbar^2}E = \frac{\psi_x''}{\psi_x} + \frac{\psi_y''}{\psi_y} + \frac{\psi_z''}{\psi_z} \tag{11}$$

Separation: $\psi_x'' = -\epsilon_x\psi_x$, $\psi_y'' = -\epsilon_y\psi_y$, $\psi_z'' = -\epsilon_z\psi_z$ where $\epsilon_x + \epsilon_y + \epsilon_z = \frac{2mE}{\hbar^2}$. The solutions to each of those equations:

$$\psi_x = A_x e^{\pm ik_x x}, \frac{\hbar^2 k_x^2}{2m} = \epsilon_x \tag{12}$$

$$\psi_y = A_y e^{\pm ik_y y}, \frac{\hbar^2 k_y^2}{2m} = \epsilon_y \tag{13}$$

$$\psi_z = A_z e^{\pm ik_z z}, \frac{\hbar^2 k_z^2}{2m} = \epsilon_z \tag{14}$$

Combining, we get

$$\frac{\hbar^2\vec{k}^2}{2m} = E \tag{15}$$

$$E = \frac{\vec{p}^2}{2m} \tag{16}$$

$$\phi_k = Ae^{i(k_x x + k_y y + k_z z)} = \phi_0 e^{i\vec{k}\cdot\vec{x}} \tag{17}$$

$$A = \frac{1}{\sqrt{2\pi}^3} \tag{18}$$

Note:

- Orthonormality:

$$\langle \phi_k | \phi_{k'} \rangle = \int d^3x \, \phi_k^*(x) \, \phi_{k'}(x) = \delta^3(k - k^{'}) \tag{19}$$

- Completeness:

$$\langle \phi_k | \phi_{k'} \rangle = \int d^3k \, \phi_k^*(x) \, \phi_k(x') = \delta^3(x - x^{'}) \tag{20}$$

- Conservation of Probability:

$$\rho = |\phi|^2 = \frac{1}{(2\pi)^3} \tag{21}$$

$$\vec{J} = \frac{\hbar}{m} Im(\phi^* \vec{Del} \phi) = \frac{\hbar \vec{k}}{m} \frac{1}{\sqrt{2\pi}^3} \tag{22}$$

Therefore,

$$\vec{J} = \rho \vec{v} \tag{23}$$

- As with the free particle in one dimension, we can build wavepackets!

$$\psi(\vec{x}, 0) = \int d^3k \tilde{\psi}(\vec{k}) \phi_{\vec{k}}(\vec{x}) \tag{24}$$

$$= \int d^3k \frac{1}{\sqrt{\pi}^3} e^{i\vec{k}\cdot\vec{x}} \tilde{\psi(\vec{k})} \tag{25}$$

$$\psi(\vec{x}, t) = \int d^3k \phi_k(x) \tilde{\psi}(\vec{k}) e^{i\frac{\hbar \vec{k}^2}{2m}} \tag{26}$$

where

$$\omega_{\vec{k}} = \frac{E_{\vec{k}}}{\hbar} \tag{27}$$

Example 2: 3D Harmonic Oscillator

$$V(\vec{r}) = \frac{1}{2}m\omega_0^2(x^2 + y^2 + z^2) = V_x(x) + V_y(y) + V_z(z) \tag{28}$$

$$E\psi(x, y, z) = \frac{-\hbar^2}{2m}[\partial_x^2 + \partial_y^2 + \partial_z^2]\psi + [V_x + V_y + V_z]\psi \tag{29}$$

We use separation of variables: $\psi = \psi_x\psi_y\psi_z$ to rewrite this as a set of three equations, of the form

$$E_x\psi_x(x, y, z) = [\frac{-\hbar^2}{2m}\partial_x^2 + V_x(x)]\psi_x(x) \tag{30}$$

etc, where

$$E = E_x + E_y + E_z \tag{31}$$

We end up with three independent harmonic oscillators.

$$\psi = \psi_l(x)\psi_m(y)\psi_n(z) \tag{32}$$

and

$$E = \hbar\omega_0(l + m + n + \frac{3}{2}) \tag{33}$$

where $N = l + m + n$ represents the "number of quanta excited". Solutions are specified by three integers, which results in degeneracy. Multiple different states can share the same energy - the degeneracy correponds to a hidden symmetry, by Noether's thoerem. Examples of degenerate states are shown below:

Table 1: Results for the relationship between trap stiffness α and laser current, from two equipartition and PSD methods. Form: y = mx + b

Energy	(l, m, n)	Degeneracy
$\frac{9}{2}\hbar\omega_0$	(3, 0, 0) (2, 1, 0) (1, 1, 1)	10
$\frac{7}{2}\hbar\omega_0$	(2, 0, 0) (1, 1, 0)	6
$\frac{5}{2}\hbar\omega_0$	(1, 0, 0) (0, 1, 0) (0, 0, 1)	3
$\frac{3}{2}\hbar\omega_0$	(0, 0, 0)	1

Example 3: 3D Square Box You'll do this in recitation and on the pset. The answer is:

$$\psi(x, y, z) = (\sqrt{\frac{2}{a}} \sin(\frac{n_x \pi x}{a}))(\sqrt{\frac{2}{b}} \sin(\frac{n_y \pi y}{b}))(\sqrt{\frac{2}{c}} \sin(\frac{n_z \pi z}{c})) \tag{34}$$

$$E_n = \frac{\pi^2 \hbar^2}{2m}[\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}] \tag{35}$$

1.2 Angular Momentum

What is the operator corresponding to $\vec{L}$?

$$\hat{\vec{L}} = \vec{\hat{r}} x \vec{\hat{p}} \tag{36}$$

$$= \hat{y}\hat{p}_z - \hat{z}\hat{p}_y; \hat{z}\hat{p}_x - \hat{x}\hat{p}_z; \hat{x}\hat{p}_y - \hat{y}\hat{p}_x \tag{37}$$

Note: $[\hat{x}, \hat{p}_y]$

In spherical coordinates:

$$\hat{L}^2 = -\hbar^2 \left(\frac{1}{\sin\theta} \partial_\theta \, sin\theta \, \partial_\theta + \frac{1}{\sin^2\theta} \partial_\phi^2\right) \tag{38}$$

$$\hat{L}_z = -i\hbar\partial_\phi \tag{39}$$

As you showed:

$$[L_x, L_y] = i\hbar L_z; [L_y, L_z] = i\hbar L_x; [L_z, L_x] = i\hbar L_y; [L^2, L_x] = [L_y, L^2] = [L_z, L^2] = 0 \tag{40}$$

Two strategies for building eigenfunctions of $\hat{L}^2$:

1. Solve PDE by brute force: not so bad for $\hat{L}_z$

   $$-i\hbar\partial_\phi Y = \hbar m Y \tag{41}$$

   so

   $$Y \propto e^{im\phi}, m \in \mathbb{Z} \tag{42}$$

   Horrible looking for $\hat{L}^2$!

2. Use operator methods, as we did for HO

Today we'll focus on (2).

First: commuting observatles.

$[x, p_x] = i\hbar\mathbb{1}$ SO WHAT?

- Suppose E $\phi_{x,p}$ which is simultaneous an eigenfunction of $\hat{x}$ and $\hat{p}$:

$$\hat{x}\phi_{x,p} = x\phi_{x,p}, \hat{p}\phi_{x,p} = p\phi_{x,p} \tag{43}$$

$$(\hat{x}\hat{p} - \hat{p}\hat{x})\phi_{xp} = (\hat{x}p - \hat{p}x)\phi_{xp} = (xp - px)\phi_{xp} = 0 \tag{44}$$

$$[\hat{x}, \hat{p}]\phi_{xp} = 0 \tag{45}$$

  We can only find simultaneous eigenstates if $[A, B] = 0$!

- Thm: $\Delta A \Delta B = \frac{1}{2} |\langle [A, B] \rangle|$

Next, given a set of observables, we can form a **complete set.** This is a set in which every element commutes with every other element.

Ex. x, p_x breaks into x or p_x.
Ex. x, y, z, p_x, p_y, p_z breaks into x, y, z or x, y, p_z.

What is the most you can know at once? $p_x, p_y, p_z, p_x, p_y, z$

Ex. L_x, L_y, L_z, L^2 or Any one L, L^2

NB $[L_x, L_y] = i\hbar L_z$ so cannot simultaneously be eigenfunctions of L_x, L_y
NB Rotational symmetry means all are equivalent. Pick coordinates st $\hat{L}_z$ simple. So, $\hat{L}_z, \hat{L}^2$

So let's find eigenfunctions Y_{lm} of $\hat{L}_z, \hat{L}^2$

$$L_z Y_{lm} = \hbar m Y_{lm} \tag{46}$$

$$L^2 Y_{lm} = \hbar^2 l(l+1) Y_{lm} \tag{47}$$

Useful tool: raising and lowering operators

$$L_+ = L_x + iL_y, L_- = L_x - iL_y \tag{48}$$

$$L_+ = (L_-)^\dagger, L_- = (L_+)^\dagger \tag{49}$$

Note the similarity to $a^\dagger = (a)^\dagger$

$$[L_+, L_-] = 2\hbar L_z, [L^2, L_\pm] = 0, [L_z, L_\pm] = \pm\hbar L_\pm \tag{50}$$

Note the similarity to $[\hat{N}, a^\dagger] = a^\dagger$ and $[N, a] = -a$

Note: $L_- L_+ = \hat{L}^2 - L_z^2 - \hbar L_z$

The point: Suppose $L_z Y_{lm} = \hbar m Y_{lm}$ and $L^2 Y_{lm} = \hbar^2 l(l+1) Y_{lm}$. Then,

$$L_z(L_+ Y_{lm}) = ([L_z, L_+] + L_+ L_z) Y_{lm} \tag{51}$$

$$= (\hbar L_+ + L_+ \hbar m) Y_{lm} = \hbar(m+1)(L_+ Y_{lm}) \tag{52}$$

$$L_z(L - Y_{lm}) = \hbar(m-1)(L - Y_{lm}) \tag{53}$$

$$L^2(L \pm Y_{lm}) = \hbar^2 l(l+1)(L_\pm Y_{lm}) \tag{54}$$

Ladder of states with fixed l is just like the ladder of harmonic oscillator states. Instead of jumping between states of different n values using a and $a^\dagger$, you jump between m, m-1, m-2, m+1, m+2, etc, using the L_- and L_+ operators. The key is: $L_\pm$ do not change l - there is a new tower for each l!