Phys. 2b 2026, Week 6 Lecture Notes (Lectures 11 & 12) (2/10-12/2026)

Key Concepts
    1. Commutators & Heisenberg's Uncertainty Principle
    2. Basis States in QM

Heisenberg Uncertainty Principle (HUP):
    Since it is not a QM postulate it must be derivable from the postulates ... It is!
    Text has all the gory details of derivation.

    Actually the wave function from HW 3 Prob. 2.21

$$\psi(x) = Ae^{-ax^2}$$

    is the Minimum Uncertainty Wave Packet.
    If we evaluate Δx for this packet we find $\Delta x = \sigma_x = \frac{1}{2\sqrt{a}}$
    and it is normalized if $A = \left(\frac{2a}{\pi}\right)^{\frac{1}{4}}$.
    It has the minimum possible uncertainty product of $\Delta x \Delta p = \frac{\hbar}{2}$ as shown in soln.

    Now some
"Fun" with Commutators:

A. General Uncertainty Relations:
    For two abitrary Hermitian operators $\hat{A}, \hat{B}$ we have a HUP given by

$$\sigma_A \sigma_B \geq \frac{1}{2i} \left\langle [\hat{A}, \hat{B}] \right\rangle \quad \text{gives e.g. } \hat{y} - \hat{p}_y \ , \hat{\theta} - \hat{L}_\theta \ , E - t \ \text{... HUP - see text}$$

    Lingo: If $\hat{A}, \hat{B}$ "commute" then $[\hat{A}, \hat{B}] = 0$: e.g., $[\hat{x}, \hat{x}^2] = 0$
            If $\hat{A}, \hat{B}$ don't commute then $[\hat{A}, \hat{B}] \neq 0$: e.g.: $[\hat{x}, \hat{p}_x] = i\hbar$

B. Commutators and the Time Development of Expectation Values

    Let's evaluate $\dfrac{d\langle A \rangle}{dt}$ for a state ψ:

$$\frac{d\langle A \rangle}{dt} = \frac{\partial \langle A \rangle}{\partial t} = \frac{\partial \langle \psi | \hat{A} \psi \rangle}{\partial t}$$

                              ↪ since all spatial dependence integrated out via $\langle \psi | \hat{A} \psi \rangle$
    The derivative operates on both ψs and $\hat{A}$ and gives us

$$\frac{d\langle A \rangle}{dt} = \langle \frac{\partial \psi}{\partial t} | \hat{A} \psi \rangle + \langle \psi | \frac{\partial \hat{A}}{\partial t} \psi \rangle + \langle \psi | \hat{A} \frac{\partial \psi}{\partial t} \rangle$$

    Now use Schrödinger's Equation $i\hbar \dfrac{\partial \psi}{\partial t} = \hat{H} \psi$ to replace $\dfrac{\partial \psi}{\partial t}$ in above:

$$\frac{d\langle A \rangle}{dt} = \left\langle \frac{1}{i\hbar}\hat{H}\psi \Big| \hat{A}\psi \right\rangle + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle + \left\langle \psi \Big| \hat{A}\frac{1}{i\hbar}\hat{H}\psi \right\rangle$$

pulling out the $i\hbar$s gives a minus sign to the first term (it's on left side of bra-ket).

$$\frac{d\langle A \rangle}{dt} = \frac{-1}{i\hbar} \left\langle \hat{H}\psi \Big| \hat{A}\psi \right\rangle + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle + \frac{1}{i\hbar} \left\langle \psi \Big| \hat{A}\hat{H}\psi \right\rangle$$

but since $\hat{H}$ Hermitian $\langle \hat{H}\psi | \hat{A}\psi \rangle = \langle \psi | \hat{H}\hat{A}\psi \rangle$ we combine the first and last terms after moving the i upstairs giving:

$$\frac{d\langle A \rangle}{dt} = \frac{i}{\hbar} \left\langle \psi(\hat{H}\hat{A} - \hat{A}\hat{H})\psi \right\rangle + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle$$

$$\therefore \quad \boxed{\frac{d\langle A \rangle}{dt} = \left(\frac{i}{\hbar}\right) \langle [\hat{H}, \hat{A}] \rangle + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle}$$

and if $\hat{A}$ is not an explicit function of time, i.e. $\hat{A} \neq \hat{A}(t)$ then

$$\frac{d\langle A \rangle}{dt} = \frac{i}{\hbar}\langle [\hat{H}, \hat{A}] \rangle$$

Example:

Consider a simple Hamiltonian,

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

and evaluate the time dependence of $\langle x \rangle$:

$$\frac{d\langle x \rangle}{dt} = \frac{i}{\hbar}\langle [\hat{H}, \hat{x}] \rangle$$

but

$$[\hat{H}, \hat{x}] = \frac{1}{2m}\underbrace{[\hat{p}_x^2, \hat{x}]}_{-2i\hbar\hat{p}_x} + [\hat{V}(x), \hat{x}] = \frac{-i\hbar\hat{p}_x}{m} \quad ; \text{ since } [\hat{V}(x), \hat{x}] = 0$$

giving

$$\frac{d\langle x \rangle}{dt} = \frac{i}{\hbar}\left\langle \left(\frac{-i\hbar\hat{p}_x}{m}\right) \right\rangle \quad \Rightarrow \quad \frac{d\langle x \rangle}{dt} = \frac{\langle p_x \rangle}{m}$$

But this is the same as the classical result ($v_x = \frac{p_x}{m}$)!

This is an example of Ehrenfest's Principle:

$\hookrightarrow$ $\boxed{\text{Quantum Mechanical expectation values are consistent with classical formulae}}$

C. Commutator Theorem (proof in book - Chap. 3 footnote 18)

If two operators commute: $[\hat{A}, \hat{B}] = 0$, then there exists a set of common eigenfunctions of $\hat{A}$ and $\hat{B}$ (non-trivial)

Example: Consider free-particle momentum eigenstates

$$\phi_p = Ae^{ip_0 x/\hbar} \quad \text{with the Hamiltonian: } \hat{H} = \frac{\hat{p}_x^2}{2m}.$$

Thus $[\hat{p}_x, \hat{H}] = 0$ since $[\hat{p}_x, \hat{p}_x^2] = 0$ and we note that ϕ_p is also an eigenfunction of $\hat{H}$: $\hat{H}\phi_p = \frac{p_0^2}{2m}\phi_p$. But it didn't have to be...

Note:

1. $\psi = A\sin(p_0 x/\hbar)$ is also an eigenfunction of $\hat{H}$, but it is *not* an eigenfunction of $\hat{p}_x$.

   Commutator theorem only says there has to be *a* set of common eigenfunctions; not that all eigenfunctions are common.

2. $Ae^{ip_0 x/\hbar}$ is not the only linearly independent eigenfunction of $\hat{H}$ with eigenvalue $\frac{p_0^2}{2m}$

   $\Rightarrow Ae^{-ip_0 x/\hbar}$ also has eigenvalue $\frac{p_0^2}{2m}$.

   Thus $Ae^{ip_0 x\hbar}$ and $Ae^{-ip_0 x\hbar}$ are degenerate eigenfunctions of $\hat{H}$

   (However they are not degenerate eigenfunctions of $\hat{p}_x$!)

D. Hilbert Space (infinite-dimensional vector space): Now: Show $\{\psi_n^{Box}\}$ to Mathematicians

$\hookrightarrow$ "An infinite, complex set of functions might be part of a Hilbert Space"

a. Space is Linear $\Rightarrow a\phi$ is an element of the space if ϕ is an element and a is a constant. Also $\phi + \psi$ is an element of the space if ψ, ϕ are elements of the space.

b. There exists an inner product: i.e. $\Rightarrow \langle\phi|\psi\rangle$ is finite

c. "Length" of an element of the space is $(\text{Length})^2 = |\phi|^2 = \langle\phi|\phi\rangle$

d. Space is complete (Math Version) i.e. there are no holes in the space $\Rightarrow$ see Griffiths

Example: The set of all 3D vectors in Euclidean space is a Hilbert space, with $\hat{x}, \hat{y}, \hat{z}$ the "basis" vectors, from which all other vectors can be constructed.

$\hookrightarrow$ Spaces of functions can also form a Hilbert space

Summary of New QM Math Tools

    I. Eigenstates of Hermitian Operators form basis states $\rightarrow$ orthogonal unit vectors of the space

  II. An arbitrary state can always be written as superposition of eigenstates of any physical observable: $\underbrace{|\psi\rangle}_{\text{arbitrary}} = \sum_{i=1}^{\infty} a_i \underbrace{|\phi_i\rangle}_{\text{eigenfuts.}}$ where a_i is called the "projection" of ψ onto ϕ_i (like components of vector)

    $\rightarrow$ Eigenstates $\{\phi_n\}$ "span" the space

    Thus

$$\langle \phi_i | \psi \rangle = \sum \langle \phi_i | a_j \phi_j \rangle = a_i$$

    Thus we can change the basis states that are used to write the wave function.

    $\Rightarrow$ Analogy to arbitrary vector expressed in different coordinate systems

        $\hookrightarrow$ can change basis vectors to cartesian, spherical, cylindrical, ...

          and re-express vector in new coordinate system.

    Thus arbitrary quantum state can be expressed in terms of momentum or position or energy (or other) eigenstates. (a_i are the components of the state vector in a particular basis); which of these (or others) to use depends on what question you ask.

 III. In general, eigenstates of Hermitian operators form a subspace of Hilbert Space

Key Concepts
    1. Schrödinger's Eq in 3D
    2. Some 3D Solutions of $\hat{H}\psi = E\psi$

Quantum Mechanics in 3D

    Start with time-dependent Schrödinger equation:

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi$$

Then in 3D cartesian coordinates:

$$\hat{H} = \frac{\hat{\vec{p}}^2}{2m} + V(x,y,z) = \frac{\hat{p}_x^2}{2m} + \frac{\hat{p}_y^2}{2m} + \frac{\hat{p}_z^2}{2m} + V(x,y,z)$$

then with $\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$, $\hat{p}_y = -i\hbar\frac{\partial}{\partial y}$, $\hat{p}_z = -i\hbar\frac{\partial}{\partial z}$
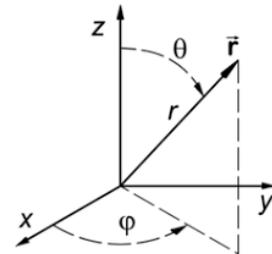
$$\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V$$

$$= -\frac{\hbar^2}{2m}\nabla^2 + V$$

All the math is in $\nabla^2 \rightarrow$ called the Laplacian (also important in E+M)
whose form depends on your coordinate system. For example:

(x, y, z) cartesian: $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$
(r, θ, ϕ) spherical: $\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial \phi^2}$

<div align="center">Spherical Coordinates Defined: ⇒</div>

Example I: Particle in a 3D Infinite Cubical Box (very useful for Ph12c/2c)

$$V(x,y,z) = \quad 0 \text{ if } 0 < x < L, \text{ and } 0 < y < L \text{ and } 0 < z < L$$
$$= \quad \infty \text{ otherwise}$$

Guess form for energy eigenstates: $\psi(x,y,z) \propto \left.\begin{array}{c}\sin k_x x \\ \sin k_y y \\ \sin k_z z\end{array}\right\}$note: product wave function clearly works!

$\psi(x,y,z) = A\sin(k_x x)\sin(k_y y)\sin(k_z z)$ satisfies the time-independent Schrodinger equation
with $A = \sqrt{\frac{8}{L_x L_y L_z}}$ but we must require $\psi = 0$ at box walls. This requirement leads to

$$k_x L = n_x \pi, \ n_x = 1, 2, 3 \ldots$$
$$k_y L = n_y \pi, \ n_y = 1, 2, 3 \ldots$$
$$k_z L = n_z \pi, \ n_z = 1, 2, 3 \ldots \ \ n_i \neq 0 \text{ why? } \rightarrow \text{ then Wave Func.} = 0$$

These n_i are called quantum numbers

and we can now write the eigenenergies:

$$E = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2)$$
$$= \frac{\hbar^2 \pi^2}{2mL^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

or

$$E = \frac{\hbar^2 \pi^2 n^2}{2mL^2}, \text{ with } n^2 = n_x^2 + n_y^2 + n_z^2$$

In this case there are many degenerate states (i.e distinguishable states with the same energy)

$$\left.\begin{matrix} n_x = 1,2,1 \\ n_y = 2,1,1 \\ n_z = 1,1,2 \end{matrix}\right\} \text{ all have same energy but W.F. is different}$$

Example II: Particle in a Spherical Box

$$V(r,\theta,\phi) = \quad 0 \text{ if } r < a$$
$$= \quad \infty \text{ if } r \geq a$$

But now we get a nasty differential equation.
How to solve for the energy eigenstates $\psi(r,\theta,\phi)$? In analogy to the Cartesian case above let's guess a "separable" solution. i.e.,

$$\psi_{Guess}(r,\theta,\phi) = A\mathbb{R}(r)\Theta(\theta)\Phi(\phi)$$

$\therefore$ must solve $-\frac{\hbar^2}{2M}\nabla^2\psi = E\psi$ for $r < a$
Substitute ψ_{Guess} into above and divide by $A\mathbb{R}\Theta\Phi$, as well as $-\frac{\hbar^2}{2M}$...

$$\frac{1}{r^2}\left[\frac{1}{\mathbb{R}}\frac{d}{dr}\left(r^2\frac{d\mathbb{R}}{dr}\right) + \frac{1}{\Theta \sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \frac{1}{\Phi\sin^2\theta}\frac{d^2\Phi}{d\phi^2}\right] + \frac{2ME}{\hbar^2} = 0$$

Now multiply by $r^2 \sin^2\theta$, giving

$$\frac{\sin^2\theta}{\mathbb{R}}\frac{d}{dr}\left(r^2\frac{d\mathbb{R}}{dr}\right) + \frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \frac{2MEr^2\sin^2\theta}{\hbar^2} = -\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} \quad \rightarrow \text{ Eq. I}$$

Now note that the above equation is valid for arbitrary r, θ, ϕ
This is only possible if both sides equal a constant. We will call this constant $m^2 \rightarrow m$ is a new quantum number. That's why we've been using M for the particle mass.

It is now easy to solve for Φ since it obeys the following equation:

$$\frac{d^2\Phi}{d\phi^2} + m^2\Phi = 0$$

giving

$$\Phi(\phi) = e^{im\phi} \text{ with } m \text{ positive or negative}$$

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and to keep Φ single-valued as we vary ϕ [i.e. $\Phi(\phi + 2\pi) = \Phi(\phi)$], m must be an integer, otherwise $\Phi(\phi + 2\pi) \neq \Phi(\phi) \rightarrow$ e.g. if $m = \frac{1}{2}$ then $\Phi(0) = 1$ but $\Phi(2\pi) = -1$.

We still need to find $\mathbb{R}$ and Θ. To do so we set the left side of Eq. I above equal to m^2 and divide by $\sin^2 \theta$ giving

$$\frac{1}{\mathbb{R}} \frac{d}{dr} \left(r^2 \frac{d\mathbb{R}}{dr} \right) + \frac{2MEr^2}{\hbar^2} = -\frac{1}{\Theta \sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) + \frac{m^2}{\sin^2 \theta}$$

again this must be valid for arbitrary values of r and θ, so both sides equal must equal a constant; let's set that constant to be $\ell(\ell + 1)$ for reasons that will be clearer next time.

We can now ask our Math colleagues for help with the solution of these two differential equations. They will tell us that the r equation is solved by a "spherical Bessel function" $\mathbb{R} = j_l(kr)$. See text for the form of this function.

We can now work out the eigenenergies from the boundary condidtion that $\mathbb{R}(r = a) = 0$. This is possible for only a discrete set of ka values - the zeros of the spherical Bessel function, which we will label with a new quantum number n. Thus we have

$$j_l(k_{ln}a) = 0$$

since for each l value there are many zeros (labeled by n). Now with the k values we can determine the eigenengies:

$$E_{nl} = \frac{\hbar^2 k_{nl}^2}{2M}$$

We still have to work out the $\Theta(\theta)$ functions.
These are conventionally combined with the Φ solutions as

$$\Theta(\theta)\Phi(\phi) = Y_\ell^m(\theta, \phi)$$

which are the "famous" Spherical Harmonics (a.k.a. the "Y el ems"). See text for their form.

Thus the full solution for the energy eigenstates for a particle in a spherical box are:

$$\psi(r, \theta, \phi) = A_{n\ell} j_\ell(k_{n\ell}r) Y_\ell^m(\theta, \phi)$$

with all of the "gory" details in the text.