Lecture 9 — Postulates IV–VI: Expansion, Expectation Values & Time Evolution

Reading: Engel 4th ed., Chapter 3 (Sections 3.4–3.6)

Learning Objectives

- Expand an arbitrary state in terms of PIB eigenfunctions and determine measurement probabilities
- Calculate expectation values using eigenfunction expansions
- Define the commutator and determine whether operators commute
- State the time-evolution postulate and describe the time-dependent behavior of quantum states

Postulate IV — Expansion & Probabilities

> **If the eigenfunctions $\{\psi_n\}$ of operator $\hat{A}$ form a complete set, then any state Ψ can be expanded as: $\Psi = \sum_n c_n \psi_n$ The probability of measuring eigenvalue a_n is $|c_n|^2$.**

Finding the Coefficients

Using orthonormality ($\int \psi_m^* \psi_n \, dx = \delta_{mn}$):

$$c_n = \int \psi_n^* \Psi \, dx$$

Completeness

$$\sum_n |c_n|^2 = 1$$

This ensures total probability is conserved.

PIB Example: Expanding an Arbitrary State

A particle in a box ($a = 1$) is prepared in the state $\Psi(x) = \sqrt{30}\, x(1 - x)$.

This is *not* an eigenstate of $\hat{H}$. To find what energies we might measure, expand in PIB eigenstates:

$c_n = \sqrt{2} \int_0^1 \sin(n\pi x) \cdot \sqrt{30}\, x(1 - x)\, dx$

Evaluating:

- $|c_1|^2 = 0.9986$ — 99.86% probability of measuring E_1
- $|c_2|^2 = 0$ — zero probability (by symmetry, Ψ is symmetric and ψ_2 is antisymmetric)
- $|c_3|^2 = 0.0013$ — tiny contribution from E_3

The parabolic state is *almost entirely* the ground state — it closely resembles ψ_1!

Postulate V — Expectation Values

> The expectation value of observable A in state Ψ is: $\langle A \rangle = \int \Psi^* \hat{A} \Psi\, dx$

If $\Psi = \sum_n c_n \psi_n$:

$\langle A \rangle = \sum_n |c_n|^2 a_n$

This is the **weighted average** of eigenvalues with probabilities $|c_n|^2$.

PIB Example: Energy of a Superposition

For the state $\Psi = \frac{1}{\sqrt{2}}\psi_1 + \frac{1}{\sqrt{2}}\psi_3$ in a PIB:

$\langle E \rangle = |c_1|^2 E_1 + |c_3|^2 E_3 = \frac{1}{2}E_1 + \frac{1}{2}(9E_1) = 5E_1$

The average energy is $5E_1$, but you never *measure* $5E_1$. Each individual measurement gives either E_1 (50% of the time) or E_3 (50% of the time).

Measurement and Collapse

After measuring observable A and obtaining eigenvalue a_n, the system **collapses** into eigenstate ψ_n. A subsequent measurement of A will yield a_n with certainty.

PIB Example: Collapse in Action

Suppose the particle is in $\Psi = \frac{1}{\sqrt{2}}\psi_1 + \frac{1}{\sqrt{2}}\psi_2$ and you measure the energy. If you obtain E_2:

1. The state immediately becomes ψ_2
2. A second energy measurement gives E_2 with 100% certainty
3. The probability density changes from the oscillating superposition to the stationary $|\psi_2|^2$

Postulate VI — Time Evolution

> **The time evolution of state Ψ is governed by the time-dependent Schrödinger equation:** $i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi$

For stationary states with definite energy E_n:

$$\Psi_n(\mathbf{r}, t) = \psi_n(\mathbf{r})\, e^{-iE_n t/\hbar}$$

For a general superposition:

$$\Psi(\mathbf{r}, t) = \sum_n c_n\, \psi_n(\mathbf{r})\, e^{-iE_n t/\hbar}$$

PIB Example: A Sloshing Superposition

For $\Psi(x, 0) = \frac{1}{\sqrt{2}}[\psi_1(x) + \psi_2(x)]$:

$$\Psi(x, t) = \frac{1}{\sqrt{2}}\left[\psi_1(x)e^{-iE_1 t/\hbar} + \psi_2(x)e^{-iE_2 t/\hbar}\right]$$

The probability density:

$$|\Psi(x,t)|^2 = \frac{1}{2}\left[|\psi_1|^2 + |\psi_2|^2 + 2\psi_1\psi_2\cos\left(\frac{(E_2-E_1)t}{\hbar}\right)\right]$$

The probability "sloshes" back and forth in the box with angular frequency $\omega = (E_2 - E_1)/\hbar = 3E_1/\hbar$. This is a quantum beat — interference between two energy eigenstates.

> [!NOTE] **Concept Check 9.2** For the sloshing PIB state above, at time $t = 0$ the probability density is peaked toward the left side of the box. At what time is it peaked toward the right side? What happens to the probability density if the particle is in a single eigenstate ψ_n?

Commutators

Definition

The **commutator** of two operators $\hat{A}$ and $\hat{B}$:

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

If $[\hat{A}, \hat{B}] = 0$, the operators **commute**.

The Canonical Commutation Relation

The most important commutator in quantum mechanics:

$$[\hat{x}, \hat{p}] = i\hbar$$

Proof: Acting on an arbitrary function $f(x)$:

$$[\hat{x}, \hat{p}]f = x\left(-i\hbar\frac{df}{dx}\right) - \left(-i\hbar\frac{d}{dx}\right)(xf)$$

$$= -i\hbar x\frac{df}{dx} + i\hbar\left(f + x\frac{df}{dx}\right) = i\hbar f$$

Therefore $[\hat{x}, \hat{p}] = i\hbar$. ∎

PIB Perspective: Why Position and Momentum Don't Commute

We showed in Lecture 8 that the PIB ground state ψ_1 is an eigenstate of $\hat{H}$ (and thus $\hat{p}^2$) but *not* of $\hat{p}$. Because $[\hat{x}, \hat{p}] \neq 0$, the particle cannot have definite position *and* definite momentum simultaneously. In the PIB:

- The particle is confined ($\Delta x \sim a$)
- Therefore it must have momentum uncertainty ($\Delta p > 0$)
- This is exactly the zero-point energy: the particle can never be at rest

Why Commutators Matter

Commutation	Physical Consequence
$[\hat{A}, \hat{B}] = 0$	A and B can be measured simultaneously with arbitrary precision; they share eigenfunctions
$[\hat{A}, \hat{B}] \neq 0$	A and B cannot be simultaneously known; measuring one disturbs the other

Common Commutators

Commutator	Value
$[\hat{x}, \hat{p}_x]$	$i\hbar$
$[\hat{x}, \hat{p}_y]$	0
$[\hat{x}, \hat{x}]$	0
$[\hat{L}_x, \hat{L}_y]$	$i\hbar\hat{L}_z$
$[\hat{L}^2, \hat{L}_z]$	0
$[\hat{H}, \hat{p}]$ (free particle)	0

Compatible Observables

If $[\hat{A}, \hat{B}] = 0$, we can find a **simultaneous eigenbasis** — functions that are eigenfunctions of both $\hat{A}$ and $\hat{B}$:

$$\hat{A}\psi = a\psi \quad \text{and} \quad \hat{B}\psi = b\psi$$

The system can have definite values of both A and B. Such observables are called **compatible**.

> [!NOTE] **Concept Check 9.3** For a **free** particle (no box), $[\hat{H}, \hat{p}] = 0$. This means $\psi = Ae^{ikx}$ is simultaneously an eigenstate of both $\hat{H}$ and $\hat{p}$. Verify this by finding the

Dirac Notation (Bra-Ket) — Brief Introduction

Dirac notation provides a compact way to write quantum expressions:

Standard	Dirac
ψ	$\lvert\psi\rangle$ (ket)
ψ^*	$\langle\psi\rvert$ (bra)
$\int \psi_m^* \psi_n \, dx$	$\langle\psi_m\lvert\psi_n\rangle$
$\int \psi^* \hat{A}\psi \, dx$	$\langle\psi\lvert\hat{A}\rvert\psi\rangle$
Eigenvalue eq.	$\hat{A}\lvert a_n\rangle = a_n\lvert a_n\rangle$

Key Equations Summary

Equation	Expression
Expansion	$\Psi = \sum_n c_n \psi_n$
Coefficients	$c_n = \int \psi_n^* \Psi \, dx$
Measurement probability	$P(a_n) = \lVert c_n \rVert^2$
Expectation value	$\langle A \rangle = \sum_n \lVert c_n \rVert^2 a_n$
Commutator	$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$
Canonical commutator	$[\hat{x}, \hat{p}] = i\hbar$
Time evolution	$\Psi(t) = \sum_n c_n \psi_n e^{-iE_n t/\hbar}$

Recent Literature Spotlight

"Agnostic Phase Estimation" *X. Song, F. Salvati, C. Gaikwad, N. Yunger Halpern, D. R. M. Arvidsson-Shukur, K. Murch*, Physical Review Letters, **2024**, 132, 260801. DOI

This work demonstrates a quantum advantage in phase estimation by entangling a probe qubit with an ancilla and measuring them in an entangled basis — extracting more information than any single-qubit sensor could. The experiment, performed on a superconducting quantum processor, illustrates how the postulates of quantum mechanics (superposition, entanglement, measurement) directly enable technologies that outperform classical approaches.

Practice Problems

1. **Expansion coefficients.** A particle in a box ($0 \leq x \leq a$) is in the state $\Psi(x) = \sqrt{30/a^5}\, x(a - x)$. Calculate the probability of measuring (a) E_1, (b) E_2, (c) E_3.

2. **Commutator calculations.** Evaluate: (a) $[\hat{x}^2, \hat{p}]$, (b) $[\hat{p}, V(x)]$, (c) $[\hat{H}, \hat{x}]$ for a particle in a potential $V(x)$.

3. **Time evolution.** A PIB system starts in the state $\Psi(0) = \frac{1}{\sqrt{2}}(\psi_1 + \psi_2)$. Write $\Psi(t)$ and show that $|\Psi(x, t)|^2$ oscillates with frequency $(E_2 - E_1)/h$.

Next lecture: The Uncertainty Principle & Problem-Solving Workshop