Lecture 1M (Part 2)

Intro: Basics of QM

1. Experimental Facts vs. Classical Predictions

2. Formal Structures: QM vs. Classical

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3. Example: Harmonic Oscillator

The harmonic oscillator is the simplest and most instructive dynamical system.
It provides a direct comparison between classical and quantum dynamics.

I. Classical Harmonic Oscillator

Hamiltonian and Rescaled Variables

The classical Hamiltonian is:

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2.$$

(0) A quick reminder

- What **"canonical"** means?
  - Two sets of variables

    $$(q_i, p_i)_{i=1}^n$$

    are called **canonical coordinates** if they satisfy the **fundamental Poisson bracket relations**

    $$\{q_i, q_j\} = 0, \quad \{p_i, p_j\} = 0, \quad \{q_i, p_j\} = \delta_{ij}$$

  - Equivalently, in matrix form:

    $$\{x_i, x_j\} = E_{ij}, \quad \text{where } x = (q_1, \dots, q_n, p_1, \dots, p_n),\ E = \begin{pmatrix} 0 & \mathbb{1}_n \\ -\mathbb{1}_n & 0 \end{pmatrix}.$$

This means the coordinates preserve the **symplectic structure**

$$\omega = \sum_i dq_i \wedge dp_i.$$

- So, “canonical” means: The coordinates define a coordinate system in which the symplectic form has the standard canonical matrix representation E.

- For the **original coordinates** (q, p) the canonical Poisson bracket is **postulated by definition** of Hamiltonian mechanics:

$$\{q, p\} = 1$$

This is not an assumption to verify

- it’s a defining property of the **canonical pair** that forms the phase-space coordinate system.
- But to **check that a change of variables preserves canonicity**, we compute the new Poisson bracket.

(1) Define rescaled variables

Define dimensionless canonical variables:

$$P = \frac{p}{\sqrt{m\omega}}, \qquad Q = \sqrt{m\omega}\, q$$

(2) Verify new variables are canonical

We must verify that this change of variables preserves the **canonical structure**:

$$\{Q, P\} = \frac{\partial Q}{\partial q}\frac{\partial P}{\partial p} - \frac{\partial Q}{\partial p}\frac{\partial P}{\partial q} = (\sqrt{m\omega})(1/\sqrt{m\omega}) - 0 = 1.$$

Hence the transformation $(q, p) \mapsto (Q, P)$ is **canonical**, i.e. it preserves the Poisson bracket and phase-space volume.

(3) Hamiltonian in rescaled canonical variables

In these variables:

$$H = \frac{\omega}{2}(Q^2 + P^2).$$

Equations of Motion and Phase-Space Trajectories

(1) Solving Hamiltonian equations

From Hamilton's equations:

$$\dot{Q} = \frac{\partial H}{\partial P} = \omega P, \qquad \dot{P} = -\frac{\partial H}{\partial Q} = -\omega Q$$

Hence, ODE governing the motion of system:

$$\ddot{Q} + \omega^2 Q = 0$$

solving which gives "trajectory" in phase space:

$$\begin{cases} Q_t = Q_0 \cos(\omega t) + P_0 \sin(\omega t), \\ P_t = -Q_0 \sin(\omega t) + P_0 \cos(\omega t). \end{cases}$$

(2) Trajectory in phase space

Thus,

$$Q_t^2 + P_t^2 = \text{const}, \qquad H = \omega \, \frac{Q_t^2 + P_t^2}{2}$$

which means trajectory in phase space is a **circle** of radius $\sqrt{2E/\omega}$, representing uniform rotation:

$$(Q_t, P_t) = R(\omega t)\,(Q_0, P_0),$$

where $R(\theta)$ is a rotation matrix in the (Q, P) plane.

Complex Variables and Rotational Flow

(1) Motivation: trajectory in phase space is a circle

Now that we have $(Q_t, P_t) = R(\omega t)\,(Q_0, P_0)$, from the perspective of "motion = (canonical) transformation of phase space", this motion corresponds to the **rotation** transformation.

Now — any rotation in a 2D real plane can be represented more compactly as **multiplication by a complex phase** $e^{-i\omega t}$ in the complex plane.

(2) Change into complex coordinates, and verify they are indeed canonical

Define complex canonical coordinates:

$$a = \frac{Q + iP}{\sqrt{2}}, \qquad a^* = \frac{Q - iP}{\sqrt{2}},$$

we verify this new set of variables is indeed canonical by checking the canonical relation:

$$\{a, a^*\} = -i.$$

> Hence, the transformation $(Q, P) \mapsto (a, a^*)$ **preserves the canonical structure** up to a constant factor: i

(3) Hamiltonian and evolution in complex canonical coordinates

Then,

$$H = \omega\, a^* a, \qquad \dot{a} = \{a, H\} = -i\omega a.$$

where the second equation is the **Hamilton equation**, of which the solution is:

$$a_t = e^{-i\omega t} a_0.$$

Hence, the phase-space flow is a **rigid rotation** in the complex plane — the shape of any probability distribution $\rho(Q, P)$ is preserved, only rotated in phase space.

Stationary Distributions in CM

A stationary probability distribution $\rho_{\text{stat}}(Q, P)$ satisfies

$$\rho_t(Q, P) = \rho_{\text{stat}}(H(Q, P)),$$

i.e., it is constant along trajectories (circular symmetry).

Examples:

- **Microcanonical**: $\rho_E(Q, P) \propto \chi_{\{E < H(Q,P) < E + \Delta E\}}$
- **Canonical**: $\rho_\beta(Q, P) = Z^{-1} e^{-\beta H(Q,P)}$

II. Quantum Harmonic Oscillator

The quantum harmonic oscillator (QHO) is the direct quantization of the classical system.
It illustrates how quantum structure reproduces classical dynamics while introducing intrinsic discreteness and uncertainty.

From Classical to Quantum Description

We start from the classical Hamiltonian:

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2.$$

In quantum mechanics, q, p become operators $\hat{q}, \hat{p}$ on a Hilbert space $\mathcal{H}$, obeying the **canonical commutation relation (CCR)**:

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

It is again convenient to introduce **dimensionless canonical operators**

$$\hat{Q} = \sqrt{m\omega}\,\hat{q}, \qquad \hat{P} = \frac{\hat{p}}{\sqrt{m\omega}}$$

so that

$$[\hat{Q}, \hat{P}] = i\hbar.$$

the Hamiltonian takes the symmetric form:

$$\hat{H} = \frac{\omega}{2}(\hat{Q}^2 + \hat{P}^2).$$

Dynamics: Heisenberg Equations of Motion

In the Heisenberg picture, observables evolve as

$$\frac{d\hat{O}}{dt} = \frac{i}{\hbar}[\hat{H}, \hat{O}].$$

Applying this to $\hat{Q}$ and $\hat{P}$ gives:

$$\dot{\hat{Q}} = \frac{i}{\hbar}[\hat{H}, \hat{Q}] = \omega \hat{P}, \qquad \dot{\hat{P}} = \frac{i}{\hbar}[\hat{H}, \hat{P}] = -\omega \hat{Q}.$$

Hence:

$$\ddot{\hat{Q}} + \omega^2 \hat{Q} = 0, \qquad \ddot{\hat{P}} + \omega^2 \hat{P} = 0.$$

Their solutions are identical in form to the classical trajectories:

$$\begin{cases} \hat{Q}_t = \cos(\omega t)\, \hat{Q}_0 + \sin(\omega t)\, \hat{P}_0, \\ \hat{P}_t = -\sin(\omega t)\, \hat{Q}_0 + \cos(\omega t)\, \hat{P}_0. \end{cases}$$

This shows that the **Heisenberg evolution is a rotation** in the $(\hat{Q}, \hat{P})$ plane — the exact quantum counterpart of the **symplectic rotation** in classical phase space.

Complex (Ladder) Operators - QM Counterpart of Complex Canonical Variables

To make the rotational structure manifest, define **complex canonical operators**:

$$\hat{a} = \frac{\hat{Q} + i\hat{P}}{\sqrt{2}}, \qquad \hat{a}^\dagger = \frac{\hat{Q} - i\hat{P}}{\sqrt{2}},$$

and one can veify the commutation relation

$$[\hat{a}, \hat{a}^\dagger] = \hbar$$

in this sense, these are complex "observables".

The Hamiltonian becomes

$$\hat{H} = \omega \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right) \hbar.$$

This form makes the **rotational invariance** of the dynamics explicit: the operator $\hat{a}$ plays the role of the complex coordinate $a = (Q + iP)/\sqrt{2}$ in classical mechanics.

Evolution of Ladder Operators

Take complex "observables" into the Heisenberg equation of motion

$$\frac{d\hat{a}}{dt} = \frac{i}{\hbar}[\hat{H}, \hat{a}] = -i\omega\hat{a}$$

of which the solution is:

$$\hat{a}_t = e^{-i\omega t}\hat{a}_0.$$

Thus the operator $\hat{a}$ **rotates rigidly in complex phase space**,
exactly like its classical analog $a_t = e^{-i\omega t}a_0$.

This rotation preserves expectation values and uncertainty shapes —
a direct manifestation of **unitary flow** in Hilbert space, the quantum analog of the **symplectic flow** in phase space.

Energy Spectrum

Consider eigenstates of the number operator $\hat{N} = \hat{a}^\dagger\hat{a}$:

$$\hat{N}|n\rangle = n\hbar\,|n\rangle.$$

From

$$[\hat{a}^\dagger\hat{a}, \hat{a}] = -\hbar\hat{a}, \qquad [\hat{a}^\dagger\hat{a}, \hat{a}^\dagger] = \hbar\hat{a}^\dagger,$$

we have

$$\hat{a}|n\rangle \propto |n-1\rangle, \qquad \hat{a}^\dagger|n\rangle \propto |n+1\rangle.$$

Hence the energy eigenvalues form an **equally spaced spectrum**:

$$E_n = \hbar\omega\left(n + \tfrac{1}{2}\right), \qquad n = 0, 1, 2, \ldots$$

with ground state satisfying $\hat{a}|0\rangle = 0$.

$$E_0 = \tfrac{1}{2}\hbar\omega.$$

Geometrical Interpretation and Classical Analogy

In classical phase space, the constant-energy surfaces are circles of radius

$$r_n = \sqrt{2E_n/\omega} = \sqrt{(2n+1)\hbar}.$$

Thus each quantum energy eigenstate corresponds to a **discrete circular orbit** in phase space, separated by an area increment of $2\pi\hbar$:

$$\Delta A = 2\pi\hbar.$$

This reflects the fundamental **quantization of phase-space area**, consistent with Bohr–Sommerfeld quantization:

$$\oint p\,dq = 2\pi\hbar(n + \tfrac{1}{2}).$$

The minimal energy $E_0 = \frac{1}{2}\hbar\omega$ corresponds to the **zero-point motion**, interpreted as quantum fluctuations that persist even in the ground state:

$$\Delta Q\,\Delta P \geq \frac{\hbar}{2}.$$

Coherent States and the Classical Limit

Define **coherent states** $|\alpha\rangle$ as eigenstates of $\hat{a}$:

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle,$$

where $\alpha = (Q + iP)/\sqrt{2\hbar}$ parameterizes a point in classical phase space.

Their expectation values follow the **classical trajectory**:

$$\begin{cases} \langle \hat{Q} \rangle_t = Q_t, \\ \langle \hat{P} \rangle_t = P_t, \end{cases} \qquad |\alpha_t\rangle = e^{-i\omega t/2}\,|\alpha e^{-i\omega t}\rangle.$$

The wavepacket thus undergoes a rigid rotation without deformation — the quantum analog of a **probability spot** rigidly rotating in classical phase space.

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4. Measurements in Quantum Mechanics

Measurement is the central concept distinguishing **quantum mechanics (QM)** from **classical mechanics (CM)**.
While classical uncertainty is ***epistemic*** (arising from ignorance of exact states), quantum uncertainty is ***intrinsic***, encoded directly in the mathematical structure of the theory.

I. From Classical to Quantum Uncertainty

- In **classical mechanics**,
  - uncertainty reflects only our ignorance of the exact state:

    $$\rho(\xi) \quad \text{represents an epistemic probability distribution in phase space.}$$

  - A pure state (a single point in phase space) allows all observables $O(\xi)$ to be known exactly.
  - **Time evolution in CM is deterministic** — uncertainty merely propagates according to Liouville's theorem.
- In **quantum mechanics**,
  - Time evolution is still deterministic (via the Schrödinger or von Neumann equations),
  - But **measurement outcomes** are inherently probabilistic, even in pure states.
    - A pure quantum state $\hat{\Pi}_\psi = |\psi\rangle\langle\psi|$ exhibits uncertainty in an observable $\hat{O}$ whenever

      $$[\hat{\Pi}_\psi, \hat{O}] \neq 0,$$

      i.e. whenever $|\psi\rangle$ is *not* an eigenstate of $\hat{O}$.

II. Quantifying Quantum Uncertainty

The **uncertainty** (variance) of an observable $\hat{O}$ in a pure state $|\psi\rangle$ is measured as:

$$(\Delta O)^2 = \langle\psi|\hat{O}^2|\psi\rangle - \langle\psi|\hat{O}|\psi\rangle^2.$$

(1) For pure state such that is also an eigenstate of $\hat{O}$, $\langle\hat{O}\rangle$ vanishes

If $|\psi\rangle$ happens to be an **eigenstate** of $\hat{O}$,

$$\hat{O}|\psi\rangle = \lambda|\psi\rangle$$

then each measurement of $\hat{O}$ always yields the same value λ, hence

$$\langle\psi|\hat{O}|\psi\rangle = \lambda, \qquad \langle\psi|\hat{O}^2|\psi\rangle = \lambda^2$$

so that

$$(\Delta O)^2 = 0.$$

- This corresponds to **complete predictability**: no statistical dispersion in outcomes.

(2) Otherwise, $(\Delta O)^2 > 0$

If $|\psi\rangle$ is *not* an eigenstate of $\hat{O}$, then the measurement outcomes of $\hat{O}$ are distributed over several eigenvalues.
Expanding in $\hat{O}$'s eigenbasis $\{|\lambda_n\rangle\}$,

$$|\psi\rangle = \sum_n c_n|\lambda_n\rangle, \qquad \hat{O}|\lambda_n\rangle = \lambda_n|\lambda_n\rangle,$$

the expected value and variance are

$$\langle\hat{O}\rangle_\psi = \sum_n |c_n|^2\lambda_n, \qquad (\Delta O)^2 = \sum_n |c_n|^2(\lambda_n - \langle\hat{O}\rangle_\psi)^2.$$

Hence $(\Delta O)^2 > 0$ unless only one coefficient c_n is nonzero — i.e., unless $|\psi\rangle$ is an eigenstate.

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(3) Geometric interpretation: orthogonal component of $\hat{O}|\psi\rangle$

To understand this geometrically, introduce the projector onto the state:

$$\hat{\Pi}_\psi = |\psi\rangle\langle\psi|$$

We can decompose $\hat{O}|\psi\rangle$ into two orthogonal components:$$\hat{O}|\psi\rangle = \underbrace{(\langle \hat{O} \rangle*psi |\psi\rangle)}*{\text{parallel part}}

- \underbrace{(\hat{O} - \langle \hat{O} \rangle*psi)|\psi\rangle*}{\text{orthogonal fluctuation}}.$The first term is **parallel** to$ $|\psi\rangle$; the second lies in the **orthogonal subspace** $(\mathbb{1} - \hat{\Pi}_\psi)\mathcal{H}$.

Because $\hat{\Pi}_\psi|\psi\rangle = |\psi\rangle$ and $(\mathbb{1} - \hat{\Pi}_\psi)|\psi\rangle = 0$,
we can write compactly:

$$(\Delta O)^2 = \langle\psi|(\hat{O} - \langle\hat{O}\rangle_\psi)^2|\psi\rangle = \langle\psi|\hat{O}(\mathbb{1} - \hat{\Pi}_\psi)\hat{O}|\psi\rangle.$$

Thus the variance measures the **squared norm of the component of $\hat{O}|\psi\rangle$ orthogonal to** $|\psi\rangle$:

$$\boxed{(\Delta O)^2 = \|(\mathbb{1} - \hat{\Pi}_\psi)\hat{O}|\psi\rangle\|^2}$$

This gives a **geometric picture** of quantum uncertainty:

> - In classical mechanics, uncertainty reflects ignorance of *which point* in phase space the system occupies.
> - In quantum mechanics, uncertainty reflects that the **state vector itself is not an eigenvector** of the observable —
>   so $\hat{O}|\psi\rangle$ has a “spread” orthogonal to $|\psi\rangle$ in Hilbert space.

(3') the variance measures the squared norm of the component of $\hat{O}|\psi\rangle$ orthogonal to $|\psi\rangle$

III. Could Quantum Uncertainty Be Classical? NO!

A natural question arises:

> Can we interpret quantum uncertainty as classical ignorance about hidden variables?

That is, can we imagine an **enlarged phase space** containing both observable variables and unobservable “hidden” variables, with an underlying probability distribution reproducing QM averages?

This idea was championed by **Einstein**, who regarded QM as an incomplete theory.

For a **single particle**, such a hidden-variable description poses no inconsistency. However, **Bell (1964)** showed that for a two-particle system, any local hidden-variable theory reproducing all quantum predictions must violate *local causality*.

This is encoded in **Bell's inequalities**, whose experimental violations (e.g., by **Aspect et al.**) demonstrate that no *local realist* model can reproduce quantum correlations.

Thus, the quantum description — and its intrinsic randomness — cannot be reduced to classical ignorance.

IV. The Measurement Postulate

Let $\hat{O}$ be an observable with spectral decomposition

$$\hat{O} = \sum_{\lambda_n \in \Sigma_0} \lambda_n \, \hat{\Pi}_{\lambda_n},$$

where $\{\hat{\Pi}_{\lambda_n}\}$ are orthogonal projection operators onto the eigenspaces of $\hat{O}$.

The **possible outcomes** of an ideal measurement are the eigenvalues λ_n.
Each corresponds to the "yes/no" proposition represented by $\hat{\Pi}_{\lambda_n}$.

Born Rule

If the system is in the state $\hat{\rho}$, the probability of obtaining a result in a subset $S \subset \Sigma_0$ is:

$$\boxed{P_S = \mathrm{Tr}(\hat{\rho}\,\hat{\Pi}_S), \qquad \hat{\Pi}_S = \sum_{\lambda_n \in S} \hat{\Pi}_{\lambda_n}}$$

this postulate is called **Born rule**.

(1) special case: single outcome

- For a single outcome λ, this reduce to:

$$P_\lambda = \mathrm{Tr}(\hat{\rho}\,\hat{\Pi}_\lambda).$$

(2) special case: pure state

- For a pure state $\hat{\rho} = |\psi\rangle\langle\psi|$, Born rule reduce to:

$$P_\lambda = \langle\psi|\hat{\Pi}_\lambda|\psi\rangle = |\langle\lambda|\psi\rangle|^2.$$

Post-Measurement State (State Collapse)

(1) Observed measurement and state collapse

In addition to Born rule, it's also postulated that: immediately after a measurement yielding outcome λ, the state collapses to:

$$\hat{\rho}_{\text{after}} = \frac{\hat{\Pi}_\lambda\,\hat{\rho}\,\hat{\Pi}_\lambda}{\text{Tr}(\hat{\rho}\,\hat{\Pi}_\lambda)}.$$

(2) Unobserved measurement yields a statistical mixture

If the measurement result is not recorded, we must average over all possible outcomes:

$$\hat{\rho}_{\text{after}} = \sum_{\lambda\in\Sigma_0} P_\lambda \frac{\hat{\Pi}_\lambda\hat{\rho}\hat{\Pi}_\lambda}{\text{Tr}(\hat{\rho}\,\hat{\Pi}_\lambda)} = \sum_{\lambda\in\Sigma_0} \hat{\Pi}_\lambda\hat{\rho}\hat{\Pi}_\lambda.$$

Thus, even if the system starts in a pure state, the unobserved measurement process yields a **statistical mixture**.

V. Measurements: Complete vs. Incomplete

(1) Non-degenerate spectrum and complete measurement

A measurement is said to be **complete** if each possible outcome uniquely determines a pure post-measurement state.
This is the case when $\hat{O}$ has a **non-degenerate spectrum** — each eigenvalue corresponds to a single eigenvector.

(2) Degenerate spectrum and incomplete measurement

If $\hat{O}$ has degenerate eigenvalues, then multiple distinct states share the same outcome.
To fully determine the post-measurement pure state, we must measure additional **compatible observables** that distinguish between degenerate subspaces.

VI. Observables: Compatible vs Incompatible

Two observables $\hat{O}_1$ and $\hat{O}_2$ are said to be **compatible** if they commute:

$$[\hat{O}_1, \hat{O}_2] = 0$$

Then they have a common eigenbasis, and can be simultaneously diagonalized.
A joint measurement of all commuting observables constitutes a single **complete measurement**.

Conversely, for **incompatible observables** ($[\hat{O}_i, \hat{O}_j] \neq 0$),
simultaneous measurement is impossible — measurement of one disturbs the other's outcomes.

> *Example:* the **Stern–Gerlach experiment** demonstrates that measuring spin along one axis destroys information about spin along perpendicular axes.

VII. The Measurement Problem

The measurement postulate introduces a **non-unitary step** (collapse) in an otherwise unitary theory.

This raises a conceptual tension:

- The total system (system + apparatus + observer) should evolve **deterministically** according to the Schrödinger equation.
- Yet, the postulate asserts a **stochastic and discontinuous** update upon measurement.

If QM is the ultimate theory of reality, what determines when and how this “collapse” occurs?

This is known as the **measurement problem** — the apparent incompatibility between deterministic unitary evolution and probabilistic measurement outcomes. Despite numerous interpretations (Copenhagen, many-worlds, decoherence, etc.), the origin of intrinsic randomness in quantum measurement remains **largely open**.

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5. Hilbert Space Representations

I. Abstract Structure of Quantum Mechanics

So far, we have encountered several “abstract” mathematical objects:

Object	Meaning
$\lvert\psi\rangle$	Abstract vector (state)
$\hat{O}$	Linear operator (observable)
$\hat{\rho}$	Density operator (statistical state)
$\mathcal{L}_{\hat{G}}$	Super-operator (acts on operators)

These objects are basis-independent and live in an abstract Hilbert space.
For explicit calculations, it is convenient to **choose a basis** and **represent** them concretely as ordered sets of numbers.

II. Representations in an Orthonormal Basis

Let $\{\lvert e_i\rangle\}_{i=1}^{D}$ be an orthonormal basis of $\mathcal{H}$.

$$\lvert\psi\rangle \;\leftrightarrow\; \begin{pmatrix}\psi_1\\ \psi_2\\ \vdots\\ \psi_D\end{pmatrix}, \quad \langle\psi\rvert \;\leftrightarrow\; (\psi_1^*, \psi_2^*, \ldots, \psi_D^*), \quad \langle\phi\vert\psi\rangle = \sum_{i=1}^{D} \phi_i^* \psi_i.$$

> Formally, $D = \dim\mathcal{H}$ may be infinite for physical systems with continuous variables (e.g. position).

Linear operators become **matrices**:

$$\hat{O} \leftrightarrow [O_{ij}], \qquad O_{ij} = \langle e_i|\hat{O}|e_j\rangle.$$

Superoperators act as linear maps on these matrices, e.g.

$$\mathcal{L}_{\hat{G}}(\hat{O}) = \frac{i}{\hbar}[\hat{G}, \hat{O}].$$

III. Example of the Harmonic Oscillator

(1) representation of ladder operators

In the **energy eigenbasis** $\{|n\rangle\}$ of the harmonic oscillator,

$$\hat{H}|n\rangle = E_n|n\rangle, \qquad E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

we define the ladder operators:

$$\hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle, \quad \hat{a}^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle.$$

Then their matrix representations are:

$$\hat{a} = \begin{pmatrix} 0 & \sqrt{1} & 0 & \cdots \\ 0 & 0 & \sqrt{2} & \cdots \\ 0 & 0 & 0 & \sqrt{3} \\ \vdots & & & \ddots \end{pmatrix}, \qquad \hat{a}^\dagger = \begin{pmatrix} 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & \cdots \\ \vdots & & & \ddots \end{pmatrix}$$

(2) Representation of Hamiltonian

From $\hat{N} = \hat{a}^\dagger\hat{a}$, we get:

$$\hat{H} = \hbar\omega\left(\hat{N} + \frac{1}{2}\right) \quad \Rightarrow \quad \hat{H} = \hbar\omega\begin{pmatrix} \frac{1}{2} & 0 & 0 & \cdots \\ 0 & \frac{3}{2} & 0 & \cdots \\ 0 & 0 & \frac{5}{2} & \cdots \\ \vdots & & & \ddots \end{pmatrix}.$$

For practical computations, one often **truncates** to finite dimension $D \gg E_{\max}/\hbar\omega$ — this effectively introduces a high-energy cutoff.

IV. Continuous Bases and Spectra

For systems with continuous observables (like position or momentum), the dimension D becomes infinite.

Position Eigenbasis and Coordinate Representation

We postulate eigenvectors of the position operator $\hat{q}$:

$$\hat{q}|x\rangle = x|x\rangle, \qquad x \in \mathbb{R}.$$

and they form a continuous orthonormal set:

$$\langle x|x'\rangle = \delta(x - x'), \qquad \int_{-\infty}^{+\infty} dx\, |x\rangle\langle x| = \mathbb{1}.$$

(1) Wave function is the coordinate representation of pure state

The **wave function** is the coordinate representation:

$$\psi(x) = \langle x|\psi\rangle, \qquad |\psi\rangle = \int dx\, \psi(x)\, |x\rangle,$$

with normalization $\int dx\, |\psi(x)|^2 = 1$.

(2) Hilbert space is isomophic to the space of square-integrable complex functions

Hence Hence, the Hilbert space of such states is **isomorphic** to the space of square-integrable complex functions:

$$\mathcal{H} \cong L^2(\mathbb{R}),$$

Momentum Eigenbasis and Corresponding Representation

Similarly, we **postulate** that the **momentum operator** $\hat{p}$ admits a continuous set of eigenstates:

$$\hat{p}|k\rangle = \hbar k\, |k\rangle, \qquad k \in \mathbb{R}.$$

They satisfy the completeness and orthonormality relations:

$$\langle k|k'\rangle = \delta(k-k'), \qquad \int_{-\infty}^{+\infty} dk\,|k\rangle\langle k| = \mathbb{1}.$$

The **momentum-space wave function** is:

$$\tilde{\psi}(k) = \langle k|\psi\rangle, \qquad |\psi\rangle = \int dk\,\tilde{\psi}(k)\,|k\rangle,$$

with normalization $\int dk\,|\tilde{\psi}(k)|^2 = 1$.

Position–Momentum Duality

(1) Postulates

We begin with the following **basic postulates**:

1. **Canonical commutation relation (CCR):**

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

2. **Spectral assumptions:**

$$\hat{q}|x\rangle = x|x\rangle, \qquad \hat{p}|k\rangle = \hbar k|k\rangle$$

where $x, k \in \mathbb{R}$, and $\{|x\rangle\}$, $\{|k\rangle\}$ are continuous orthonormal sets:

$$\langle x|x'\rangle = \delta(x-x'), \qquad \langle k|k'\rangle = \delta(k-k'), \qquad \int dx\,|x\rangle\langle x| = \int dk\,|k\rangle\langle k| = \mathbb{1}$$

3. **Action of $\hat{p}$ in the position representation:**

$$\langle x|\hat{p}|\psi\rangle = -i\hbar\frac{d}{dx}\langle x|\psi\rangle.$$

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(2) Direct consequence of the postulates: inner product of position and momentum eigenbasis defines the plane-wave kernel

Applying $\hat{p}|k\rangle = \hbar k|k\rangle$ and inserting the position resolution of identity gives:

$$\langle x|\hat{p}|k\rangle = \hbar k\langle x|k\rangle.$$

But in the position representation

$$\langle x|\hat{p}|k\rangle = -i\hbar\frac{d}{dx}\langle x|k\rangle.$$

Hence, $\langle x|k\rangle$ satisfies the differential equation

$$-i\hbar\frac{d}{dx}\langle x|k\rangle = \hbar k\,\langle x|k\rangle,$$

whose solution is

$$\langle x|k\rangle = C\,e^{ikx}.$$

To fix C, impose the orthonormality condition

$$\langle k|k'\rangle = \int dx\,\langle k|x\rangle\langle x|k'\rangle = |C|^2\int dx\,e^{-i(k-k')x} = 2\pi|C|^2\delta(k-k'),$$

which yields $|C|^2 = 1/(2\pi)$.

Thus, we choose (up to a global phase convention)

$$\boxed{\langle x|k\rangle = \frac{1}{\sqrt{2\pi}}\,e^{ikx}}$$

This is the **plane-wave kernel** linking the position and momentum bases.

(2') The wave functions in the two representations are related by the unitary Fourier transform

For any state $|\psi\rangle$,

$$\psi(x) = \langle x|\psi\rangle, \qquad \tilde{\psi}(k) = \langle k|\psi\rangle.$$

Inserting the identity $\int dk\,|k\rangle\langle k| = \mathbb{1}$ gives:

$$\psi(x) = \int dk\,\langle x|k\rangle\,\tilde{\psi}(k) = \frac{1}{\sqrt{2\pi}}\int dk\,e^{ikx}\,\tilde{\psi}(k).$$

Similarly,

$$\tilde{\psi}(k) = \int dx\,\langle k|x\rangle\,\psi(x) = \frac{1}{\sqrt{2\pi}}\int dx\,e^{-ikx}\,\psi(x).$$

These are **unitary Fourier transforms** relating the coordinate and momentum representations.
Their unitarity guarantees normalization equivalence:

$$\int dx\, |\psi(x)|^2 = \int dk\, |\tilde{\psi}(k)|^2 = 1.$$

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(3) Position and momentum operators in coordinate representation

In the coordinate basis, the position operator acts *multiplicatively*:

$$(\hat{q}\psi)(x) = \langle x|\hat{q}|\psi\rangle = x\langle x|\psi\rangle = x\,\psi(x).$$

To find the momentum operator's form, insert the completeness relation in $|x\rangle$:

$$\langle x|\hat{p}|\psi\rangle = \int dx'\, \langle x|\hat{p}|x'\rangle\, \langle x'|\psi\rangle. \$\$ Wecancomputeitskernelfromthe CCR: \$\$[\hat{q},\hat{p}] = i\hbar \quad \Rightarrow$$

Hence in coordinate space:

$$\boxed{\hat{q} = x, \qquad \hat{p} = -i\hbar\,\frac{d}{dx}.}$$

These operators satisfy $[\hat{q},\hat{p}] = i\hbar$ as expected.

(4) Position and momentum operators in coordinate representation

By symmetry, we can express everything in the momentum basis.
The momentum operator acts multiplicatively:

$$(\hat{p}\tilde{\psi})(k) = \hbar k\,\tilde{\psi}(k)$$

To find $\hat{q}$, we use the Fourier kernel $\langle k|x\rangle = \frac{1}{\sqrt{2\pi}}e^{-ikx}$:

$$\langle k|\hat{q}|\psi\rangle = \int dx\, \langle k|x\rangle\, x\, \langle x|\psi\rangle = \int dx\, \frac{e^{-ikx}}{\sqrt{2\pi}}\, x\,\psi(x).$$

Integrating by parts and using

$$xe^{-ikx} = i\,\frac{d}{dk}e^{-ikx},$$

we obtain

$$(\hat{q}\tilde{\psi})(k) = i\hbar\,\frac{d}{dk}\tilde{\psi}(k).$$

Thus in momentum space:

$$\boxed{\hat{p} = \hbar k, \qquad \hat{q} = i\hbar\,\frac{d}{dk}.}$$

V. Schrödinger Equation in Coordinate Representation

With $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{q})$, we identify

$$\hat{p} \leftrightarrow -i\hbar\frac{d}{dx}, \quad \hat{q} \leftrightarrow x.$$

hence, Schrödinger's equation becomes:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x,t).$$

For stationary states $\psi(x,t) = e^{-iEt/\hbar}\psi_E(x)$,

$$\hat{H}\psi_E = E\psi_E \quad \Longleftrightarrow \quad -\frac{\hbar^2}{2m}\frac{d^2\psi_E}{dx^2} + V(x)\psi_E(x) = E\psi_E(x).$$

VI. Continuous Spectrum and Projection-Valued Measures

- For discrete spectra:

$$\hat{O} = \sum_n \lambda_n |\lambda_n\rangle\langle\lambda_n|.$$

- For continuous spectra (von Neumann's generalization):

$$\hat{O} = \int_\Sigma \lambda \, d\hat{\Pi}(\lambda),$$

where $d\hat{\Pi}(\lambda)$ is a **projection-valued measure (PVM)** satisfying

$$\hat{\Pi}(S)\hat{\Pi}(S') = \hat{\Pi}(S \cap S'), \qquad \hat{\Pi}(\Sigma) = \mathbb{1}.$$

This allows treating both discrete and continuous spectra in a unified formalism.

VII. Example: Free Particle and Wave Packets

For a free particle, $\hat{H} = \frac{\hat{p}^2}{2m}$.

Since $[\hat{H}, \hat{p}] = 0$, $\hat{H}$ and $\hat{p}$ share eigenstates:

$$\hat{H}|k\rangle = \frac{\hbar^2 k^2}{2m}|k\rangle.$$

- The energy spectrum is continuous: $E_k = \hbar^2 k^2/2m \geq 0$.
- States $|+k\rangle$ and $|-k\rangle$ have the same energy: **twofold degeneracy**.

Coordinate representation:

$$\langle x|k\rangle = \frac{1}{\sqrt{2\pi}} e^{ikx}.$$

The **probability density** of a pure momentum eigenstate is uniform:

$$|\psi_k(x)|^2 = \text{const.}$$

Such states are **non-normalizable**, representing "improper eigenvectors."

(a) Wave Packets and Normalizable States

A realistic state must be normalizable, i.e. a **superposition** of momentum eigenstates over a finite interval:

$$|\psi_{k_0,\Delta k}\rangle = \frac{1}{\sqrt{\Delta k}} \int_{k_0 - \Delta k/2}^{k_0 + \Delta k/2} |k\rangle \, dk.$$

In position space:

$$\psi_{k_0,\Delta k}(x) = \frac{1}{\sqrt{\Delta k}} \int_{k_0-\Delta k/2}^{k_0+\Delta k/2} e^{ikx}\, dk \;\approx\; \frac{\sin(\Delta k\, x/2)}{x/2} e^{ik_0 x}.$$

This represents a **wave packet** with carrier wavenumber k_0 and envelope width $\sim 1/\Delta k$.

> **Heisenberg tradeoff:**
> The narrower the packet in momentum space ($\Delta k \to 0$),
> the broader its envelope in position space ($\Delta x \sim 1/\Delta k$).

(b) Energy Expectation and Classical Limit

$$\langle \hat{H} \rangle_{\psi_{k_0,\Delta k}} \simeq \frac{\hbar^2 k_0^2}{2m} + \mathcal{O}((\Delta k)^2)$$

As $\Delta k \to 0$, the packet approaches a plane wave and becomes increasingly classical in the sense that the **energy–momentum relation** becomes sharply defined.

V. Uncertainty Relations ("Indeterminacy Principle")

I. Motivation: From Noncommutativity to Uncertainty

We have already defined the variance (uncertainty) of an observable $\hat{A}$ in a normalized state $|\psi\rangle$:

$$(\Delta A)^2 = \langle \psi | (\hat{A} - \langle \hat{A} \rangle)^2 | \psi \rangle.$$

- If two observables $\hat{A}$ and $\hat{B}$ **commute**, i.e. $[\hat{A}, \hat{B}] = 0$, they can be simultaneously diagonalized and thus simultaneously have definite values in some states.
- **Noncommutativity** implies that no state can have both variances zero simultaneously — this is the origin of the **uncertainty principle**.

Derivation: Schrödinger–Robertson Inequality

Let us prove that for arbitrary Hermitian operators $\hat{A}$ and $\hat{B}$,

$$(\Delta A)^2(\Delta B)^2 \ge \frac{1}{4}|\langle[\hat{A},\hat{B}]\rangle|^2.$$

(1) Centering operators

Define the “fluctuation” operators:

$$\hat{A}' = \hat{A} - \langle\hat{A}\rangle, \qquad \hat{B}' = \hat{B} - \langle\hat{B}\rangle.$$

For any real parameter λ, consider the positive norm:

$$\|(\hat{A}' + i\lambda\hat{B}')|\psi\rangle\|^2 \ge 0.$$

Expanding the expectation value gives:$$\langle (\hat{A}' - i\lambda \hat{B}')(\hat{A}'
+ i\lambda \hat{B}') \rangle
= \langle \hat{A}'^2 \rangle + \lambda^2 \langle \hat{B}'^2 \rangle

- i\lambda \langle [\hat{A}', \hat{B}'] \rangle \ge 0.$$

(2) Quadratic form in λ

This inequality must hold for all real λ.
Hence, the discriminant of the quadratic expression must be non-positive:

$$\left(\mathrm{Im}\,\langle[\hat{A}',\hat{B}']\rangle\right)^2 \le 4\langle\hat{A}'^2\rangle\langle\hat{B}'^2\rangle.$$

Recognizing

$$\langle\hat{A}'^2\rangle = (\Delta A)^2, \qquad \langle\hat{B}'^2\rangle = (\Delta B)^2,$$

and $\langle[\hat{A}',\hat{B}']\rangle = \langle[\hat{A},\hat{B}]\rangle$,
we obtain the **Schrödinger–Robertson uncertainty relation**:

$$\boxed{(\Delta A)^2(\Delta B)^2 \ge \frac{1}{4}|\langle[\hat{A},\hat{B}]\rangle|^2.}$$

Special Case: Heisenberg Uncertainty

For the canonical pair $(\hat{q}, \hat{p})$ satisfying $[\hat{q}, \hat{p}] = i\hbar$, we get:

$$\boxed{\Delta q \, \Delta p \geq \frac{\hbar}{2}.}$$

This bound is **saturated** for Gaussian wave packets, in particular for the **ground state of the harmonic oscillator**:

$$\psi_0(x) \propto e^{-m\omega x^2/2\hbar}, \qquad \Delta q \, \Delta p = \frac{\hbar}{2}.$$

For a free particle, Δp can be made arbitrarily small, but then Δq diverges, consistent with the inequality.

Geometric Interpretation

Uncertainty arises because in Hilbert space, $|\psi\rangle$ cannot be an eigenvector of both some $\hat{A}$ and some $\hat{B}$ when the two operators do not commute.
The inequality quantifies the minimal "spread" allowed by the algebraic incompatibility:

$$[\hat{A}, \hat{B}] \neq 0 \quad \Rightarrow \quad \text{nonzero minimal uncertainty.}$$

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von Neumann's Operational Interpretation

In real measurements, no observable can be measured with infinite precision.
Continuous-spectrum operators (like $\hat{q}$ and $\hat{p}$) are replaced by **coarse-grained** versions that correspond to finite experimental resolution:

$$\hat{q} \;\to\; \hat{q}_{\Delta}, \qquad \hat{p} \;\to\; \hat{p}_{\Delta'},$$

with resolutions Δq, Δp determined by the apparatus.

The commutator between such coarse-grained operators effectively vanishes if their resolution exceeds the quantum scale:

$$[\hat{q}_{\Delta}, \hat{p}_{\Delta'}] \approx 0 \quad \text{only if} \quad \Delta q \, \Delta p \gg \hbar$$

Thus, **simultaneous measurability** is restored approximately for macroscopic scales where $\Delta q \Delta p \gg \hbar$, while quantum effects become dominant only when measurement precision approaches the fundamental limit $\Delta q \Delta p \sim \hbar$.