Lecture 1M (Part 1)

This set of notes is bassed on the graduate course "*Advanced Quantum Mechanics*" instructed by Prof. Alessio Lerose at KU Leuven. The labels "M,S,P,X" following lecture number stand for "Main, Supplementary, Problems, and Xplorings", notes labeled "M" are mostly based on Prof. Alessio Lerose's handwritten lecture notes, with personal extensions which may not be scientifically rigourous or even wrong (please kindly contact zhengshen@physics.run if you find any mistake).

Intro: Basics of QM

1. Experimental Facts vs. Classical Predictions

Classical mechanics works well until experimentalist started to use EM radiation as a probe to investigate the behavior of matter:

- **Blackbody radiation** (EM radiation emitted by a piece of matter in thermal equilibrium) does not obey the basic laws of classical statistical mechanics.
  - In particular, **the classical equipartition theorem** predicts that each electromagnetic mode should carry an average energy of $k_B T$, leading to an **infinite total energy density** when integrating over all frequencies — a contradiction known as the **ultraviolet catastrophe**.
  - Experimental measurements, however, show that the energy density peaks at a finite frequency and falls off exponentially at high frequencies.
  - This discrepancy revealed the breakdown of classical physics at microscopic scales and led **Planck** to propose that electromagnetic energy is **quantized** in units of $E = h\nu = \hbar\omega$ marking the birth of **quantum theory**.
- **Heat capacity of solids** (thermal energy stored in atomic vibrations within a crystal lattice) also fails to follow the predictions of classical statistical mechanics.
  - In particular, according to the **Dulong–Petit law** derived from the **equipartition theorem**, each atom in a solid should contribute an average energy of $3k_B T$, leading to a constant molar heat capacity

$$C_V = 3R$$

independent of temperature.

- Experimentally, however, the heat capacity of solids **drops sharply at low temperatures** and approaches zero as $T \to 0$.
- This deviation indicates that lattice vibrations (phonons) cannot have a continuous range of energies as classical theory assumes. Instead, their energies are **quantized** in units of $E = \hbar\omega$, as described by the **Einstein** and later **Debye models**, which successfully explain the observed temperature dependence of C_V.

- **Atomic and molecular spectra** (the absorption and emission of light by gases) also violate classical predictions.
  - In classical electrodynamics, an electron orbiting a nucleus behaves like an accelerating charge and should **continuously radiate electromagnetic waves**.
  - The emitted radiation would have **a continuous range of wavelengths**, determined by the **orbital frequency** of the electron,

$$\lambda = \frac{2\pi c}{\omega_{\text{orbit}}}$$

    and since the electron could spiral inward smoothly, every intermediate orbital frequency would contribute — producing a **continuous emission spectrum**, not the discrete lines seen experimentally.
  - Moreover, the radiated power of an accelerating charge is given by the **Larmor formula**,

$$P = \frac{e^2 a^2}{6\pi\varepsilon_0 c^3}$$

    which implies that the electron would **lose energy rapidly** and spiral into the nucleus.
  - Estimating the radiative loss for a hydrogen atom gives a classical **lifetime of about 10^{-11} seconds**, meaning the atom would collapse almost instantly — in stark contrast to the observed stability of matter.
  - In reality, atoms emit and absorb light **only at discrete wavelengths**, corresponding to **quantized energy level transitions**

$$\Delta E = h\nu = hc/\lambda,$$

as first explained by **Bohr's model** and later generalized in **quantum mechanics**.

- **Photoelectric effect** (emission of electrons from a metal surface under illumination) provides another clear failure of classical physics.
  - The classical prediction is that electrons would be ejected once the accumulated energy per electron exceeds the work function Φ, with

    $$E_{\text{kin}} \propto I_{\text{light}},$$

    where I_{light} is the light intensity, and the emission should occur for **any frequency** given sufficient intensity.
  - In contrast, experiments show that electrons are emitted **only if** the incident light has a frequency **above a threshold** ν_0, regardless of its intensity. The maximum kinetic energy of emitted electrons follows

    $$E_{\text{kin}} = h\nu - \Phi,$$

    increasing **linearly with frequency**, not with intensity.
  - Furthermore, the emission occurs **without measurable delay**, contradicting the classical accumulation picture.
  - This behavior can only be explained if electromagnetic radiation consists of **discrete quanta of energy** $E = h\nu$, each capable of ejecting one electron — a result first proposed by **Einstein (1905)**, marking a foundational step in **quantum theory**.
- **Scattering of X-rays and γ-rays by matter** also exposes the breakdown of classical physics.
  - In the **classical Thomson scattering** picture, electromagnetic waves scatter elastically off free electrons. The scattered wave should have **the same frequency** as the incident one, and the total scattering cross-section should be **independent of photon energy**.
  - Experimentally, however, high-energy photons (X-rays, γ-rays) scattered from electrons are observed to have a **lower frequency** (longer wavelength) than the incident radiation. The wavelength shift depends only on the **scattering angle** θ,

$$\Delta\lambda = \lambda' - \lambda = \frac{h}{m_e c}(1 - \cos\theta),$$

where $\frac{h}{m_e c}$ is the **Compton wavelength** of the electron.

- This **Compton effect** cannot be explained by wave theory, since classical waves cannot change wavelength through elastic scattering.
- The correct explanation comes from **treating light as particles (photons)** carrying energy $E = h\nu$ and momentum $p = h/\lambda$. The observed wavelength shift then follows directly from **energy-momentum conservation** in a photon–electron collision:

$$h\nu + m_e c^2 = h\nu' + \sqrt{(p_e c)^2 + (m_e c^2)^2}.$$

- This experiment provided decisive evidence for the **particle-like nature of light** and confirmed the quantum relation between energy and momentum of photons.

Furthermore, why not reason these phenomena in some complicated non-linear many-body interaction?

1. **Each failure is systematic and universal**, not material-specific.
   - The **blackbody spectrum**, **photoelectric effect**, **atomic spectra**, **heat capacities**, and **Compton scattering** all show *precisely the same kind of deviation* from classical predictions — across vastly different systems.
   - Nonlinear or many-body effects in classical physics typically depend on the details of the material (density, lattice structure, impurities, etc.), whereas these quantum behaviors depend **only on fundamental constants** (h, k_B, c, m_e).
2. **Quantitative predictions match only when energy quantization is assumed.**
   - Planck's law, Einstein's photoelectric equation, Bohr's line spectra, Debye's $C_V \propto T^3$ law, and the Compton shift

$$\Delta\lambda = \frac{h}{m_e c}(1 - \cos\theta)$$

   all follow from a single postulate: **energy and momentum exist in discrete quanta**.

  - No classical nonlinear model reproduces *exactly* these functional forms with the correct constants.
3. **Microscopic measurements show discreteness, not chaos.**
   - If the effects were due to nonlinear many-body interactions, measured spectra would be irregular or chaotic.
   - Instead, we observe **discrete, sharply defined lines and quantized steps**, matching integer multiples of $h\nu$ — a clear signature of underlying quantization.
4. **Experiments at single-particle level confirm quantization.**
   - Individual photon or electron detection (e.g., in photoelectric or Compton experiments) shows **discrete energy transfer events**, one quantum at a time.
   - The statistical distribution of counts follows **Poisson or quantum statistics**, not classical intensity fluctuations.
   - **BUT** are these experiments really "single particle", what if there are some hidden interaction with environment that is "many-body" and result in a statistical result that looks "quantum"?
     - I'd rather believe in emergent quantum mechanics than believing the word is ruled by QM/QFT...
5. **Quantum theory unifies all of them with one principle.**
   - The same formalism — wavefunctions, operators, and the postulate

     $$E = h\nu, \quad p = \hbar k$$

     — consistently explains blackbody radiation, atomic stability, line spectra, photoelectric emission, and scattering, with quantitative precision.

Hence, scientists concluded that these are not the result of some hidden nonlinearities in classical mechanics, but rather reflect a **fundamental discreteness of energy and probability**, requiring the **quantum mechanical framework**.

---

2. Formal Structures: QM vs. Classical

I. Classical Mechanics

Phase space $\mathcal{P}$

The basic object in classical mechanics (CM) is the **phase space** $\mathcal{P}$.

- $\mathcal{P}$ is a smooth manifold of even dimension $d = 2n$.
- A point in phase space is

$$\xi = (q, p) \in \mathcal{P},$$

  where $q = (q_1, \ldots, q_n)$ are generalized coordinates and $p = (p_1, \ldots, p_n)$ are their conjugate momenta.
  Thus, $\mathcal{P}$ represents the space of all possible **states** of a system.

State ρ

(1) A state is a probability distribution on phase space

A **state** is a probability distribution on phase space:

$$\rho(\xi) \geq 0, \qquad \int_{\mathcal{P}} d\xi \, \rho(\xi) = 1.$$

- $\rho(\xi)$ represents our **epistemic uncertainty** about the true configuration of the system.
- The probability of finding the system in a small phase-space volume h^n around ξ is $\rho(\xi)h^n$.
- **Notice**: a state is a **probability distribution** $\rho(\xi)$ on the phase space where ξ lives, rather than a specific value of ξ (for instance, $\xi = \xi_0$)

(2) CM allows arbitray precise measurement, and thus assumes the existence of uncertainty-free states called pure states

In principle, classical mechanics allows **arbitrarily precise** measurements:

- The measurement resolution h can be made arbitrarily small.
- Hence, the theory assumes the existence of **uncertainty-free states**:

$$\rho_{\xi_0}(\xi) = \delta(\xi - \xi_0)$$

  corresponding to exact knowledge of both q and p.

    - We call state such that with **Kronecker delta** probability distribution, i.e. state that is **uncertainty-free**, a **pure state**.
    - **Notice**: again, a pure state is the distribution $\rho_{\xi_0}(\xi) = \delta(\xi - \xi_0)$ rather than the specific state value ξ_0

(3) States can be constructed via statistical mixture, and the set of all states form a convex

Statistical mixtures of states are allowed:

$$\rho(\xi) = p\,\rho_1(\xi) + (1-p)\,\rho_2(\xi), \qquad 0 \le p \le 1$$

- The set of all states forms a **convex set**.
- **Pure states** are the **extremal points** (corners), while **mixed states** lie inside the convex region.
    - In what sense a **convex**?

In what sense the set of all states forms a **convex** set?

1. **Set of classical states**
   Define the set of all valid probability distributions on phase space:

   $$\mathcal{S}_{\text{cl}} = \Big\{ \rho : \mathcal{P} \to \mathbb{R}_{\ge 0} \;\Big|\; \int_{\mathcal{P}} d\xi\, \rho(\xi) = 1 \Big\}.$$

   Each ρ is a legitimate state of the system.
2. **Definition of convexity**
   A subset C of a vector space is *convex* if, for any $x_1, x_2 \in C$, all convex combinations

   $$x_\lambda = \lambda x_1 + (1-\lambda) x_2, \qquad 0 \le \lambda \le 1$$

   also belong to C.
3. **Why $\mathcal{S}_{\text{cl}}$ is convex**
   For $\rho_1, \rho_2 \in \mathcal{S}_{\text{cl}}$, define

   $$\rho_\lambda(\xi) = \lambda \rho_1(\xi) + (1-\lambda)\rho_2(\xi).$$

   Then:
   - Non-negativity: $\rho_\lambda(\xi) \ge 0$.

- Normalization:

$$\int d\xi\, \rho_\lambda(\xi) = \lambda \int \rho_1 + (1-\lambda) \int \rho_2 = \lambda + (1-\lambda) = 1$$

  Hence $\rho_\lambda \in \mathcal{S}_{\mathrm{cl}}$, proving convexity.

4. **Geometric interpretation**
   - The **pure states** $\rho_{\xi_0}(\xi) = \delta(\xi - \xi_0)$ are **extremal points** — they cannot be written as mixtures of others.
   - **Mixed states** lie *inside* the convex hull, representing probabilistic mixtures of pure states.
5. **Conceptual meaning**
   - Convexity encodes the idea that **classical uncertainty is epistemic** — a mixed state represents ignorance about which pure state the system is actually in.
   - Later, in quantum mechanics, the state space is also convex, but *pure states* themselves have a fundamentally different, non-epistemic meaning.

So basically, from the perspective of convex geometry, a **pure state** distinguishes from mixed states in a sense that it **can not be expressed as a mixture** of mixed states or pure states;

"Epistemic" means **pertaining to knowledge** (from Greek *epistēmē*, "knowledge"). So an **epistemic uncertainty** is one that arises because **we don't know** something — not because nature itself is indeterminate.
Take harmonic oscillartor as an example,:

- A pure state means we know exactly the position and momentum. There is *no uncertainty* — if we know the initial condition, we know everything forever.
- A mixed state corresponds to a *distribution* of possible initial conditions. Physically, this means we have a **cloud of oscillators**, or a single oscillator whose initial position/momentum are uncertain. Each member of the ensemble follows its own deterministic trajectory, but we don't know which one.
  So physically:
- A **pure state** corresponds to *one definite trajectory* in phase space.
- A **mixed state** corresponds to an *ensemble of possible trajectories*, weighted by probability.

(3') A pure state corresponds to *one definite trajectory* in phase space; a mixed state corresponds to an *ensemble of possible trajectories*, weighted by probability.

Observable $O : \mathcal{P} \to \mathbb{R}$ and Measurement

(1) An observable is a smoon real-valued function on phase space

An **observable** is a smooth real-valued function on phase space:

$$O : \mathcal{P} \to \mathbb{R}$$

Examples: energy $H(q, p)$, position q_i, momentum p_i, etc.

(2) Expectation value $\langle O \rangle$ of an observable on a given state is an integral

For a given state ρ, the **expectation value** of an observable O is

$$\langle O \rangle_\rho = \int_{\mathcal{P}} d\xi\, \rho(\xi)\, O(\xi).$$

This is the average result of many measurements performed on identically prepared systems.

(3) The probability of an experimental measurement gives an outcome in an interval is an integral

A real measurement of O gives an outcome in an interval $(\lambda_j, \lambda_j + \Delta)$ with probability:

P(O \in [\lambda_j, \lambda_j + \Delta]) = \int_{\mathcal{P}_\Delta=\{\lambda -

- χ_Ω represents the **yes/no question** "Is the system's state ξ inside the region Ω?" Measuring χ_Ω thus tells us whether the system's microstate lies within Ω.
- The **expectation value**

$$\langle \chi_\Omega \rangle_\rho = \int_{\mathcal{P}} d\xi\, \rho(\xi)\, \chi_\Omega(\xi) = \int_\Omega d\xi\, \rho(\xi)$$

gives the **probability** that the system is found in Ω.

- Any general (smooth) observable $O(\xi)$ can then be constructed as a **weighted combination** of such elementary ones:

$$O(\xi) = \int_{\mathbb{R}} d\lambda \, \lambda \, \chi_{\Omega_\lambda}(\xi), \qquad \Omega_\lambda = \{\xi \in \mathcal{P} \mid O(\xi) = \lambda\}.$$

  Conceptually, each χ_{Ω_λ} picks out the phase-space region where O takes a specific value λ, and $O(\xi)$ aggregates these values with their weights λ.

Hence, the **elementary observables** χ_Ω serve as the **building blocks** of all classical observables, linking the abstract function $O(\xi)$ to experimentally measurable yes/no events in phase space.

Phase-Space Transformations and Dynamics

The central idea of Hamiltonian mechanics is that the evolution of a physical system can be understood as **a special kind of continuous (active) transformation on phase space**.
We start from the general notion of phase-space transformation, identify the physically meaningful subclass (canonical transformations),
and finally see how all such transformations — including time evolution — can be expressed **in terms of Poisson brackets**.

Notice:

- When we use the terminology **transformation**, it is actually always **active**, namley it's an **map from a space to another**; what many refer as "passive transformation" should actually be called "re-parameterization of space".
- Despite that **transformation** refers to general map from a space to another, in physical context, physicists often use the word "transfomation" for "invertible, and even structure-preserving" transformation, namely an **isomorphism**; and sometimes we use "transformation" for **automorphism**
- **However, in this set of notes, we shall always (at least try to) adapt the rigourous terminology**.

Word	Mathematical meaning	Physicist's typical usage
Transformation	Any map $f: X \to Y$, not necessarily invertible or structure-preserving	Usually means an invertible, structure-preserving map (an automorphism)
Automorphism	A structure-preserving bijection $f: X \to X $	Rarely used explicitly; its meaning is implied when we say "transformation"
Isomorphism	A structure-preserving bijection $f: X \to Y$ between possibly different objects	Physicists often just call this a "transformation between equivalent descriptions"

(1) Phase-Space Transformations: Physical Meaning

An **(active) phase-space transformation** is a smooth map

$$\Phi : \mathcal{P} \to \mathcal{P}, \qquad \xi \mapsto \eta = \Phi(\xi),$$

that moves each phase-space point (the physical state) to another one.

- Physically, Φ represents a **change of the system's state**:
  the representative point moves along some curve in $\mathcal{P}$.
- The **time evolution** of a closed system is the most fundamental example of such a transformation.

(For reference: a *passive* coordinate change $(q, p) \mapsto (Q, P)$ merely relabels points of $\mathcal{P}$. It is mathematically compatible with the same symplectic structure but does not correspond to a physical motion.)

(2) Canonical Transformations: (Structure-Preserving) Automorphisms of phase space

> **Notice**: When we use the word "**automorphism**", it means the map from a space to itself that is **structure-preserving** and **invertible**, we explicitly wite these conditions only to enphasize how canonical transformations distinguish from general phase-space trabsformations.

Among all maps $\Phi : \mathcal{P} \to \mathcal{P}$, the physically admissible ones are those that preserve the **symplectic structure** (of the phase space manifold) characterized by the

$2n \times 2n$ matrix

$$\mathbf{E} = \begin{pmatrix} 0 & \mathbf{1}_n \\ -\mathbf{1}_n & 0 \end{pmatrix}.$$

Let $J = \frac{\partial \Phi}{\partial \xi}$ be the Jacobian of Φ. Then Φ is **canonical** if and only if

$$J^\top \mathbf{E} J = \mathbf{E}.$$

- Later we will see that such transformation ensures that the fundamental relations between coordinates and momenta

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

  are invariant after canonical transformations
- One can show that canonical transformations preserve phase-space volume (Liouville's theorem) and the form of Hamilton's equations.
  - **Notice** not all diffeomorphism(automorphism on manifold) preserve volume:
    - A *volume* on an n-dimensional manifold M is specified by a nowhere-vanishing top form (volume form) $\Omega \in \Omega^n(M)$. The volume of a region $U \subset M$ is

      $$\mathrm{Vol}(U) = \int_U \Omega$$

    - A diffeomorphism $f : M \to M$ is **volume-preserving** if

      $$f^*\Omega = \Omega.$$

      In local coordinates, this reduces to the Jacobian condition $\det\left(\frac{\partial f}{\partial x}\right) = 1$ with respect to the density underlying Ω.
    - On a **symplectic** manifold $(\mathcal{P}, \omega)$ of dimension $2n$, the **Liouville volume form** is

      $$\Omega_{\mathrm{L}} \equiv \frac{1}{n!}\,\omega^n = dq_1 \wedge dp_1 \wedge \cdots \wedge dq_n \wedge dp_n.$$

      A **canonical (symplectic) transformation** $\Phi : \mathcal{P} \to \mathcal{P}$ is defined by

      $$\Phi^*\omega = \omega.$$

Taking the n-fold wedge,

$$\Phi^*\Omega_{\mathrm{L}} = \Phi^*\left(\tfrac{1}{n!}\omega^n\right) = \tfrac{1}{n!}\left(\Phi^*\omega\right)^n = \tfrac{1}{n!}\omega^n = \Omega_{\mathrm{L}}$$

so every canonical transformation preserves the Liouville volume (this is **Liouville's theorem**).

- Notice **Not every diffeomorphism is volume-preserving.** In general, for $f : M \to M$,

$$f^*\Omega = (\det J_f)\,\Omega \quad \text{(in local frames)},$$

so unless $\det J_f \equiv 1$, volumes change.

- **Volume-preserving is weaker than symplectic.** If a diffeomorphism preserves a given volume form Ω (equivalently $\det J_f = 1$ in adapted coordinates), it need not preserve the symplectic form:

$$f^*\Omega_{\mathrm{L}} = \Omega_{\mathrm{L}} \quad \not\Rightarrow \quad f^*\omega = \omega$$

In contrast, **symplectic** $\Rightarrow$ **volume-preserving**:

$$\Phi^*\omega = \omega \quad \Rightarrow \quad \Phi^*\Omega_{\mathrm{L}} = \Omega_{\mathrm{L}}.$$

- In canonical coordinates $\xi = (q, p)$, the symplectic condition can be written as a Jacobian constraint

$$J^\top \mathbf{E} J = \mathbf{E}, \qquad \mathbf{E} = \begin{pmatrix} 0 & \mathbf{1}_n \\ -\mathbf{1}_n & 0 \end{pmatrix}$$

which in particular implies $\det J = 1$ (hence Liouville preservation), but is strictly stronger than $\det J = 1$.

- They form a **group** under composition: if Φ_1 and Φ_2 are canonical, so is $\Phi_2 \circ \Phi_1$.

---

(3) Infinitesimal canonical transformations and the rise of the Poisson Bracket

We now ask: **how do canonical transformations arise continuously, and what algebraic structure encodes their infinitesimal form?**

(a) Continuous family of canonical transformations

Consider a **one-parameter family** of canonical transformations

$$\Phi_\tau : \mathcal{P} \to \mathcal{P}, \qquad \Phi_0 = \mathrm{id},$$

that moves each point $\xi \in \mathcal{P}$ smoothly along a curve. For instance, for a point ξ_0, this family of canonical transfomations moves it to a curve, points on the curve can then be parameterized by τ:

$$\xi_0(\tau) = \Phi_\tau(\xi_0)$$

The **velocity field** describing this motion is

$$X(\xi) = \frac{d\xi}{d\tau}\Big|_{\tau=0}.$$

(We call this a field because it's a function of phase-space points).
Since every Φ_τ is canonical, it preserves the symplectic matrix $\mathbf{E}$:

$$J_\tau^\top \mathbf{E} J_\tau = \mathbf{E}, \qquad \text{where } J_\tau = \frac{\partial \Phi_\tau}{\partial \xi}.$$

Differentiating this relation at $\tau = 0$ (where $J_0 = \mathbf{1}$) gives the **infinitesimal canonical condition** in terms of velocity field derivatives:

$$(\partial X)^\top \mathbf{E} + \mathbf{E}(\partial X) = 0, \qquad \partial X = \frac{\partial X}{\partial \xi}.$$

(b) Existence of a generating function
The above condition is a **constraint for a family of transformations to be canonical**, the constraint is expressed in terms of velocity field; and conversely it can be viewed as a **constraint for velocity field X itself to be "allowed"**.
Essentially, it states that X is a **Hamiltonian vector field**, i.e. it preserves the symplectic form to first order. A fundamental result from symplectic geometry says that such a vector field can always be expressed as

$$X(\xi) = \mathbf{E}\,\nabla_\xi G(\xi),$$

for some scalar function $G : \mathcal{P} \to \mathbb{R}$, called the **generator** (or Hamiltonian function) of the transformation.
Thus, every infinitesimal canonical transformation is generated by a single scalar function G.

(c) Change of an observable along the flow
(We shall first clarify: By saying "change of an observable" it does not mean we are changing the function O itself — the observable remains the same rule $O(\xi)$; What

changes is the **value** of O **when evaluated on the transformed state**.)
Let $O(\xi)$ be any observable (a smooth function on $\mathcal{P}$).
As the phase-space point moves according to the vector field X, O changes as

$$\frac{dO}{d\tau} = \nabla_\xi O \cdot \frac{d\xi}{d\tau} = \nabla_\xi O \cdot X = \nabla_\xi O \cdot (\mathbf{E}\,\nabla_\xi G) = (\nabla_\xi O)^\top \mathbf{E}\,\nabla_\xi G.$$

We now define this bilinear operation between O and G as the **Poisson bracket**:$$\boxed{
{O, G}
= (\nabla\xi O)^\top \mathbf{E}, \nabla\xi G
= \sum_{i=1}^n
\left(
\frac{\partial O}{\partial q_i}\frac{\partial G}{\partial p_i}

- \frac{\partial O}{\partial p_i}\frac{\partial G}{\partial q_i}
  \right).
  }

  Hencetheinfinitesimalchangeofanyobservableunderacanonicalflowgeneratedby$G$is

  \frac{dO}{d\tau} = {O, G}.$$
  (d) Logical emergence of the Poisson bracket

1. **Start** with canonical transformations that preserve the symplectic form ($J^\top \mathbf{E} J = \mathbf{E}$).
2. **Differentiate** to obtain the condition for infinitesimal flows ($(\partial X)^\top \mathbf{E} + \mathbf{E}(\partial X) = 0$), this is the constraint for "physically allowed flows in phase space"
3. **Solve** this condition: the general solution is $X = \mathbf{E}\nabla G$, meaning that "for every physically allowed flow in phase space, there is a **generator** associated"
4. **Compute** how any observable's evaluation on an initial state changes under this flow: $\frac{dO}{d\tau} = (\nabla O)^\top \mathbf{E}\nabla G$.
5. **Define** this expression as $\{O, G\}$ — the **Poisson bracket**.
   Thus, the **Poisson bracket is not postulated** but arises *inevitably* as the unique bilinear operation that encodes the infinitesimal canonical flow on phase space.

(e) Physical interpretation

- The generator $G(\xi)$ defines a small canonical motion of the system.
- The quantity $\{O, G\}$ measures **how the observable O's evaluation on a given initial state changes** when the state moves infinitesimally along the flow generated by G.
- When the generator G is the Hamiltonian H, this motion becomes **real time evolution**:

  $$\dot{O} = \{O, H\}.$$

  Hence, the Poisson bracket represents the **infinitesimal generator of physical motion** in phase space — it is the algebraic shadow of the underlying symplectic geometry.

---

(4) Poisson Bracket: Definition and Structure

For two observables $O_1(\xi)$ and $O_2(\xi)$,
the **Poisson bracket** is defined as

$$\{O_1, O_2\} = \sum_{j=1}^{n} \left(\frac{\partial O_1}{\partial q_j} \frac{\partial O_2}{\partial p_j} - \frac{\partial O_1}{\partial p_j} \frac{\partial O_2}{\partial q_j} \right) = (\nabla_\xi O_1)^\top \mathbf{E} \nabla_\xi O_2.$$

Properties:

- **Antisymmetry:** $\{O_1, O_2\} = -\{O_2, O_1\}$.
- **Leibniz rule:** $\{O_1 O_2, O_3\} = O_1\{O_2, O_3\} + O_2\{O_1, O_3\}$.
- **Jacobi identity:** $\{O_1, \{O_2, O_3\}\} + \text{cyclic} = 0$.

The set of smooth observables with this bracket forms a **Lie algebra**, and the corresponding canonical flows are the **Lie group** actions generated by it.

Refer to Lecture 1S for a short reminder of **topological groups, Lie groups and Lie algebra**.

(5) Fundamental Poisson Brackets and Canonical Variables

Viewing q_i and p_i themselves as observables gives the **fundamental brackets**

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

A new coordinate system (Q_i, P_i) on $\mathcal{P}$ is **canonical** if it satisfies the same relations:

$$\{Q_i, Q_j\} = 0, \qquad \{P_i, P_j\} = 0, \qquad \{Q_i, P_j\} = \delta_{ij}.$$

This provides an intrinsic criterion for identifying canonical coordinates.

---

(6) Hamiltonian Flow and Dynamics Generated by an Observable

Each observable $G(\xi)$ defines a **Hamiltonian vector field**

$$X_G = \mathbf{E}\,\nabla_\xi G,$$

which generates a one-parameter family of canonical transformations Φ_τ^G satisfying

$$\frac{d\xi}{d\tau} = X_G(\xi).$$

In coordinates,

$$\dot{q}_i = \frac{\partial G}{\partial p_i}, \qquad \dot{p}_i = -\frac{\partial G}{\partial q_i}.$$

For any observable $O(\xi)$,

$$\frac{dO}{d\tau} = \{O, G\}$$

Hence, the Poisson bracket encodes the **infinitesimal change of any quantity** under the canonical flow generated by G.

When $G = H$ (the Hamiltonian),
this becomes the **equation of motion**:

$$\dot{O} = \{O, H\},$$

and in particular,

$$\dot{q}_i = \{q_i, H\} = \frac{\partial H}{\partial p_i}, \qquad \dot{p}_i = \{p_i, H\} = -\frac{\partial H}{\partial q_i}.$$

The integral curves $\xi(\tau)$ form a **one-parameter Abelian group**
of canonical transformations:

$$\Phi_0^G = \mathrm{id}, \quad \Phi_{\tau_1+\tau_2}^G = \Phi_{\tau_1}^G \circ \Phi_{\tau_2}^G, \quad (\Phi_\tau^G)^{-1} = \Phi_{-\tau}^G.$$

Since $\nabla_\xi \cdot X_G = 0$, each Φ_τ^G preserves phase-space volume (Liouville's theorem).

Time Evolution and Liouville Dynamics in Classical Mechanics

Having established that infinitesimal canonical transformations are generated by the Poisson bracket, we now systematically apply this structure to describe **time evolution** — the continuous motion of a system along the canonical flow generated by the **Hamiltonian function** $H(\xi)$.

(1) Time Evolution as a Canonical Flow

The **Hamiltonian flow** Φ_t^H generated by H determines how every phase-space point moves in time:

$$\frac{d\xi}{dt} = X_H(\xi) = \mathbf{E}\,\nabla_\xi H(\xi)$$

Formally, this defines a one-parameter group of canonical transformations

$$\Phi_t^H : \xi_0 \mapsto \xi_t, \qquad \Phi_{t+s}^H = \Phi_t^H \circ \Phi_s^H, \quad \Phi_0^H = \mathrm{id}.$$

Time evolution thus acts as a **canonical automorphism** of the phase space.

---

(2) Evolution of Mixed States (Probability Distributions)

Let $\rho_t(\xi)$ be the probability density on phase space at time t. **Classical causality** demands that the probability of being found in a given region
evolves consistently with the deterministic flow of states.
Formally:

$$\rho_t(\xi) = \rho_0\big(\Phi_{-t}^H(\xi)\big),$$

meaning that the probability of "being at ξ at time t
equals the probability that "the system was initially at the point
such that evolves into ξ after time t'.

Differentiating with respect to time:

$$\frac{d\rho_t(\xi)}{dt} = -(\nabla_\xi \rho_t)\cdot \frac{d\xi}{dt} = -\nabla_\xi \rho_t \cdot (\mathbf{E}\,\nabla_\xi H) = -\{\rho_t, H\}.$$

Hence, the **Liouville equation**:

$$\boxed{\frac{d\rho_t}{dt} = -\{\rho_t, H\} \quad \text{or equivalently} \quad \partial_t \rho_t = \{H, \rho_t\}.}$$

This expresses the conservation of probability density along the Hamiltonian flow.

(3) Conservation of Total Probability (Liouville's Theorem)

Integrating over the whole phase space,

$$\frac{d}{dt}\int d\xi\, \rho_t(\xi) = -\int d\xi\, \nabla_\xi \cdot (\rho_t X_H) = -\int d\xi\, (\nabla_\xi \rho_t)\cdot X_H - \int d\xi\, \rho_t (\nabla_\xi \cdot X_H).$$

Since $\nabla_\xi \cdot X_H = 0$
(the Hamiltonian flow is volume-preserving), both terms vanish,
so the total probability is conserved:

$$\frac{d}{dt}\int d\xi\, \rho_t(\xi) = 0.$$

(4) Liouville Operator and Formal Solution

The Liouville equation can be written in operator form:

$$\frac{d\rho_t}{dt} = \mathcal{L}_H \rho_t, \qquad \mathcal{L}_H(\,\cdot\,) := \{\, H, \,\cdot\, \},$$

where $\mathcal{L}_H$ is called the **Liouville operator**
or the **Lie derivative** along the Hamiltonian flow.

The formal solution is:

$$\rho_t = e^{\,t\mathcal{L}_H} \rho_0.$$

This describes how any initial probability distribution is transported
along the trajectories of the Hamiltonian vector field.

---

(5) Time Evolution of Observables

The expectation value of an observable $O(\xi)$ at time t is

$$\langle O\rangle_t = \int d\xi\, \rho_t(\xi)\, O(\xi) = \int d\xi\, \rho_0(\xi)\, O\big(\Phi_t^H(\xi)\big).$$

This expression shows that time evolution can equivalently be thought of as acting either on **states** or on **observables**:

$$\rho_t = e^{t\mathcal{L}_H}\rho_0 \quad \Longleftrightarrow \quad O_t = e^{-t\mathcal{L}_H}O_0,$$

so that the expectation value remains invariant:

$$\langle O_t\rangle_{\rho_0} = \langle O_0\rangle_{\rho_t}.$$

Differentiating O_t gives the **Heisenberg-type equation of motion**:

$$\frac{dO_t}{dt} = \{O_t, H\},$$

which is the same relation obtained earlier for single trajectories.

(6) Summary: States vs. Observables

Viewpoint	Object that evolves	Equation	Interpretation
Schrödinger picture	Probability distribution ρ_t	$\dot{\rho}_t = \{H, \rho_t\}$	The distribution is carried by the flow
Heisenberg picture	Observable O_t	$\dot{O}_t = \{O_t, H\}$	The observable changes along the flow
Invariant quantity	Expectation value	$\frac{d}{dt}\langle O_t\rangle_{\rho_0} = 0$	Probabilistic consistency (Liouville theorem)

---

(7) Conceptual Summary

- Time evolution in classical mechanics is a **canonical transformation** generated by the Hamiltonian.

- The **Liouville equation** governs the evolution of mixed states (probability densities).
- Observables evolve according to the same Poisson-bracket law.
- The **expectation value** of any observable is invariant under this joint evolution.

Hence, classical dynamics can be viewed equivalently as acting on **states** or on **observables** — a duality that anticipates the Schrödinger and Heisenberg pictures of quantum mechanics.

II. Quantum Mechanics

Hilbert Space $\mathcal{H}$

The basic space of QM is a **Hilbert space** $\mathcal{H}$:
a complex vector space equipped with an inner product $\langle\phi|\psi\rangle$.

The basic mathematical structure underlying Quantum Mechanics is a **Hilbert space** $\mathcal{H}$.
Formally, a Hilbert space is a **complex vector space** equipped with a **Hermitian inner product**

$$\langle\cdot|\cdot\rangle : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$$

such that satisfies the following properties for all $|\phi\rangle, |\psi\rangle, |\chi\rangle \in \mathcal{H}$ and all $a, b \in \mathbb{C}$:

1. **Linearity in the second argument:**
   $\langle\phi|a\psi + b\chi\rangle = a\langle\phi|\psi\rangle + b\langle\phi|\chi\rangle.$
2. **Conjugate symmetry:**
   $\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^*$ and
3. **Positive definiteness:**
   $\langle\psi|\psi\rangle \geq 0$, with equality if and only if $|\psi\rangle = 0.$
4. (1+2 naturally lead to conjugate linearity in first argument, this is automatically satisfied)

It's also good to know that the norm on $\mathcal{H}$ is defined by

$$\| \, |\psi\rangle \, \| = \sqrt{\langle\psi|\psi\rangle},$$

and $\mathcal{H}$ is **complete** with respect to this norm.

States

(1) Pure state represented as ray, a pure state as an equivalent class

A **pure state** of a quantum system is represented by a *ray* in $\mathcal{H}$ —
that is, by an equivalence class of nonzero vectors

$$|\psi\rangle \sim e^{i\alpha}|\psi\rangle, \qquad \alpha \in \mathbb{R}$$

which define the same physical state.

(1') A pure state is often represented by a representative (normalized) vector of the ray

In practice, one may use normalized vector $|\psi\rangle$ of the ray it belongs to to represent a pure state.

(2) Pure stated represented as rank-1 orthogonal projector Π_ψ

Equivalently, each pure state can be represented by a **rank-1 orthogonal projector**

$$\Pi_\psi = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}, \qquad |\psi\rangle \neq 0.$$

In practice we work with normalized vectors $\langle\psi|\psi\rangle = 1$, so that $\Pi_\psi = |\psi\rangle\langle\psi|$.
The set of all pure states therefore corresponds to the **complex projective Hilbert space**

$$\mathbb{P}(\mathcal{H}) = (\mathcal{H} \setminus \{0\})/U(1),$$

where $U(1)$ acts by global phase multiplication $|\psi\rangle \mapsto e^{i\alpha}|\psi\rangle$.

---

(3) Mixed state as probability distribution, represented by density operator ρ

Like in classical mechanics, we may lack complete knowledge of the system's state. This **epistemic uncertainty** is represented by a **mixed state** (statistical ensemble) described by a **density operator** $\hat{\rho}$.

- Let be a probability distribution over normalized vectors on $\mathcal{H}$, satisfying

$$\rho(|\psi\rangle) \geq 0, \qquad \int_{\mathcal{H}} d\psi\, \rho(|\psi\rangle) = 1.$$

  We associate to it the **density operator**

$$\hat{\rho} = \int_{\mathcal{H}} d\psi\, \rho(|\psi\rangle)\, |\psi\rangle\langle\psi|,$$

  which acts on $\mathcal{H}$ and encodes the same statistical information.
- For a discrete ensemble $\{\, |\psi_i\rangle, p_i \,\}$, this reduces to

$$\hat{\rho} = \sum_i p_i\, |\psi_i\rangle\langle\psi_i|, \qquad p_i \geq 0, \quad \sum_i p_i = 1.$$

(4) Properties of the Density Operator

A valid density operator $\hat{\rho}$ satisfies:

$$\langle\phi|\hat{\rho}|\phi\rangle \geq 0, \qquad \hat{\rho}^\dagger = \hat{\rho}, \qquad \mathrm{Tr}\,\hat{\rho} = 1.$$

It can always be diagonalized:

$$\hat{\rho} = \sum_n p_n\, |n\rangle\langle n|, \qquad p_n \geq 0, \quad \sum_n p_n = 1,$$

where $\{|n\rangle\}$ are orthonormal eigenvectors.
Historically, $\hat{\rho}$ is called the **density matrix**.

(5) All density operators form a convex set, with pure states as extremal points

The operator $\hat{\rho}$ is thus a **compact, positive semidefinite, trace-one** operator on $\mathcal{H}$:

$$\hat{\rho} \geq 0, \qquad \mathrm{Tr}\,\hat{\rho} = 1.$$

The space of all such operators,

$$\mathcal{S}_{\mathrm{QM}} = \{\, \hat{\rho} \in \mathcal{B}(\mathcal{H}) \mid \hat{\rho} \geq 0,\ \mathrm{Tr}\hat{\rho} = 1 \,\}$$

forms a **convex set**:
if $\hat{\rho}_1, \hat{\rho}_2 \in \mathcal{S}_{\rm QM}$ and $0 \le p \le 1$,
then $p\hat{\rho}_1 + (1-p)\hat{\rho}_2 \in \mathcal{S}_{\rm QM}$.

- **Pure states** are the **extremal points** of this set (they cannot be written as nontrivial mixtures).
- **Mixed states** are convex combinations of pure ones, representing statistical mixtures rather than definite quantum states.

Observable and Measurement

(1) Observables are Hermitian operators

An **observable** in QM is represented by a **self-adjoint operator** $\hat{O} = \hat{O}^\dagger$ acting on $\mathcal{H}$, namely an Hermitian operator. i.e. an operator satisfying:

$$\langle \phi, \hat{A}\psi \rangle = \langle \hat{A}\phi, \psi \rangle, \quad \forall \phi, \psi \in \mathcal{D}(\hat{A}),$$

(2) Thus, observables admit a spectral decomposition

Such operators have real eigenvalues and admit a **spectral decomposition**:

$$\hat{O} = \sum_n \lambda_n \, \Pi_{\lambda_n}, \qquad \Pi_{\lambda_n} = |\lambda_n\rangle\langle\lambda_n|, \qquad \langle\lambda_m|\lambda_n\rangle = \delta_{mn}.$$

where each Π_{λ_n} is an **elementary yes/no observable**, and any function of $\hat{O}$ is defined spectrally:

$$f(\hat{O}) = \sum_n f(\lambda_n) \, \Pi_{\lambda_n}.$$

This spectral structure is the quantum analog of the decomposition of classical observables into level sets on phase space.

---

(3) Probability of a measurement

When an observable $\hat{O}$ (a self-adjoint operator) is measured on a system in state , its possible outcomes are the **eigenvalues** λ_n of $\hat{O}$, and the probability of obtaining λ_n

is given by the **Born rule**:

$$P(\lambda_n) = \mathrm{Tr}(\hat\rho\,\Pi_{\lambda_n}), \qquad \Pi_{\lambda_n} = |\lambda_n\rangle\langle\lambda_n|.$$

For a **pure state** $|\psi\rangle$, this reduce to

$$P(\lambda_n) = \langle\psi|\Pi_{\lambda_n}|\psi\rangle = |\langle\lambda_n|\psi\rangle|^2$$

(4) Expectation value of an observable

The **expectation value** of $\hat O$ in state $\hat\rho$ is then the statistical mean
of all possible measurement results:

$$\langle \hat O\rangle_{\hat\rho} = \sum_n \lambda_n\, P(\lambda_n) = \sum_n \lambda_n\, \mathrm{Tr}(\hat\rho\,\Pi_{\lambda_n}) = \mathrm{Tr}(\hat\rho\,\hat O). \$\$ or a pure state, this reduces to : \$\$ \langle \hat O\rangle_{\psi}$$

In classical mechanics this probability would be purely *epistemic* (reflecting ignorance), but in QM, it reflects **intrinsic uncertainty** of measurement outcomes — even for pure states.

Hilbert Space Transformations and Dynamics

Quantum mechanics, like classical mechanics, admits transformations acting on its state space. However, here the state space is the **Hilbert space** $\mathcal{H}$, and the relevant structure to preserve is not the **symplectic form** but the **inner product**, which encodes probability amplitudes.

(1) General Transformations of States

A general transformation of states is a linear map

$$|\psi\rangle \;\longmapsto\; |\psi'\rangle = \hat T\,|\psi\rangle,$$

where $\hat T$ is an operator acting on $\mathcal{H}$.

In general, $\hat T$ may not preserve the inner product:

$$\langle\psi'|\phi'\rangle = \langle\psi|\hat T^\dagger \hat T|\phi\rangle \neq \langle\psi|\phi\rangle.$$

Such transformations distort probability amplitudes and thus are **not physically admissible**.

(2) Structure-Preserving Transformations: Unitary and Antiunitary Maps

The physically admissible transformations are those preserving inner products:

$$\langle \psi' | \phi' \rangle = \langle \psi | \phi \rangle,$$

which implies

$$\hat{T}^\dagger \hat{T} = \mathbb{1}.$$

These are **unitary transformations**.
(If the map is antilinear and still preserves the norm, it is **antiunitary**;
such maps appear, for instance, in time-reversal symmetry, but we focus on the unitary case.)

Unitary transformations preserve:

- The **norm of state vectors**, hence normalization of probabilities;
- The **inner product structure**, hence all transition probabilities $|\langle \phi | \psi \rangle|^2$.

(2') Thus, **unitary transformations are the quantum analog of canonical transformations** in classical mechanics

They preserve the fundamental structure of the theory — probability amplitudes instead of phase-space volume.

---

(3) Infinitesimal Unitary Transformations: generator of a transformation and the rise of commutator

A one-parameter family of unitary transformations $\hat{U}_\tau$
forms a **continuous group**:

$$\hat{U}_\tau^\dagger \hat{U}_\tau = \mathbb{1}, \qquad \hat{U}_{\tau_1 + \tau_2} = \hat{U}_{\tau_1} \hat{U}_{\tau_2}.$$

Any such family can be written as an exponential of a **Hermitian generator** $\hat{G}$:

$$\hat{U}_\tau = e^{-\frac{i}{\hbar} \tau \hat{G}}, \qquad \hat{G}^\dagger = \hat{G}$$

Differentiating at $\tau = 0$ gives the infinitesimal form:

$$\frac{d}{d\tau}|\psi_\tau\rangle = -\frac{i}{\hbar}\hat{G}|\psi_\tau\rangle.$$

Here $\hat{G}$ plays the same role as the generating function in classical mechanics: it defines a **flow on the Hilbert space** that preserves the underlying structure.

Now **recall our workflow of introducing the concept of Poisson braket in CM** [(3) Infinitesimal canonical transformations and the rise of the Poisson Bracket], where we followed the logic chain:

1. **Start** with canonical transformations that preserve the symplectic form ($J^\top \mathbf{E} J = \mathbf{E}$).
2. **Differentiate** to obtain the condition for infinitesimal flows ($(\partial X)^\top \mathbf{E} + \mathbf{E}(\partial X) = 0$), this is the constraint for "physically allowed flows in phase space"
3. **Solve** this condition: the general solution is $X = \mathbf{E}\nabla G$, meaning that "for every physically allowed flow in phase space, there is a **generator** associated"
4. **Compute** how any observable's evaluation on an initial state changes under this flow: $\frac{dO}{d\tau} = (\nabla O)^\top \mathbf{E}\nabla G$.
5. **Define** this expression as $\{O, G\}$ — the **Poisson bracket**.
   Analogically, since we have we shall continue from the **4th** step: **compute** how any **observable's evaluation on an initial state changes under the flow induced by an infinitesimal unitary transformation**.

(c). Evolve of evaluation of an observable
Let $\hat{U}_\tau = e^{-\frac{i}{\hbar}\tau\hat{G}}$ act on an initial state $|\psi\rangle$.
The evolved state is:

$$|\psi_\tau\rangle = \hat{U}_\tau|\psi\rangle.$$

The expectation value of an observable $\hat{O}$ in the evolved state is

$$\langle\hat{O}\rangle_\tau = \langle\psi_\tau|\hat{O}|\psi_\tau\rangle = \langle\psi|\hat{U}_\tau^\dagger\,\hat{O}\,\hat{U}_\tau|\psi\rangle.$$

Differentiating with respect to τ gives:

$$\frac{d}{d\tau}\langle\hat{O}\rangle_\tau = \frac{i}{\hbar}\,\langle\psi|[\hat{G}, \hat{O}_\tau]|\psi\rangle, \qquad \hat{O}_\tau = \hat{U}_\tau^\dagger\hat{O}\hat{U}_\tau.$$

Hence, the rate of change of an observable's expectation value under a transformation generated by $\hat{G}$ is determined by the **commutator** $[\hat{G}, \hat{O}]$.

(4) Definition of the Quantum Poisson Bracket (Commutator)

By analogy with the classical expression

$$\dot{O} = \{O, G\},$$

we define the **quantum Poisson bracket** as

$$\{\hat{O}, \hat{G}\}_{\mathrm{QM}} = \frac{1}{i\hbar}[\hat{O}, \hat{G}] = \frac{1}{i\hbar}(\hat{O}\hat{G} - \hat{G}\hat{O}).$$

This identifies the commutator (up to the factor $1/i\hbar$)
as the **quantum analog of the Poisson bracket**.

It governs both:

- infinitesimal evolution of expectation values
    - this is from a **straightforward analog** with CM, in a sense "evaluation of anobservable on a system with given initial (pure) state" corresponds to "measurement (expectation value) of an observable on a system with given initial (pure) state", and thus their evolution
- infinitesimal transformations of observables
    - this is **not** a direct analog from CM, this only make sense when we introduce the so called Heisenberg picture

Thus, at this stage, we can (at least) say:
If $\hat{G}$ generates a unitary flow, the corresponding evolution of the expectation value of observables is:

$$\boxed{\frac{d\langle\hat{O}\rangle}{d\tau} = \frac{i}{\hbar}\langle[\hat{G}, \hat{O}]\rangle}$$

---

(5) Active vs. Passive Interpretations of the Flow : Heisenberg Picture

In the previous discussion, the **state** $|\psi\rangle$ evolved under a unitary flow generated by $\hat{G}$
:

$$|\psi_\tau\rangle = \hat{U}_\tau|\psi\rangle, \qquad \hat{U}_\tau = e^{-\frac{i}{\hbar}\hat{G}\tau}.$$

This is called the **active interpretation** — the physical state itself moves in Hilbert space, while observables remain fixed.

Alternatively, we can adopt a **passive interpretation**, where the state is kept fixed, and instead we view the **observables** as evolving according to

$$\hat{O}_\tau = \hat{U}_\tau^\dagger\,\hat{O}\,\hat{U}_\tau.$$

This defines the **Heisenberg picture** of quantum mechanics.

Both descriptions are **physically equivalent**, since they yield identical expectation values:

$$\langle\psi_\tau|\hat{O}|\psi_\tau\rangle = \langle\psi|\hat{O}_\tau|\psi\rangle.$$

This equivalence mirrors the classical duality between two ways of describing canonical transformations:

- **Active viewpoint:** points in phase space (the states) move under the Hamiltonian flow Φ_t.
- **Passive viewpoint:** the coordinate functions (observables) are transformed while the point is held fixed.
  Thus, the Schrödinger and Heisenberg pictures in quantum mechanics correspond precisely to these two classical perspectives on phase-space evolution.

Differentiating $\hat{O}_\tau = \hat{U}_\tau^\dagger\hat{O}\hat{U}_\tau$ with respect to τ gives

$$\boxed{\frac{d\hat{O}_\tau}{d\tau} = \frac{1}{i\hbar}\,[\hat{O}_\tau, \hat{G}]}$$

which is the **Heisenberg equation of motion**.

Thus, the commutator $\frac{1}{i\hbar}[\cdot,\cdot]$ governs

- infinitesimal transformations of **observables** in the **Heisenberg picture** — the exact quantum analog of the Poisson bracket $\{\cdot, \cdot\}$ in classical mechanics.
- in addition to "infinitesimal evolution of **expectation values** in **Schrodinger's picture**" which we have discussed in last subsection.

---

(6) Canonical Commutation Relations as Structural Consequences

From the viewpoint of infinitesimal unitary transformations,
the **canonical commutation relations**

$$[\hat{q}_i, \hat{p}_j] = i\hbar\, \delta_{ij}, \qquad [\hat{q}_i, \hat{q}_j] = [\hat{p}_i, \hat{p}_j] = 0,$$

express how position and momentum operators
transform under each other's generated flows:

- The flow generated by $\hat{p}_j$ shifts $\hat{q}_i$:

$$\frac{d\hat{q}_i}{d\tau} = \frac{i}{\hbar}[\hat{p}_j, \hat{q}_i] = \delta_{ij}.$$

- The flow generated by $\hat{q}_i$ shifts $\hat{p}_j$ oppositely:

$$\frac{d\hat{p}_j}{d\tau} = \frac{i}{\hbar}[\hat{q}_i, \hat{p}_j] = -\delta_{ij}.$$

Hence, the CCR are **not arbitrary postulates**: they encode the infinitesimal structure of unitary flows that preserve the Hilbert-space inner product,
just as the Poisson bracket structure encodes the infinitesimal canonical flows that preserve the symplectic form in classical mechanics.

Generators, Commutation, and Quantum Dynamics

Once the structure of allowed transformations is understood, we can describe how **dynamics** arises as a continuous unitary flow generated by a particular observable — the Hamiltonian.

(1) Generator of Time Evolution: the Hamiltonian Operator

Physical time evolution is a unitary flow generated by the **Hamiltonian** $\hat{H}$:

$$i\hbar \frac{d}{dt}|\psi_t\rangle = \hat{H}\,|\psi_t\rangle.$$

Its formal solution is

$$|\psi_t\rangle = \hat{U}_t^H\,|\psi_0\rangle, \qquad \hat{U}_t^H = e^{-\frac{i}{\hbar}t\hat{H}}.$$

For non-relativistic particles,

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

---

(2) Liouville–von Neumann Equation for Mixed States

For a mixed state $\hat{\rho}$, causality implies that probabilities evolve consistently under the same unitary flow:

$$\hat{\rho}_t = \hat{U}_t^H\,\hat{\rho}_0\,(\hat{U}_t^H)^\dagger.$$

Differentiating gives the **Liouville–von Neumann equation**:

$$\frac{d\hat{\rho}_t}{dt} = -\frac{i}{\hbar}[\hat{H}, \hat{\rho}_t] \equiv \mathcal{L}_H\,\hat{\rho}_t$$

The super-operator $\mathcal{L}_H = -\frac{i}{\hbar}[\hat{H}, \cdot\,]$
is the quantum analog of the **Liouville operator** in classical mechanics.

---

(3) Stationary States

A state $\hat{\rho}_{\text{stat}}$ is **stationary** if it commutes with $\hat{H}$:

$$[\hat{\rho}_{\text{stat}}, \hat{H}] = 0$$

Such states are mixtures of energy eigenstates Π_{E_n}, and evolve trivially in time:

$$\hat{\rho}_{\text{stat}}(t) = \hat{\rho}_{\text{stat}}.$$

---

(4) Time Evolution of Observables: Heisenberg Picture

Because expectation values $\langle \hat{O} \rangle_t = \mathrm{Tr}(\hat{\rho}_t \hat{O})$ must remain invariant, time evolution can equivalently be represented as acting on observables:

$$\hat{O}_t = (\hat{U}_t^H)^\dagger \, \hat{O} \, \hat{U}_t^H,$$

so that

$$\langle \hat{O} \rangle_t = \mathrm{Tr}(\hat{\rho}_0 \, \hat{O}_t) = \mathrm{Tr}(\hat{\rho}_t \, \hat{O}).$$

Differentiating gives the **Heisenberg equation of motion**:

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

This is the direct quantum counterpart of

$$\frac{dO}{dt} = \{O, H\}$$

in classical mechanics.

III. Classical–Quantum Parallel

Concept / Structure / Dynamics	Classical Mechanics	Quantum Mechanics
State space	Phase space $\mathcal{P}$	Hilbert space $\mathcal{H}$
Pure state	Point ξ_0 or $\rho(\xi) = \delta(\xi - \xi_0)$	Ray $\psi\rangle$ or projector $\psi\rangle\langle\psi$
Mixed state	Probability density $\rho(\xi)$	Density operator (matrix) $\hat{\rho}$
Observable	Real function $O(\xi)$ on $\mathcal{P}$	Hermitian operator $\hat{O}$ on $\mathcal{H}$
Expectation value	$\langle O \rangle = \int d\xi \, \rho(\xi) O(\xi)$	$\langle \hat{O} \rangle = \mathrm{Tr}(\hat{\rho} \, \hat{O})$
Elementary observable	Indicator function of region in $\mathcal{P}$	Projector $\Pi = \phi\rangle\langle\phi$ (yes/no proposition)
Transformation of states	Canonical transformation $\xi \mapsto \eta(\xi)$	Unitary transformation $\psi\rangle \mapsto \hat{U}\psi\rangle$

Concept / Structure / Dynamics	Classical Mechanics	Quantum Mechanics
Structure preserved	Symplectic form $\omega = dq \wedge dp$ (volume and Poisson structure)	Inner product $\langle \phi \psi \rangle$ (probabilities)
Infinitesimal generator	Function $G(q, p)$ generating Hamiltonian vector field $X_G = \mathbf{E} \nabla G$	Hermitian operator $\hat{G}$ generating unitary flow $\hat{U}_\tau = e^{-i\tau\hat{G}/\hbar}$
Infinitesimal structure (bracket)	Poisson bracket $\{A, B\} = (\nabla A)^\top \mathbf{E} \nabla B$	Commutator $\frac{1}{i\hbar}[\hat{A}, \hat{B}]$
Canonical pair	(q_i, p_j) with $\{q_i, p_j\} = \delta_{ij}$	$(\hat{q}_i, \hat{p}_j)$ with $[\hat{q}_i, \hat{p}_j] = i\hbar\,\delta_{ij}$
Transformation of observables	$O \mapsto O' = O \circ \eta^{-1}$ (pullback)	$\hat{O} \mapsto \hat{O}' = \hat{U}^\dagger \hat{O} \hat{U}$
Evolution of state	$\dot{\rho} = \{H, \rho\}$ (Liouville equation)	$\dot{\hat{\rho}} = -\frac{i}{\hbar}[\hat{H}, \hat{\rho}]$ (von Neumann equation)
Evolution of observable	$\dot{O} = \{O, H\}$ (Hamilton's equations)	$\dot{\hat{O}} = \frac{i}{\hbar}[\hat{H}, \hat{O}]$ (Heisenberg equations)
Generator of motion	Hamiltonian function $H(q, p)$	Hamiltonian operator $\hat{H}$
Flow on state space	Hamiltonian flow Φ_t^H (symplectic, volume-preserving)	Unitary flow $\hat{U}_t^H = e^{-it\hat{H}/\hbar}$ (inner-product preserving)
Stationary state / invariant distribution	$\{H, \rho_{\text{stat}}\} = 0$	$[\hat{H}, \hat{\rho}_{\text{stat}}] = 0$
Geometric structure preserved by dynamics	Symplectic form ω, phase-space volume (Liouville's theorem)	Inner product $\langle \psi \phi \rangle$ (unitarity)
Physical interpretation of $\hbar$	—	Quantization scale of phase-space area, $[q_i, p_j] = i\hbar$
Classical limit ($\hbar \to 0$)	—	$\frac{1}{i\hbar}[\hat{A}, \hat{B}] \to \{A, B\}$

In this unified view:

- **Symplectic** $\leftrightarrow$ **Unitary**
  captures the structure-preserving transformations in both theories.
- **Poisson bracket** $\leftrightarrow$ **Commutator**
  provides the algebraic skeleton of dynamics.
- **Hamiltonian flow** $\leftrightarrow$ **Unitary evolution**
  connects the generator to physical time evolution.

The **formal structure** of QM mirrors that of classical mechanics:
both are built on

- a convex set of states,
- observables forming a real vector space with a bilinear bracket,
- dynamics generated by a distinguished element (the Hamiltonian).

However:

- In CM, uncertainty is *epistemic* (lack of knowledge about ξ);
- In QM, uncertainty is *intrinsic*, arising from **non-commutativity** of observables. Planck's constant $\hbar$ quantifies this deviation: as $\hbar \to 0$, commutators reduce to Poisson brackets and the quantum theory tends to its classical limit.

3. Example: Harmonic Oscillator (Part 2)

4. Measurement in QM (Part2)