Unitary Time Evolution

Quantum Foundations · Module 2 — Postulates

Node 2.4

Position in Knowledge Graph

System: Quantum Foundations **Structural Domain:** Postulates of Quantum Mechanics **Node:** 2.4

This postulate gives the formalism its dynamics. The state postulate (2.1) and the observable postulate (2.2) define a static theory of states and questions; the Born rule (2.3) turns it into a theory of measurement statistics. Time evolution is what makes it a theory of how states change between measurements.

Formal Statement

The time evolution of an isolated quantum system is generated by a self-adjoint operator H — the **Hamiltonian**, identified with the system's total energy observable — via the **Schrödinger equation**:

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle.$$

Equivalently, evolution is implemented by a two-parameter family of **unitary operators** $U(t_2, t_1) : \mathcal{H} \to \mathcal{H}$:

$$|\psi(t_2)\rangle = U(t_2, t_1)|\psi(t_1)\rangle,$$

satisfying $U^\dagger(t_2, t_1)U(t_2, t_1) = I$, the composition law $U(t_3, t_1) = U(t_3, t_2)U(t_2, t_1)$, and the boundary condition $U(t, t) = I$.

For a time-independent Hamiltonian the solution is explicit:

$$U(t) = e^{-iHt/\hbar}, \qquad |\psi(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle.$$

For a time-dependent Hamiltonian $H(t)$, the formal solution is the **time-ordered exponential**

$$U(t, 0) = \mathcal{T}\exp\left(-\frac{i}{\hbar}\int_0^t H(s)\,ds\right).$$

Intuition

Unitary evolution is the formal expression of two physical demands:

1. **Probabilities are conserved.** The total probability of all possible measurement outcomes must remain one at every instant; otherwise the theory predicts the disappearance (or creation) of probability mass, which is empirically absurd.
2. **Evolution is linear and deterministic.** The superposition principle survives dynamics: if $|\psi_1(t)\rangle$ and $|\psi_2(t)\rangle$ are solutions, so is $\alpha|\psi_1(t)\rangle + \beta|\psi_2(t)\rangle$, with the same coefficients at every time.

Unitarity is the unique class of operators on a Hilbert space that is both linear and norm-preserving. It is therefore the only kind of map that can represent the closed-system dynamics demanded by the postulates.

The Hamiltonian plays a double role: as the energy observable (a Hermitian operator whose eigenvalues are the possible energy measurement outcomes) and as the generator of time evolution (whose exponential supplies the unitary). This double role is not a coincidence: it is the quantum version of Noether's theorem for time translation (Node 2.6).

Structural Role

Unitary evolution is the postulate that separates **closed systems** from **open systems**:

- A closed system evolves unitarily under a fixed Hamiltonian, and its state remains pure (Node 5.1).
- An open system coupled to an environment does not evolve unitarily on its own; its effective dynamics are described by completely positive trace-preserving maps (Node 7.3) and generated by Lindblad operators (Node 8.2).

Every structural feature of Module 8 (open systems) is derived by starting from a unitary evolution on a larger system and tracing out part of it. Unitarity is therefore not merely the dynamics of closed systems; it is the axiom from which all other quantum dynamics are built.

Unitary evolution is also the fundamental resource of the VQA course: quantum circuits are products of unitary gates, each implementing $U(\theta) = e^{-iG\theta}$ for some generator G.

Mathematical Development

Why unitary? The Wigner argument

Suppose evolution $|\psi\rangle \mapsto T|\psi\rangle$ preserves all transition probabilities: $|\langle T\phi|T\psi\rangle|^2 = |\langle\phi|\psi\rangle|^2$ for all $|\phi\rangle, |\psi\rangle$. Wigner's theorem asserts that T must be either unitary (linear, inner-product preserving) or anti-unitary (antilinear, conjugate-inner-product preserving). Continuous time evolution rules out the anti-unitary case by a continuity-from-the-identity argument, leaving unitarity as the unique option.

Stone's theorem

Theorem (Stone). A one-parameter group $U(t)$ of unitary operators on a Hilbert space is strongly continuous if and only if there exists a (possibly unbounded) self-adjoint operator H such that

$$U(t) = e^{-iHt/\hbar}.$$

The operator H is called the **infinitesimal generator** of the group. Stone's theorem is the rigorous statement that "continuous unitary evolution" and "Hermitian Hamiltonian" are two sides of the same structural object.

Probability conservation

If $|\psi(t)\rangle = U(t)|\psi(0)\rangle$ with $U(t)$ unitary, then

$$\langle\psi(t)|\psi(t)\rangle = \langle\psi(0)|U^\dagger U|\psi(0)\rangle = \langle\psi(0)|\psi(0)\rangle,$$

so norms (hence Born-rule total probabilities) are conserved exactly.

The three pictures

Time dependence can be assigned to states or operators:

- **Schrödinger picture.** States evolve: $|\psi_S(t)\rangle = U(t)|\psi(0)\rangle$. Operators are time-independent. This is the default.
- **Heisenberg picture.** States are fixed; operators evolve: $A_H(t) = U^\dagger(t)AU(t)$. The Heisenberg equation reads $\frac{dA_H}{dt} = \frac{i}{\hbar}[H, A_H]$.
- **Interaction picture.** For $H = H_0 + V(t)$, the fast part H_0 is absorbed into the operators and the slow part V drives the remaining evolution of the states. Used for perturbation theory.

Expectation values are identical across pictures: $\langle\psi_S(t)|A|\psi_S(t)\rangle = \langle\psi(0)|A_H(t)|\psi(0)\rangle$.

Ehrenfest's theorem

For any observable A,

$$\frac{d}{dt}\langle A\rangle_{\psi(t)} = \frac{i}{\hbar}\langle[H, A]\rangle_{\psi(t)} + \left\langle\frac{\partial A}{\partial t}\right\rangle.$$

The classical limit recovers Hamilton's equations: $\dot{q} = \partial H/\partial p$, $\dot{p} = -\partial H/\partial q$, with Poisson brackets replacing commutators by $\{\cdot,\cdot\} \leftrightarrow \frac{1}{i\hbar}[\cdot,\cdot]$.

Worked Example

Larmor precession of a qubit

A spin-$\frac{1}{2}$ particle in a static magnetic field along $\hat{z}$ has Hamiltonian

$$H = \frac{\hbar\omega}{2}Z, \qquad \omega = \gamma B,$$

where γ is the gyromagnetic ratio and B the field strength. The time evolution operator is

$$U(t) = e^{-iHt/\hbar} = e^{-i\omega tZ/2} = \cos(\omega t/2)I - i\sin(\omega t/2)Z.$$

Evolution of $|+\rangle$

Initial state: $|\psi(0)\rangle = |+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$.

$$|\psi(t)\rangle = U(t)|+\rangle = \tfrac{1}{\sqrt{2}}\left(e^{-i\omega t/2}|0\rangle + e^{+i\omega t/2}|1\rangle\right).$$

Up to an overall phase, this is

$$|\psi(t)\rangle \simeq \tfrac{1}{\sqrt{2}}\left(|0\rangle + e^{i\omega t}|1\rangle\right) = \cos\left(\tfrac{\omega t}{2}\right)|+\rangle - i\sin\left(\tfrac{\omega t}{2}\right)|-\rangle.$$

Expectation values

Track $\langle X\rangle, \langle Y\rangle, \langle Z\rangle$:

$$\langle X(t)\rangle = \cos(\omega t), \qquad \langle Y(t)\rangle = -\sin(\omega t), \qquad \langle Z(t)\rangle = 0.$$

The Bloch vector $\vec{r}(t) = (\cos\omega t, -\sin\omega t, 0)$ precesses clockwise around the z-axis with angular frequency ω. This is Larmor precession — one of the most directly testable consequences of the Schrödinger equation and the experimental basis of NMR and MRI.

Energy measurement

If instead we measure the energy $H = (\hbar\omega/2)Z$ on $|\psi(t)\rangle$, the outcomes are $\pm\hbar\omega/2$ with probabilities $1/2, 1/2$ — constant in time, because $[H, H] = 0$ makes energy a conserved quantity. Expectation value $\langle H\rangle = 0$ throughout the precession.

Cross-Links

- **Linear Algebra:** Unitary matrices, matrix exponentials, and the operator-valued functional calculus.
- **VQA:** Parameterized circuits are products of unitary gates $U_k(\theta_k) = e^{-iG_k\theta_k}$; gradients are computed via the parameter-shift rule that exploits the unitary structure.
- **Quantum Information:** Quantum gates are unitaries; the universal gate set is a generating set for $U(2^n)$.
- **Quantum Thermodynamics:** Unitary evolution is reversible and conserves von Neumann entropy; the second law arises only when part of the system is coarse-grained away (Module 8).
- **Systems Thinking:** Unitary evolution is the canonical example of a deterministic, reversible, information-preserving dynamical flow.
- **Module 10 (Foundations):** The universal unitarity of closed-system quantum mechanics is in tension with the non-unitary projection postulate — the formal statement of the measurement problem.

Structural Compression

Invariant: Probability conservation, realized as inner-product preservation.

Mechanism: $U^\dagger U = I$, generated via Stone's theorem by a self-adjoint Hamiltonian.

Cross-System Echo: Symplectic flow in classical Hamiltonian mechanics preserves phase-space volume (Liouville's theorem). Unitary flow in quantum mechanics preserves the inner product. Both are the "time-translation symmetry" of their respective state spaces, and both identify the Hamiltonian as the generator.

Exercises

1. Verify that $U(t) = e^{-iHt/\hbar}$ is unitary for any Hermitian H. (Use $(e^{-iHt/\hbar})^\dagger = e^{+iHt/\hbar}$ and commutativity of H with itself.)
2. Derive the Heisenberg equation of motion $dA_H/dt = (i/\hbar)[H, A_H]$ from the definition $A_H(t) = U^\dagger(t)AU(t)$.
3. Prove Ehrenfest's theorem in the Schrödinger picture by differentiating $\langle\psi(t)|A|\psi(t)\rangle$ directly.
4. For $H = (\hbar\omega/2)X$, compute $U(t)$ and apply it to the initial state $|0\rangle$. Sketch the trajectory of the Bloch vector on the sphere.
5. For a two-level system with Hamiltonian $H = \omega_1 X + \omega_2 Z$, find the eigenvalues and eigenvectors of H. Write $U(t)$ in closed form.
6. Show that energy expectation values are constant in time under unitary evolution with a time-independent Hamiltonian. What is the corresponding statement when $H = H(t)$?
7. Explain, structurally, why the projection postulate (Node 2.3) cannot be unitary, and why this discontinuity is the precise location of the measurement problem.

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Concepts: unitary-evolution, dynamical-systems, linear-operators
Prerequisites: 2.1, 2.2, 1.5
Enables: 4.1, 8.1

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