Postulates of QM (C-T III)

① States are normalized kets $|\psi\rangle$, $\|\psi\| = \sqrt{\langle\psi|\psi\rangle} = 1$

Phase doesn't matter

② Measurable quantities are Hermitian operators $\hat{A}^\dagger = \hat{A}$

(But an act of measurement does <u>not</u> correspond to $\hat{A}|\psi\rangle$!)

③ Outcomes of a measurement of $\hat{A}$ are eigenvalues $\{a_j\}_j$ of $\hat{A}$. Upon measuring $\hat{A}$, the jth outcome occurs with probability

$$\boxed{\Pr(a_j) = \langle\psi|\hat{P}_j|\psi\rangle = \sum_\alpha |\langle a_{j\alpha}|\psi\rangle|^2} \quad \text{(Born rule)}$$

Projection operator $\hat{A} = \sum_j a_j \hat{P}_j = \sum_{j\alpha} a_j |a_{j\alpha}\rangle\langle a_{j\alpha}|$

In other words, $\Pr(a_j) = \sum_\alpha |c_{j\alpha}|^2$ where the $c_{j\alpha}$'s are the expansion coefficients of $|\psi\rangle$ in the A-representation

$$|\psi\rangle = \sum_{j\alpha} c_{j\alpha} |a_{j\alpha}\rangle$$

The state after the measurement is $\boxed{\dfrac{\hat{P}_j|\psi\rangle}{\sqrt{\langle\psi|\hat{P}_j|\psi\rangle}}}$ (Projection postulate)

In non-degenerate cases, Postulate ③ reduces to $\Pr(a_j) = |\langle a_j|\psi\rangle|^2$ and the state collapses to the eigenvector $|a_j\rangle$.

Schrödinger–Robertson inequality

The variance of a random variable A is $\langle (A-\langle A\rangle)^2\rangle = \langle A^2\rangle - \langle A\rangle^2$.
For the quantum case, define the deviation operator

$$\hat{A}_\Delta \equiv \hat{A} - \langle \hat{A}\rangle .$$

Note that $\langle \hat{A}\rangle = \langle \psi|\hat{A}|\psi\rangle$ depends on the choice of state $|\psi\rangle$.

Properties ① $\langle \hat{A}_\Delta\rangle = 0$ ② $[\hat{A}_\Delta, \hat{B}_\Delta] = [\hat{A}, \hat{B}]$

Before stating the inequality and the proof, let us define one more thing: the (symmetrized) covariance $\Gamma_{ab} = \frac{1}{2}\langle \hat{A}_\Delta\hat{B}_\Delta + \hat{B}_\Delta\hat{A}_\Delta\rangle$.

$$\boxed{\Delta A \Delta B \geq \sqrt{|\Gamma_{ab}|^2 + \frac{1}{4}|\langle[\hat{A},\hat{B}]\rangle|^2} \geq \frac{1}{2}|\langle[\hat{A},\hat{B}]\rangle|}$$

- $$\Delta A \Delta B = \sqrt{(\langle\psi|\hat{A}_\Delta)(\hat{A}_\Delta|\psi\rangle)(\langle\psi|\hat{B}_\Delta)(\hat{B}_\Delta|\psi\rangle)}$$

$$\geq |\langle\psi|\hat{A}_\Delta\hat{B}_\Delta|\psi\rangle| \qquad \text{Cauchy-Schwarz}$$

$$= \left|\langle\psi| \frac{\hat{A}_\Delta\hat{B}_\Delta + \hat{B}_\Delta\hat{A}_\Delta + \hat{A}_\Delta\hat{B}_\Delta - \hat{B}_\Delta\hat{A}_\Delta}{2} |\psi\rangle\right|$$

$$= \left|\Gamma_{ab} + \frac{1}{2}\langle[\hat{A}_\Delta, \hat{B}_\Delta]\rangle\right|$$

$$= \left|\underbrace{\Gamma_{ab}}_{\text{Real part}} + \frac{1}{2}\underbrace{\langle[\hat{A},\hat{B}]\rangle}_{\text{Imaginary part}}\right| \qquad \text{Property ①}$$

$$= \sqrt{|\Gamma_{ab}|^2 + \frac{1}{4}|\langle[\hat{A},\hat{B}]\rangle|^2} \geq \frac{1}{2}|\langle[\hat{A},\hat{B}]\rangle| \qquad \square$$

Wigner's theorem states that the only maps $\hat{U}$ (not necessary linear a priori) that preserve the inner product are unitary and antiunitary ones.

$$\hat{U}^{\dagger} = \hat{U}^{-1}$$

Linear ↙ ↘ Antilinear

$$\hat{U}(a|\psi\rangle + b|\varphi\rangle) = a\hat{U}|\psi\rangle + b\hat{U}|\varphi\rangle$$

$$\hat{V}(a|\psi\rangle + b|\varphi\rangle) = a^*\hat{U}|\psi\rangle + b^*\hat{U}|\varphi\rangle$$

(Complex conjugation is basis-dependent!)

$$\langle \hat{U}\phi | \hat{U}\psi\rangle = \langle \phi | \hat{U}^{\dagger}\hat{U}|\psi\rangle = \langle \phi|\psi\rangle$$

But antilinear maps are not closed under multiplication.

$$\hat{V}_1\hat{V}_2(a|\psi\rangle + b|\varphi\rangle) = \hat{V}_1(a^*\hat{V}_2|\psi\rangle + b^*\hat{V}_2|\varphi\rangle)$$

Linear

$$= a\hat{V}_1\hat{V}_2|\psi\rangle + b\hat{V}_1\hat{V}_2|\varphi\rangle$$

So only linear, unitary maps can be the continuous-time evolution operators $\hat{U}(t_2,t_1)\hat{U}(t_1,t_0) = \hat{U}(t_2,t_0)$

Suppose that the effect of $\frac{d}{dt}$ on a state vector is a linear operator, which we denote by $\hat{G}$.

$$\frac{d}{dt}\langle\psi(t)|\psi(t)\rangle = \left(\frac{d}{dt}\langle\psi(t)|\right)|\psi(t)\rangle + \langle\psi(t)|\frac{d}{dt}|\psi(t)\rangle$$

$$= \langle\psi(t)|\left(\hat{G}^{\dagger} + \hat{G}\right)|\psi(t)\rangle$$

For the LHS to be 0, $\hat{G}$ must be anti-Hermitian.

Equivalently, $\hat{G}$ is i times a Hermitian operator.

$$\frac{d}{dt}|\psi(t)\rangle = \hat{G}(t)|\psi(t)\rangle$$

$$\left[\frac{d}{dt}\hat{U}(t,0)\right]|\psi(0)\rangle = \hat{G}(t)\,\hat{U}(t,0)|\psi(0)\rangle$$

Since this equation is true for any initial state $|\psi(0)\rangle$, it can be considered to be an operator equation,

$$\frac{d\hat{U}(t,0)}{dt} = \hat{G}(t)\,\hat{U}(t),$$

which for time-independent $\hat{G}$, has the solution

$$\hat{U}(t,0) = e^{\hat{G}t}.$$

Classically, such $\hat{G}$ would be proportional to the generator of time translation, that is, the Hamiltonian H. Thus, for dimensional reason, we choose $\hat{G} = \frac{1}{i\hbar}\hat{H} \leftarrow$ Hamiltonian operator

TDSE

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle \longrightarrow \boxed{i\hbar \frac{d}{dt}\hat{U}(t,t_0) = \hat{H}(t)\hat{U}(t,t_0)}$$

Operator version of the TDSE

Initial condition

$$\hat{U}(t_0,t_0) = \hat{\mathbb{1}}$$

Group property $\hat{U}(t_2,t_0) = \hat{U}(t_2,t_1)\hat{U}(t_1,t_0)$

$$\hat{U}^{-1}(t,t_0) = \hat{U}(t_0,t)$$

$$\hat{U}(t_0+dt,t_0) = \underbrace{\hat{U}(t_0,t_0)}_{\hat{\mathbb{1}}} + dt\,\underbrace{\frac{d\hat{U}}{dt}(t,t_0)\Big|_{t=t_0}}_{-\frac{i}{\hbar}\hat{H}(t_0)\hat{\mathbb{1}}} + \mathcal{O}(dt^2)$$

zeroth order :

$$= \hat{\mathbb{1}} - \frac{i}{\hbar}\hat{H}(t_0)\,dt + \mathcal{O}(dt^2) \quad *$$

Strategy: Divide time into steps with size $\epsilon = \frac{\Delta t}{N}$, $\Delta t = t - t_0$

Group property $\hat{U}(t,t_0) = \prod_{n=1}^{N} \hat{U}(t_0+n\epsilon,\, t_0+(n-1)\epsilon)$ ← Watch out for the ordering!

Case I: $\hat{H}$ is independent of time

Take $\epsilon \to 0$ and we the result $*$ for infinitesimal dt

$$\hat{U}(t,t_0) = \left(\mathbb{1} - \frac{i}{\hbar}\hat{H}\frac{\Delta t}{N}\right)^N = e^{-i\hat{H}(t-t_0)/\hbar}$$

Case II : $[\hat{H}(t_n), \hat{H}(t_m)] = 0$

$$\hat{U}(t,t_0) = \prod_{n=1}^{N} \left\{ \hat{\mathbb{1}} - \frac{i\epsilon}{\hbar}\hat{H}[t-(n-1)\epsilon] \right\}$$

As $\epsilon \to 0$ or equivalently $N \to \infty$,

$$t_0 + (N-1)\epsilon = t_0 + \underbrace{(N-1)}_{N}\Delta t \to t$$

The $\hat{H}(t_n)$'s commute at different times $\Rightarrow$ Can combine the exponentials

$$\hat{U}(t,t_0) = \lim_{\epsilon \to 0} \exp\left\{ \frac{-i\epsilon}{\hbar} \sum_{n=0}^{N-1} \hat{H}[t-(n-1)\epsilon] \right\}$$

$$\lim_{N\to\infty} \sum_{k=0}^{N-1} \frac{\Delta t}{N} H(t_0 + k\epsilon) = \int_{t_0}^{t} dt\, \hat{H}(t)$$

$$\boxed{\hat{U}(t,t_0) = \exp\left[\frac{-i}{\hbar}\int_{t_0}^{t} H(t)\,dt \right] \quad \text{if } [H(t_n), H(t_m)] = 0}$$

Case III : General

With the initial condition $\hat{U}(t_0,t_0) = \hat{\mathbb{1}}$, we can write generally,

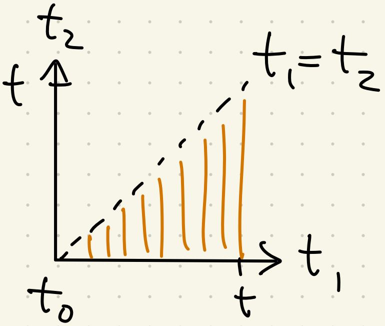
$$\hat{U}(t,t_0) = \hat{\mathbb{1}} - \frac{i}{\hbar}\int_{t_0}^{t} dt'\, \hat{H}(t')\hat{U}(t',t_0),$$

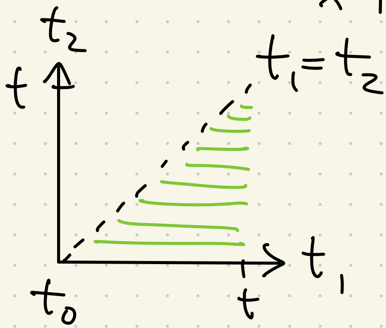
and iteratively solve for $\hat{U}$:

$$\hat{U}(t,t_0) = \hat{\mathbb{1}} - \frac{i}{\hbar}\int_{t_0}^{t} dt'\, \hat{H}(t')\left[\hat{\mathbb{1}} - \frac{i}{\hbar}\int_{t_0}^{t'} dt''\, \hat{H}(t'')\hat{U}(t'',t_0) \right]$$

Up to the Nth order,

$$\hat{U}_N(t,t_0) = \hat{\mathbb{1}} + \sum_{n=1}^{N} \left(\frac{-i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n$$
$$\times\ \hat{H}(t_1)\hat{H}(t_2)\cdots\hat{H}(t_n)$$





$t_0 < t_1 < t \xrightarrow{\text{Change order of integration}} t_2 < t_1 < t \longleftarrow$ Integrate first (on the right)

$t_0 < t_2 < t_1 \qquad\qquad t_0 < t_2 < t \longleftarrow$ — " — second

$$\hat{U}_2(t,t_0) = \hat{\mathbb{1}} + \sum \left(\frac{-i}{\hbar}\right)^n \boxed{\int_{t_0}^{t} dt_2 \int_{t_2}^{t} dt_1\, \hat{H}(t_1)\hat{H}(t_2)} \quad \star$$

We will switch to integrating over the whole square $[t_0,t] \times [t_0,t]$ and then halving the area.

Define the time-ordered product,

$$\mathcal{T}\left[\hat{H}(t_1)\hat{H}(t_2)\cdots\hat{H}(t_n)\right] = \hat{H}(t_{j_1})\hat{H}(t_{j_2})\cdots\hat{H}(t_{j_n})$$

$\longrightarrow$ Past

where $t_{j_1} > t_{j_2} > \cdots > t_{j_n}$

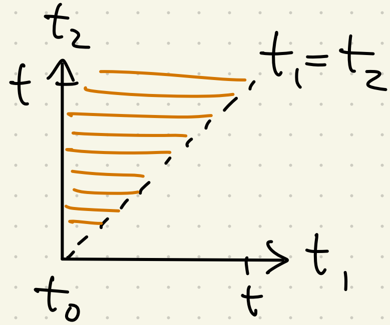
$$\star = \mathcal{T}\left[\hat{H}(t_1)\hat{H}(t_2)\right]$$

If we relabel the integral ☆, swapping t_1 and t_2, we obtain

$$\int_{t_0}^{t} dt_1 \int_{t_1}^{t} dt_2\, \hat{H}(t_2)\hat{H}(t_1) = \int_{t_0}^{t} dt_1 \int_{t_1}^{t} dt_2\, \mathcal{T}\left[\hat{H}(t_1)\hat{H}(t_2)\right]$$

$t_1 < t_2$

∴ We can change all the integral limits to $[t_0, t]$



$$\frac{1}{2}\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2\, \mathcal{T}\left[\hat{H}(t_1)\hat{H}(t_2)\right]$$

General order N

$$\frac{1}{N!}\int_{t_0}^{t_1} dt_1 \int_{t_0}^{t_2} dt_2 \cdots \int_{t_0}^{t} dt_N\, \mathcal{T}\left[\prod \hat{H}(t_n)\right]$$

$\hat{U}(t, t_0)$

$$= \hat{\mathbb{1}} + \sum_{N=1}^{\infty} \frac{1}{N!}\left(\frac{-i}{\hbar}\right)^N \int_{t_0}^{t_1} dt_1 \int_{t_0}^{t_2} dt_2 \cdots \int_{t_0}^{t} dt_N\, \mathcal{T}\left[\prod \hat{H}(t_n)\right]$$

$$\equiv \mathcal{T}\left\{ e^{-i/\hbar \int_{t_0}^{t} dt\, \hat{H}(t)} \right\}$$ (Dyson series)

Now that we know the form that time evolutions of quantum states must take, we can figure out the time evolution of expectation values (and therefore any statistical moment of any observable)

$$\frac{d}{dt}\langle \hat{A} \rangle = \left(\frac{d}{dt}\langle \psi(t)|\right) \hat{A} |\psi(t)\rangle + \langle \psi(t)| \hat{A} \frac{d}{dt}|\psi(t)\rangle$$

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

$$= \frac{1}{i\hbar}\langle [\hat{A}, \hat{H}] \rangle$$

If $\hat{A}$ itself is time-dependent (in the Schrödinger picture)

$$\boxed{\frac{d}{dt}\langle \hat{A} \rangle = \frac{1}{i\hbar}\langle [\hat{A}, \hat{H}] \rangle + \frac{\partial \langle \hat{A} \rangle}{\partial t}}$$

Dirac quantization: Poisson bracket $\{\ ,\ \} \rightarrow \frac{1}{i\hbar}[\ ,\ ]$

Classical $\qquad \dot{A} = \{A, H\}$

Ehrenfest theorem: If $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$, then

$$\boxed{\frac{d\langle \hat{x} \rangle}{dt} = \frac{\langle \hat{p} \rangle}{m} \qquad \frac{d\langle \hat{p} \rangle}{dt} = -\langle \vec{\nabla} V(\hat{x}) \rangle}$$

If the potential is linear or quadratic in $\hat{x}$
$\Rightarrow$ The quantum expectation values follow exactly the classical trajectories

CEx $\quad V(x) = -kx^4 \quad$ But $-\vec{\nabla} V(\langle \hat{x} \rangle)$

$$\langle -\vec{\nabla} V(x) \rangle = 4k\langle x^3 \rangle \neq 4k\langle x \rangle^3$$

Symmetries and Conservation Laws

... in classical mechanics

(Noether) In systems that can be described by a Lagrangian or a Hamiltonian, conservation laws correspond to symmetries and vice versa

Symmetry under translation in a generalized coordinate q

$$q_j \mapsto q_j + \delta q_j \Leftrightarrow \frac{\partial L}{\partial q_j} = 0$$

Canonical momentum $p_j = \frac{\partial L}{\partial \dot{q}_j}$ conserved by Lagrange eq.

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}\right) - \frac{\partial L}{\partial q_j} = 0.$$

Hamiltonian: $\frac{dp_j}{dt} = 0 \Leftrightarrow \frac{\partial H}{\partial q_j} = 0$

Constants of motion in QM

If $[\hat{A}, \hat{H}] = 0$ then $\frac{d}{dt}\langle \hat{A} \rangle = 0$ in any state we are taking the expectation value w.r.t.

Not to be confused with stationary states, whose expectation value of any operator remains constant in time.

When we calculate expectation values (or any statistical quantities related to measurements) of the form $\langle \hat{A} \rangle$, we have the choice to attach the time dependence to the state,

$$\underbrace{\left[\langle \psi(0)| \hat{U}^\dagger(t,0)\right]}_{\langle \psi(t)|} \hat{A} \underbrace{\left[\hat{U}(t,0)|\psi(0)\rangle\right]}_{|\psi(t)\rangle},$$ (Schrödinger picture)

or the operator,

$$\langle \psi(0)| \underbrace{\left[\hat{U}^\dagger(t,0)\hat{A}\hat{U}(t,0)\right]}_{\hat{A}(t)} |\psi(0)\rangle$$ (Heisenberg picture)

When we want to be very clear, we would put the S or H subscripts under the state vector/operator

$$|\psi_H\rangle = \hat{U}(t,0)|\psi_S(t)\rangle = |\psi_S(0)\rangle$$

$$A_H(t) = \hat{U}^\dagger(t,0)\hat{A}_S\hat{U}(t,0)$$

$$i\hbar \frac{dA_H}{dt} = i\hbar\left(\frac{d\hat{U}^\dagger}{dt}\hat{A}_S\hat{U} + \hat{U}^\dagger\hat{A}_S\frac{d\hat{U}}{dt}\right)$$

$$= i\hbar\left(-\frac{1}{i\hbar}\hat{U}^\dagger\hat{H}_S\hat{A}_S\hat{U} + \frac{1}{i\hbar}\hat{U}^\dagger\hat{A}_S H_S\hat{U}\right)$$

$$= \hat{U}^\dagger[\hat{A}_S,\hat{H}_S]\hat{U} = [\hat{A}_H,\hat{H}_H]$$

$$\boxed{\frac{d\hat{A}_H}{dt} = \frac{1}{i\hbar}[\hat{A},\hat{H}] + \frac{\partial\hat{A}}{\partial t}}$$

The time evolution op. $\hat{U}$ itself is not in any picture; it defines the picture.

$$H_H = \hat{U}^\dagger H_S\hat{U}$$
$$= \hat{U}^\dagger\hat{U}H_S$$
$$= H_S$$