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$\boxed{\text{Time evolution in QM}}$ (cf. Sakurai 2.1)

☆ Time evolution operator

pure state at $t = t_0$ $\quad |\psi(t_0)\rangle$

at later time t $\quad |\psi(t)\rangle$

They should be related by a linear operator $U(t, t_0)$.

$$|\psi(t)\rangle = U(t, t_0)\, |\psi(t_0)\rangle$$

$U(t, t_0)$ has following 3 properties.

① $U(t_0, t_0) = \mathbb{1}$

② $U(t, t_0)^{-1} = U(t, t_0)^{\dagger}$ — unitary to preserve probabilities.

If NR, no particle is created or destroyed. $1 = \text{Prob}(\text{finding a particle in } V)$
$= \text{Prob}(\text{finding a particle in } V \text{ at a later time})$

③ $U(t_2, t_1)\, U(t_1, t_0) = U(t_2, t_0)$

☆ like translation, U also forms a unitary group.

☆ Hamiltonian

consider $t \to t + \epsilon \qquad \epsilon \ll 1$

$$U(t+\epsilon, t) = \mathbb{1} - i\epsilon\,\Omega(t) + \cdots$$

$$\Omega(t) \equiv i \frac{\partial}{\partial t'} U(t', t)\Big|_{t'=t}$$

this "i" makes Ω Hermitian, by $UU^{\dagger} = \mathbb{1} - i\epsilon(\Omega - \Omega^{\dagger}) \cdots$

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* $\Omega(t)$ is regarded as the generator of time translation in QM. (operator)

It advances a state from time t to $t+\epsilon$,
and many infinitesimal advances results in finite Δt evolution.

* $\Omega(t)$ is Hermitian, $\leadsto$ some physical observables?

* From the CM poisson bracket

$$\frac{d}{dt}A = \frac{\partial A}{\partial q}\frac{dq}{dt} + \frac{\partial A}{\partial p}\frac{dp}{dt} + \frac{\partial A}{\partial t}^{0}$$

if no explicit time dependence.

$$= \{A, H\}_{\text{poisson}},$$

$$\Rightarrow A(t+\epsilon) \simeq \cancel{\mathbb{1}}A \pm \epsilon\{\cancel{H}, A\}_p + O(\epsilon^2)$$

$$A(t+\Delta t) = \lim_{N\to\infty}\left(\mathbb{1} - \frac{\Delta t}{N}\{H, \ \}\right)^N A(t)$$

$$= \exp^{-:\Delta t H:} A(t)$$

* We guess that $\Omega(t)$ is closely related to the operator that we should define as the QM version Hamiltonian. $\hat{H}$.

* Dimensionality

$$[\Omega] = \left[\frac{\partial}{\partial t}\right] = \frac{1}{[T]}$$

$$[\text{energy}] = \frac{ML^2}{T^2}$$

$$\frac{ML^2}{T}$$

we need a converting factor with this dimensionality

What is it? Not surprisingly $\hbar$ again!!

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☆ So, $\hat{H}(t) = \hbar\Omega(t)$

with this,

$$U(t+\epsilon, t) = \mathbb{1} - \frac{i}{\hbar}\epsilon \hat{H}(t) + \cdots$$

* In CM, H could be time-dependent, e.g. charged particle in an EM wave, ...

☆ Similar question arise when we write

$$\boxed{\hat{P} = \hbar\hat{k}} \quad \& \quad \boxed{\hat{H}(t) = \hbar\Omega(t)}$$

How do we know these two operators share the same $\hbar$?!

* 1900's Einstein ⇒ light (photon) $E = \hbar_1\omega$, $\vec{P} = \hbar_2\vec{k}$
by Maxwell's theory $\omega = c|\vec{k}|$ ⇒ $\hbar_1 = \hbar_2$

* tested in Compton scattering (1923)

* Another ~~way~~ reason that these 2 $\hbar$'s must be the same is from special relativity.

$P^\mu = (E, \vec{P})$. They are equally footing, diff in diff frame
⇒ only one $\hbar$

☆ <u>Differential Equation for Time Evolution</u>

$$\frac{\partial U(t,t_0)}{\partial t} = \lim_{\epsilon\to 0} \frac{U(t+\epsilon,t_0) - U(t,t_0)}{\epsilon}$$

$$= \lim_{\epsilon\to 0} \frac{(U(t+\epsilon,t) - \mathbb{1})}{\epsilon} U(t,t_0) = -\frac{i}{\hbar}\cdot \hat{H}(t) U(t,t_0)$$

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$$\Rightarrow \boxed{i\hbar \frac{\partial U(t,t_0)}{\partial t} = \hat{H}(t)\, U(t,t_0)}$$

Giving the initial conditions, the solution is unique.

So,

$$i\hbar \frac{\partial}{\partial t}|\Psi(t)\rangle = i\hbar\frac{\partial}{\partial t}\left(U(t,t_0)\,|\Psi(t_0)\rangle \right)$$

$$= \left(i\hbar \frac{\partial}{\partial t} U(t,t_0) \right)|\Psi(t_0)\rangle$$

$$= \hat{H}(t)\, U(t,t_0)\,|\Psi(t_0)\rangle = \hat{H}(t)\,|\Psi(t_0)\rangle$$

$$\Rightarrow \boxed{i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}(t)\,|\Psi(t)\rangle}$$

This is our old friend, the Schrödinger Eq.

- If $\hat{H}$ is independent of time, $\frac{\partial \hat{H}}{\partial t} = 0$.

$$\Rightarrow U(t,t_0) = \exp\left(-\frac{i\hat{H}}{\hbar}(t-t_0)\right)$$

By choosing $t_0 = 0$,
$$U(t) = \exp\left(-\frac{i\hat{H}t}{\hbar}\right)$$

- In general, if $\hat{H}$ is time-dependent, no simple solution for $U(t,t_0)$

& $\hat{H}(t)$ does NOT commute with $U(t,t_0)$.

In general $[\hat{H}(t), \hat{H}(t')] \neq 0$

2. The Poisson bracket helped Dirac to establish the formal structure of QM on the CM.

$$\underbrace{\frac{1}{i\hbar}[A,B]}_{QM} \longrightarrow \{A,B\}_{\text{poisson}}$$

For example spin has no CM counterpart

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Heisenberg picture

diff by a time dependent unitary transformation

Up to now, we have used the Schrödinger picture :
⇒ kets evolve according to the Schrödinger Eq.
& operators do not evolve !

But, sometimes, the so called Heisenberg picture is useful.
⇒ kets do not evolve
but operators evolve according to the Heisenberg Eq.

Denote $|\psi_S(t)\rangle = |\psi(t)\rangle$: time-dependent state vector in the Schrödinger picture.

$$|\psi_H\rangle = U(t,t_0)^\dagger |\psi_S(t)\rangle \quad : \text{state vector in the Heisenberg picture}$$
$$= |\psi_S(t_0)\rangle$$

If the operator $A_S(t) = A(t)$ ← allow an explicite time dependence

then in the Heisenberg picture

$$A_H(t) = \underbrace{U(t,t_0)^\dagger A_S(t)\, U(t,t_0)}_{\text{implicit time dependence}}$$

no evolution for $|\psi_H\rangle$

$$i\hbar \frac{dA_H}{dt} = -U(t,t_0)^\dagger \hat{H}_S \underset{UU^\dagger = 1}{\vee} A_S U(t,t_0) + U^\dagger A_S \underset{UU^\dagger = \mathbb{I}}{\wedge} \hat{H}_S \underset{UU^\dagger}{\vee} U$$
$$+ i\hbar\, U^\dagger \frac{\partial A_S}{\partial t} U$$

$$\left(\because\ i\hbar \frac{\partial U}{\partial t}(t,t_0) = \hat{H}_S(t)\, U(t,t_0) \right.$$
$$\left. -i\hbar \frac{\partial}{\partial t} U(t,t_0)^\dagger = U(t,t_0)^\dagger \hat{H}_S(t) \right)$$

$$= -(U^\dagger \hat{H}_S U)(U^\dagger A_S U) + (U^\dagger A_S U)(U^\dagger \hat{H}_S U) + i\hbar\, U^\dagger \frac{\partial A_S}{\partial t} U = \boxed{[A_H, \hat{H}_H] + i\hbar \frac{\partial A_H}{\partial t}}$$

This is to compare with the CM equation !

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* All physical observables can be expressed in terms of matrix elements of the form of $\langle \phi | A | \psi \rangle$.
These are the <u>same</u> in both the Heisenberg & Schrödinger picture

$$\langle \phi_s(t) | A_s | \psi_s(t) \rangle = \langle \phi_H | A_H(t) | \psi_H \rangle$$

- If you know one solution in one picture, it's easy to ~~get~~ transfer it to another picture.

$\Rightarrow$ $\boxed{\text{The two pictures are physically equivalent.}}$

* For some problem, e.g. S.H.O. the Heisenberg picture is easier to use.

* If, in the special case, $\hat{H}_s$ is independent of time, the operator $U(t, t_0)$ is a function of $\hat{H}_s$ and thus $[U, \hat{H}_s] = 0$. then $\hat{H}_H = U^+ \hat{H}_s U = \hat{H}_s$

* Another useful picture : interaction picture
is usually adopted in dealing with time-dependent perturbation calculation.

$$\hat{H} = \underbrace{\hat{H}_0}_{\substack{\downarrow \\ H_H \\ \text{free}}} + \underbrace{\hat{H}_1}_{\substack{\downarrow \\ H_s \\ \text{perturbation}}}$$

the time evolution of kets due to H_0 is absorbed into $\hat{H}_0 \rightarrow \hat{H}_H$ and leave the time evolution due to $\hat{H}_1$ to the kets

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Time evolution of the density operator

Here, we work in the Schrödinger picture.
and consider the density operator for a discrete ensemble of pure state $|\psi_i\rangle$ with statistical weight f_i.

$\Rightarrow \hat{\rho}$ is a function of time, because $|\psi_i\rangle$ is.

At $t = t_0$

$$\hat{\rho}(t_0) = \sum_i f_i |\psi_i(t_0)\rangle\langle\psi_i(t_0)|$$

and at the final time it is

$$\hat{\rho}(t) = \sum_i f_i |\psi_i(t)\rangle\langle\psi_i(t)| = U(t,t_0) \sum_i f_i |\psi_i(t_0)\rangle\langle\psi_i(t_0)| U^{\dagger}(t,t_0)$$
$$= U(t,t_0)\hat{\rho}(t_0)U(t,t_0)^{\dagger}$$

Differentiating it with respect to time

$$i\hbar\frac{\partial}{\partial t}\hat{\rho}(t) = \hat{H}U\hat{\rho}(t_0)U^{\dagger} - U\hat{\rho}(t_0)U^{\dagger}\hat{H} = [\hat{H},\hat{\rho}]$$

$$\left(\frac{\partial U}{\partial t} = \frac{-i}{\hbar}\hat{H}U, \quad \frac{\partial U^{\dagger}}{\partial t} = \frac{+i}{\hbar}U^{\dagger}\hat{H}\right)$$

$$\boxed{i\hbar\frac{\partial}{\partial t}\hat{\rho} = [\hat{H},\hat{\rho}]}$$

$\Rightarrow$ This replaces the Schrödinger eq when we are facing the mixed state.

or $\dfrac{\partial\hat{\rho}}{\partial t} - \dfrac{i}{\hbar}[\hat{\rho},\hat{H}] = 0$

looks like the classical Liouville eq.

also looks like the Heisenberg eq, but totally different.

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