Three pictures of quantum dynamics

(1) The Schrödinger picture:

\[ i\hbar \frac{d}{dt} |\psi_s(t)\rangle = \hat{H}_S(t) |\psi_s(t)\rangle \]

States evolve with time; for time-independent systems, \( \hat{H}_S \) is independent of time.

We can solve this Schrödinger equation formally as follows:

\[ |\psi_s(t)\rangle = \hat{U}_S(t, t_0) |\psi_s(t_0)\rangle \]

where the time evolution operator \( \hat{U}_S \) satisfies the EOM

\[ it\hbar \frac{d\hat{U}_S(t, t_0)}{dt} = \hat{H}_S(t) \hat{U}_S(t, t_0) \]

\[ \Rightarrow \hat{U}_S(t, t_0) = \frac{1}{N!} \prod_{n=0}^{N-1} \left( e^{-\frac{i}{\hbar} \int_{t_n}^{t_{n+1}} \hat{H}_S(t') dt'} \right) \]

with \( \Delta = \frac{t - t_0}{N} \)

We remind ourselves of the following properties:

\[ \hat{U}^+ \hat{U} = \hat{I} = \hat{U}(t, t) \]

\[ \hat{U}(t_2, t_1) \hat{U}(t_3, t_1) = \hat{U}(t_3, t_1); \quad \hat{U}^+(t_2, t_1) = \hat{U}(t_1, t_2) \]
(2) The Heisenberg picture

The Heisenberg picture is obtained from the Schrödinger picture by a (time-dependent) unitary transformation

\[ |\Psi_H\rangle = \hat{U}_S(t,0) |\Psi_S(t)\rangle \quad \iff \quad \langle \Psi_H | = \langle \Psi_S(t) | \hat{U}_S^\dagger(t,0) \]

Since \[ |\Psi_S(t)\rangle = \hat{U}_S(t,0) |\Psi_S(0)\rangle \], we see that

\[ |\Psi_H\rangle = |\Psi_S(0)\rangle \]

independent of time.

This unitary transformation shifts all time evolution to the operators:

\[ \langle \Psi_S(t) | \hat{\hat{\Omega}}_S(t) |\Psi_S(t)\rangle = \langle \Psi_H(t) | \hat{\hat{\Omega}}_H(t) |\Psi_H(t)\rangle \]

\[ = \langle \Psi_S(t) | \hat{U}_S(t,0) \hat{\hat{\Omega}}_S(t) \hat{U}_S^\dagger(t,0) |\Psi_S(0)\rangle \]

\[ \rightarrow \hat{\hat{\Omega}}_H(t) = \hat{U}_S(t,0) \hat{\hat{\Omega}}_S(t) \hat{U}_S^\dagger(t,0) \quad \text{for any observable} \]

Even if the observable is time-independent in the Schrödinger picture, it is represented by a time-dependent operator in the Heisenberg picture.

In the Heisenberg picture we have

\[ \frac{d}{dt} |\Psi_H\rangle = 0 \]

and
\[ i\hbar \frac{d\hat{\Omega}_H}{dt} = i\hbar \frac{d\hat{U}_s(0,t)\hat{\Omega}_s(t)\hat{U}_s(t,0)}{dt} + \hat{U}_s(0,t)i\hbar \frac{d\hat{\Omega}_s(t)}{dt} \hat{U}_s(t,0) \]

\[ = (-i\hbar \frac{d}{dt} \hat{U}_s(t,0))^+ \hat{\Omega}_s(t)\hat{U}_s(t,0) + \hat{U}_s(0,t)i\hbar \frac{d\hat{\Omega}_s(t)}{dt} \hat{U}_s(t,0) \]

\[ = -\hat{U}_s(0,t)\hat{H}_s(t)\hat{U}_s(t,0)\hat{U}_s(0,t)\hat{\Omega}_s(t)\hat{U}_s(t,0) \]

\[ + i\hbar \hat{U}_s(0,t)\frac{d\hat{\Omega}_s(t)}{dt} \hat{U}_s(t,0) \]

\[ + \hat{U}_s(0,t)\hat{\Omega}_s(t)\hat{U}_s(t,0)\hat{U}_s(0,t)\hat{H}_s(t)\hat{U}_s(t,0) \]

\[ = [\hat{\Omega}_H(t), \hat{H}_H(t)] + i\hbar \left( \frac{\partial \hat{\Omega}_H(t)}{\partial t} \right)_H \]

\[ \Rightarrow \quad i\hbar \frac{d\hat{\Omega}_H}{dt} = [\hat{\Omega}_H(t), \hat{H}_H(t)] + i\hbar \left( \frac{\partial \hat{\Omega}_H}{\partial t} \right)_H \]

**Heisenberg equation of motion.**

The overlap between Heisenberg picture state is time independent.
\[ \langle \Phi_H | \Psi_H \rangle = \text{independent of time} \]

This overlap matrix element represents the following overlap of Schrödinger picture states:

\[
\begin{align*}
\langle \Phi_H | \Psi_H \rangle &= \langle \Phi_s(t) | \hat{U}(t,0) \hat{U}_s(0,t) | \Psi_s(t) \rangle \\
&= \langle \Phi_s(t) | \Psi_s(t) \rangle \quad \text{(which is therefore also time independent)} \\
&= \langle \Phi_s(t) | \hat{U}_s(t,t_0) | \Psi_s(t_0) \rangle \\
&= \langle \Phi_s(\infty) | \hat{U}_s(\infty,-\infty) | \Psi_s(-\infty) \rangle
\end{align*}
\]

(3) The interaction picture

If we split \( \hat{H}(t) \) into an unperturbed ("non-interacting") part and an interaction term ("perturbation"),

\[ \hat{H}(t) = \hat{H}_0(t) + \hat{H}_I(t) = \hat{H}_0(t) + \hat{V}(t) \]

we can split the time evolution between the state and the operators such that the operators evolve with \( \hat{H}^0 \) and the state evolve only with the perturbation. This is called the interaction picture.
In most applications one splits $\hat{H}(t)$ such that in the S-picture $\hat{H}_S^0$ is independent of time and all time-dependence goes into $\hat{V}(t)$. But let us develop the interaction picture first for the general case.

We define a "non-interacting" time-evolution operator $\hat{U}_S^0(t,t_0)$ by

$$i\hbar \frac{d}{dt} \hat{U}_S^0(t,t_0) = \hat{H}_S^0(t) \hat{U}_S^0(t,t_0)$$

and the interaction picture state vectors through

$$|\psi_I(t)\rangle = (\hat{U}_S^0(t,t_0))^\dagger |\psi_S(t)\rangle$$

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

$$|\psi_I(0)\rangle = |\psi_S(0)\rangle$$

This is similar to the Heisenberg picture, except that we use only the non-interacting part of the Hamiltonian for our unitary transformation. If there are no interactions, $\hat{V} \equiv 0$, then the interaction picture states $|\psi_I(t)\rangle$ are time independent — interaction and Heisenberg picture agree in this case. Any time dependence of $|\psi_I(t)\rangle$ is thus entirely caused by $\hat{V}(t)$. 

76
in the interaction picture, the states evolve with \( \hat{V}(t) \) in time, while the time evolution of the observables is due to \( \hat{H}^0(t) \).

Let's check this:

\[
\frac{\text{i} \hbar}{\text{d}t} |\psi_I(t)\rangle = \frac{\text{i} \hbar}{\text{d}t} \left( \hat{U}^0_s(t,0) |\psi_s(t)\rangle \right)
\]

\[
= \left( -\frac{\text{i} \hbar}{\text{d}t} \hat{U}^0_s(t,0) \right)^* |\psi_s(t)\rangle + \hat{U}^0_s(0,t) \frac{\text{i} \hbar}{\text{d}t} |\psi_s(t)\rangle
\]

\[
= (-\hat{H}^0_s(t) \hat{U}^0_s(t,0))^* |\psi_s(t)\rangle + \hat{U}^0_s(0,t) \hat{H}_s(t) |\psi_s(t)\rangle
\]

\[
= \hat{U}^0_s(0,t) \left[ -\hat{H}^0_s(t) + \hat{H}_s(t) \right] |\psi_s(t)\rangle
\]

\[
= \hat{U}^0_s(0,t) \hat{V}_s(t) \hat{U}^0_s(t,0) \hat{U}^0_s(0,t) |\psi_s(t)\rangle
\]

\[
\hat{V}_I(t) = \text{interaction in interaction picture}
\]

\[
\Rightarrow \frac{\text{i} \hbar}{\text{d}t} |\psi_I(t)\rangle = \hat{V}_I(t) |\psi_I(t)\rangle
\]

\( \text{I-states evolve with } \hat{V}_I(t) \)

For the operators:

\[
\hat{S}_I(t) = \hat{U}^0_s(0,t) \hat{S}_s(t) \hat{U}^0_s(t,0)
\]

\[
\frac{\text{i} \hbar}{\text{d}t} \hat{S}_I(t) = \frac{\text{i} \hbar}{\text{d}t} \left( \hat{U}^0_s(0,t) \hat{S}_s(t) \hat{U}^0_s(t,0) \right)
\]

\[
= -\text{i} \hbar \hat{U}^0_s(0,t) \hat{H}^0_s(t) \hat{S}_s(t) \hat{U}^0_s(t,0)
\]

\[
+ \hat{U}^0_s(0,t) \frac{\text{i} \hbar}{\text{d}t} \hat{U}^0_s(t,0)
\]

\[
+ \hat{U}^0_s(0,t) \hat{S}_s(t) \hat{H}_s(t) \hat{U}^0_s(t,0)
\]
\[
= -\hat{U}_s^0(0,t) \hat{H}_s^0(t) \hat{U}_s^0(t,0) \hat{U}_s^0(0,t) \hat{\Omega}_s(t) \hat{U}_s^0(t,0)
+ \hat{U}_s^0(0,t) (i \hbar \frac{\partial}{\partial t}) \hat{U}_s^0(t,0)
+ \hat{U}_s^0(t) \hat{\Omega}_s(t) \hat{U}_s^0(t,0) \hat{U}_s^0(0,t) \hat{H}_s^0(t) \hat{U}_s^0(t,0)
\]

\[
\Rightarrow i \hbar \frac{d \hat{\Omega}_I(t)}{dt} = \left[ \hat{\Omega}_I(t), \hat{H}_I^0(t) \right] + i \hbar \left( \frac{\partial \hat{\Omega}_I(t)}{\partial t} \right)
\]

interaction picture observables evolve with $\hat{H}_I^0(t)$

Let us now define the propagator $\hat{U}_I$ in the interaction picture:

\[
|\psi_I(t)\rangle = \hat{U}_I(t,t_0) |\psi_I(t_0)\rangle
\]

Because of $i \hbar \frac{d}{dt} |\psi_I(t)\rangle = \hat{V}_I(t) |\psi_I(t)\rangle$, this propagator satisfies the E.O.M.

\[
\frac{i \hbar}{2} \frac{d}{dt} \hat{U}_I(t,t_0) = \hat{V}_I(t) \hat{U}_I(t,t_0)
\]

We can relate $\hat{U}_I$ to $\hat{U}_s$ and $\hat{U}_s^0$:

\[
|\psi_I(t)\rangle = \hat{U}_I(t,t_0) |\psi_I(t_0)\rangle
\]

\[
\hat{U}_s^0(0,t) |\psi_s(t)\rangle = \hat{U}_I(t,t_0) \hat{U}_s^0(0,t_0) |\psi_s(t_0)\rangle
\]
\[ \hat{U}_S(0,t) \hat{U}_S(t,t_0) | \psi_s(t_0) \rangle = \hat{U}_I(t,t_0) \hat{U}_S(t_0,0) | \psi_s(t_0) \rangle \]

\[ \implies \hat{U}_I(t,t_0) = \hat{U}_S(0,t) \hat{U}_S(t,t_0) \hat{U}_S(t_0,0) \]

I-propagator \hspace{2cm} S-propagator

(transforms like any other operator)

For \( t_0 = 0 \) (i.e. at the time when the 3 pictures coincide) this simplifies to

\[ \hat{U}_I(t,0) = \hat{U}_S(0,t) \hat{U}_S(t,0) \]

or

\[ \hat{U}_S(t,0) = \hat{U}_S(t,0) \hat{U}_I(t,0) \]

We chose to make the 3 pictures coincide at \( t = 0 \); we could, however, have chosen any other reference time \( t_{ref} \). We can change this simply a posteriori by replacing all time arguments "0" by "ref." For example:

\[ \hat{U}_I(t_1,t_2) = \hat{U}_S(t_{ref},t_1) \hat{U}_S(t_2,t_{ref}) \hat{U}_S(t_{ref},0) \]

Note: Shankar uses the notation \( t_0 \) for \( t_{ref} \).

His \( t_0 \) should not be confused with our \( t_0 \) which is a free time parameter unrelated to the reference time where the pictures coincide.
Perturbation theory in the interaction picture:

In the interaction picture, the states evolve only in response to the interaction:

\[ |\Psi_I(t)\rangle = \hat{U}_I(t, t_0) |\Psi_I(t_0)\rangle \]
\[ \dot{\psi} + \frac{i}{\hbar} |\Psi_I(t)\rangle = \hat{V}_I(t) |\Psi_I(t)\rangle \]
\[ \dot{\hat{U}}_I(t, t_0) = \hat{V}_I(t) \hat{U}_I(t, t_0) \]

We can solve the last equation formally by integrating both sides from \( t_0 \) to \( t \):

\[ \hat{U}_I(t, t_0) = \hat{I} - \frac{i}{\hbar} \int_{t_0}^{t} dt' \hat{V}_I(t') \hat{U}_I(t', t_0) \]

except that this is not really a solution but an integral equation for \( \hat{U}_I \). It is useful because it can be solved iteratively, with each iteration corresponding to the next higher order in the perturbative series:

**Zeroth order:** drop all terms containing \( \hat{V} \)

\[ \Rightarrow \hat{U}_I^{(0)}(t, t_0) = \hat{I} , \quad |\Psi_I^{(0)}(t)\rangle = |\Psi_I^{(0)}(t_0)\rangle \]

The interaction-picture state does not evolve.
First order  

Keep only linear terms in $\hat{V}$

\[ \Rightarrow \text{can set } \hat{U}_I(t, t_0) = \hat{U}_I^{(0)}(t, t_0) = 1 \]

on the r.h.s.

\[ \Rightarrow \hat{U}_I^{(1)}(t, t_0) = \mathbf{1} - \frac{i}{\hbar} \int_{t_0}^{t} dt' \hat{V}_I(t') \]

Let us use this to compute

\[ C_f(t) = \langle f_s | e^{i E_0^f(t-t_{ref})} \hat{U}_S(t, t_{ref}) | i_s^0 \rangle \]

i.e. the transition amplitude to the state $| f_s \rangle$ at time $t$ for a system that started (in the Schrödinger picture) in state $| i_s^0 \rangle$ at the reference time $t_{ref}$.

We assume here (as we had earlier) that $\hat{H}_S$ is time independent. Then $\hat{U}_S(t, t_{ref})$ is simply

\[ \hat{U}_S(t, t_{ref}) = e^{-\frac{i}{\hbar} \hat{H}_S(t-t_{ref})} \]

Using Eq. (x) on p. 79 for $0 \rightarrow t_{ref}$ we can rewrite $C_f(t)$ as

\[ C_f(t) = \langle f_s | \hat{U}_I^{(0)}(t, t_{ref}) \hat{U}_S(t, t_{ref}) | i_s^0 \rangle \]

\[ = \langle f_s | \hat{U}_I(t, t_{ref}) | i_s^0 \rangle \]

This holds with the exact interaction picture propagator $\hat{U}_I(t, t_{ref})$. 

(81)
Using the first-order approximation for $\hat{e}^i_t$ we find
\[
\hat{e}^{(1)}_t = \langle f_s | \hat{I} - \frac{i}{\hbar} \int_{t_{ref}}^t dt' \hat{V}_I(t') | i_s \rangle \\
= \delta_{fi} - \frac{i}{\hbar} \int_{t_{ref}}^t dt' \langle f_s | \hat{V}_I(t') | i_s \rangle \\
= \delta_{fi} - \frac{i}{\hbar} \int_{t_{ref}}^t dt' \langle f_s | \hat{U}_s(t_{ref}, t') \hat{V}_I(t') \hat{U}_s^\dagger(t_{ref}, t) | i_s \rangle \\
= \delta_{fi} - \frac{i}{\hbar} \int_{t_{ref}}^t dt' \langle f_s | e^{-\frac{i}{\hbar} E_0^{(2)} (t_{ref} - t') \hat{V}_I(t')} e^{-\frac{i}{\hbar} E_0^{(2)} (t_{ref} - t_f) \hat{V}_I(t_f)} | i_s \rangle \\
= \delta_{fi} - \frac{i}{\hbar} \int_{t_{ref}}^t dt' \langle f_s | \hat{V}_I(t') | i_s \rangle e^{i \omega_f (t - t_{ref})}
\]

This agrees with our earlier result if we set $t_{ref} = 0$.

**Higher orders:** If we keep feeding the result for $\hat{U}_I(t, t_{ref})$ at a given order into the right hand side of the integral equation to generate the next higher order approximation, we get
\[
\hat{U}_I(t, t_{ref}) = \hat{I} - \frac{i}{\hbar} \int_{t_{ref}}^t dt' \hat{V}_I(t') + \left( \frac{i}{\hbar} \right)^2 \int_{t_{ref}}^t dt' \int_{t_{ref}}^t dt'' \hat{V}_I(t') \hat{V}_I(t'') + \left( \frac{i}{\hbar} \right)^3 \int_{t_{ref}}^t dt' \int_{t_{ref}}^t dt' \int_{t_{ref}}^t dt'' \hat{V}_I(t') \hat{V}_I(t'') \hat{V}_I(t''') + \ldots
\]
Note that the $\hat{V}$ factors under the integral are time-ordered, with largest time agreement to the left and smallest to the right.

With a little trick we can resum this series:

We write

$$\int_{\text{ref}}^{t} \int_{\text{ref}}^{t} \hat{V}(t') \hat{V}(t'') = \frac{1}{2} \int_{\text{ref}}^{t} \int_{\text{ref}}^{t} \hat{V}(t') \hat{V}(t'') + \frac{1}{2} \int_{\text{ref}}^{t} \int_{t'}^{t} \hat{V}(t') \hat{V}(t'')$$

$$= \frac{1}{2} \int_{\text{ref}}^{t} \int_{\text{ref}}^{t'} \hat{V}(t') \hat{V}(t'') + \frac{1}{2} \int_{\text{ref}}^{t'} \int_{t'}^{t} \hat{V}(t') \hat{V}(t'')$$

$$= \frac{1}{2} \int_{\text{ref}}^{t} \int_{\text{ref}}^{t'} \hat{V}(t') \hat{V}(t'') + \frac{1}{2} \int_{\text{ref}}^{t} \int_{t'}^{t} \hat{V}(t') \hat{V}(t'')$$

$$= \frac{1}{2} \int_{\text{ref}}^{t} \int_{\text{ref}}^{t'} \hat{V}(t') \hat{V}(t'')$$

$$= \frac{1}{2} \int_{\text{ref}}^{t} \int_{\text{ref}}^{t'} [\hat{V}(t') \hat{V}(t'') + \hat{V}(t'') \hat{V}(t')]$$

where

$$\hat{V}(t') \hat{V}(t'') = \Theta(t' - t'') \hat{V}(t') \hat{V}(t'') + \Theta(t' - t) \hat{V}(t'') \hat{V}(t')$$

$$= \{ \hat{V}(t') \hat{V}(t'') \text{ if } t' > t'' \}
\{ \hat{V}(t'') \hat{V}(t') \text{ if } t'' > t' \}$$

is the time-ordered product of $\hat{V}(t')$ and $\hat{V}(t'')$.

$$\Rightarrow \hat{U}_{\text{ref}}(t; \text{ref}) = \hat{1} - \frac{i}{\hbar} \int_{\text{ref}}^{t} \hat{V}(t') + \frac{1}{2} \left( \frac{i}{\hbar} \right)^2 \int_{\text{ref}}^{t} \int_{\text{ref}}^{t} \hat{V}(t') \hat{V}(t'') + \frac{1}{3} \left( \frac{i}{\hbar} \right)^3 \int_{\text{ref}}^{t} \int_{\text{ref}}^{t} \int_{\text{ref}}^{t} \hat{V}(t') \hat{V}(t'') \hat{V}(t'') + \ldots$$
The complete Schrödinger picture propagator is a sum of terms with $\theta, 1, 2, \ldots$ actions of $\mathcal{U}$ at intermediate times.

We can also get the Schrödinger picture propagator for the Taylor expansion of the exponential function.

\[
\mathcal{U}(t, t') = \frac{1}{t - t'} \mathcal{U}_0(t, t') \mathcal{U}(t', t)
\]

\[\mathcal{U}(t, t') = e^{i \frac{1}{2} \mathcal{H}_0 (t-t') \mathcal{U}_0(t, t') (t-t')} + \ldots\]
The intermediate times when \( \hat{U} \) acts are integrated over from initial time \( t_{\text{ref}} \) to final time \( t \).

For the transition amplitude this implies

\[
\langle f_s | U(t, t_{\text{ref}}) | i_s^0 \rangle = \langle f_s^0 | U_5(t_{\text{ref}}, t) U_5(t, t_{\text{ref}}) | i_s^0 \rangle \\
= \langle f_s^0 | e^{-\frac{i}{\hbar} E_0 (t_{\text{ref}}-t)} U_5(t, t_{\text{ref}}) | i_s^0 \rangle \\
= S_{fi} - \frac{i}{\hbar} \int_{t_{\text{ref}}}^{t} dt' e^{-i \frac{E_0 (t_{\text{ref}}-t')}{\hbar}} \langle f_s^0 | v_5(t') | i_s^0 \rangle e^{-i \frac{E_0 (t'-t_{\text{ref}})}{\hbar}} \\
+ \left( \frac{i}{\hbar} \right)^2 \int_{t_{\text{ref}}}^{t} dt' \int_{t_{\text{ref}}}^{t} dt'' \sum_n e^{-i \frac{E_0 (t_{\text{ref}}-t')}{\hbar}} \langle f_s^0 | v_5(t') | n \rangle \langle n | v_5(t'') | i_s^0 \rangle e^{-i \frac{E_0 (t''-t_{\text{ref}})}{\hbar}} \\
\times e^{-i \frac{E_0 (t'-t'')}{\hbar}} \langle n | v_5(t'') | i_s^0 \rangle e^{-i \frac{E_0 (t''-t_{\text{ref}})}{\hbar}} + \ldots
\]

Dropping the \( 5 \) subscripts everywhere and simplifying this gives

\[
\langle f_s | U(t, t_{\text{ref}}) | i_s^0 \rangle = e^{-i \frac{\omega_{fi} t_{\text{ref}}}{\hbar}} \left[ S_{fi} - \frac{i}{\hbar} \int_{t_{\text{ref}}}^{t} dt' \langle f_s^0 v_5(t') | i_s^0 \rangle e^{i \frac{\omega_{fi} t'}{\hbar}} \\
+ \left( \frac{i}{\hbar} \right)^2 \int_{t_{\text{ref}}}^{t} dt' \int_{t_{\text{ref}}}^{t} dt'' \sum_n \langle f_s^0 v_5(t') | n \rangle \langle n | v_5(t'') | i_s^0 \rangle e^{i \frac{\omega_{fi} t''}{\hbar}} \\
+ \ldots \right]
\]