I.06. Time Evolution Operator

The time evolution operator is defined by the eq.

$$i\hbar \frac{\partial}{\partial t} \hat{U}(t, t') = \hat{H}(t)\, \hat{U}(t, t') \qquad (1.233)$$

Comparing with the Schrodinger eq., we see that

$$|\, \Psi(t) \rangle = \hat{U}(t, t')\, |\, \Psi(t') \rangle \qquad (1.233a)$$

Since $\hat{U}$ governs the evolution of the states, it must satisfies the following group properties

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

$$\hat{U}(t, t') = \hat{U}(t, t_a)\, \hat{U}(t_a, t') \qquad \forall\ t < t_a < t' \qquad (1.233b)$$

$$\rightarrow \qquad \hat{U}(t, t_a)\, \hat{U}(t_a, t) = 1$$

$$\therefore \qquad \hat{U}^{-1}(t, t') = \hat{U}(t', t) \qquad (1.236)$$

For a time-independent Hamiltonian, the Schrodinger eq. can be integrated to get

$$|\, \Psi(t) \rangle = e^{-i(t-t')\hat{H}/\hbar}\, |\, \Psi(t') \rangle \qquad (1.231)$$

i.e.,

$$\hat{U}(t, t') = e^{-i(t-t')\hat{H}/\hbar} \qquad (1.232)$$

Validity of (1.231) can be verified by time differentiation, whereupon the Schrodinger eq. is recovered.

For a time-independent and hermitian $\hat{H}$, (1.236) & (1.232) imply

$$\hat{U}^{-1}(t, t') = e^{i(t-t')\hat{H}/\hbar} = \hat{U}^{+}(t, t') \qquad (1.236)$$

$$\rightarrow \qquad \hat{U}^{-1} = \hat{U}^{+} \qquad (1.235)$$

i.e., $\hat{U}$ is unitary.

For a time-dependent Hamiltonian $\hat{H} = H(\hat{\mathbf{x}}, \hat{\mathbf{p}}, t)$, (1.233) can be integrated by iteration. Integrating once gives

$$\hat{U}(t, t') = 1 + \frac{1}{i\hbar} \int_{t'}^{t} d t_1\, \hat{H}(t_1)\, \hat{U}(t_1, t') \qquad (1.237a)$$

where the 1st eq. in (1.233b) was used.

Using (1.237a) on itself, we have

$$\hat{U}(t, t') = 1 + \frac{1}{i\hbar} \int_{t'}^{t} d t_1\, \hat{H}(t_1) \left[1 + \frac{1}{i\hbar} \int_{t'}^{t_1} d t_2\, \hat{H}(t_2)\, \hat{U}(t_2, t') \right]$$

$$= 1 + \frac{1}{i\hbar} \int_{t'}^{t} d t_1\, \hat{H}(t_1) + \frac{1}{(i\hbar)^2} \int_{t'}^{t} d t_1 \int_{t'}^{t_1} d t_2\, \hat{H}(t_1)\, \hat{H}(t_2)\, \hat{U}(t_2, t')$$

Applying again (1.237a) gives

$$\hat{U}(t, t') = 1 + \frac{1}{i\hbar} \int_{t'}^{t} d t_1\, \hat{H}(t_1) + \frac{1}{(i\hbar)^2} \int_{t'}^{t} d t_1 \int_{t'}^{t_1} d t_2\, \hat{H}(t_1)\, \hat{H}(t_2)$$

$$+ \frac{1}{(i\hbar)^3} \int_{t'}^{t} d t_1 \int_{t'}^{t_1} d t_2 \int_{t'}^{t_2} d t_3\, \hat{H}(t_1)\, \hat{H}(t_2)\, \hat{H}(t_3)\, \hat{U}(t_3, t')$$

Continuing the iteration, we get the Neumann-Liouville expansion (also called the Dyson series),

$$\hat{U}(t, t') = \sum_{n=0}^{\infty} \frac{1}{(i\hbar)^n} \int_{t'}^{t} d t_1 \int_{t'}^{t_1} d t_2 \ldots \int_{t'}^{t_{n-1}} d t_n\, \hat{H}(t_1) \ldots \hat{H}(t_n) \qquad (1.239)$$

with the understanding that the $n = 0$ term is equal to 1. Note that

$$t \geq t_1 \geq \ldots \geq t_n \geq t' \tag{1.239a}$$

The time-ordered operator rearranges the order of a product of operators so that the one on the left always has a later time:

$$\hat{T}\left[\hat{O}_1(t_1) \ldots \hat{O}_n(t_n)\right] = \hat{O}_{i_1}(t_{i_1}) \ldots \hat{O}_{i_n}(t_{i_n}) \tag{1.241}$$

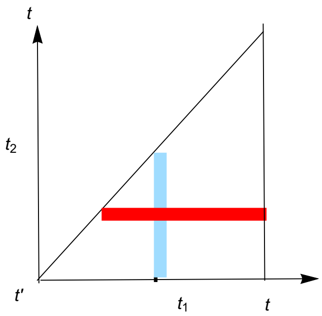
whre $(i_1, \ldots, i_n)$ is the rearrangement of $(1, \ldots, n)$ such that

$$t_{i_1} \geq \ldots \geq t_{i_n} \tag{1.242}$$

Consider now the 2nd order term in (1.239).

$$\mathcal{I}_2 = \frac{1}{(i\hbar)^2} \int_{t'}^{t} d\,t_1 \int_{t'}^{t_1} d\,t_2\, \hat{H}(t_1)\, \hat{H}(t_2) \qquad (\, t_1 \geq t_2 \,)$$

With reference to the figure below, this treats the integration area as consisting of parallel vertical blue bars.



Reversing the order of integration (integration area consists of parallel horizontal red bars in figure above) gives

$$\mathcal{I}_2 = \frac{1}{(i\hbar)^2} \int_{t'}^{t} d\,t_2 \int_{t_2}^{t} d\,t_1\, \hat{H}(t_1)\, \hat{H}(t_2)$$

Switching the names of the dummy variables gives

$$\mathcal{I}_2 = \frac{1}{(i\hbar)^2} \int_{t'}^{t} d\,t_1 \int_{t_1}^{t} d\,t_2\, \hat{H}(t_2)\, \hat{H}(t_1) \qquad (\, t_2 \geq t_1)$$

Combining the two gives

$$\mathcal{I}_2 = \frac{1}{2\,(i\hbar)^2} \int_{t'}^{t} d\,t_1 \int_{t'}^{t} d\,t_2\, \hat{T}\left[\hat{H}(t_1)\, \hat{H}(t_2)\right] \tag{1.248}$$

$$= \frac{1}{2\,(i\hbar)^2}\, \hat{T}\left(\int_{t'}^{t} d\,t_1\, \hat{H}(t_1) \right)^2 \tag{1.249}$$

Since there are $n!$ permutations for n time points, the n^{th} order term consists of $n!$ time-orderings so that

$$\mathcal{I}_n = \frac{1}{n!\,(i\hbar)^n}\, \hat{T}\left(\int_{t'}^{t} d\,t_1\, \hat{H}(t_1) \right)^n \tag{1.250}$$

and (1.239) simplifies to

$$\hat{U}(t, t') = \hat{T} \sum_{n=0}^{\infty} \frac{1}{n!\,(i\hbar)^n} \left(\int_{t'}^{t} d\,t_1\, \hat{H}(t_1) \right)^n$$

$$= \hat{T} \exp\left[-\frac{i}{\hbar} \int_{t'}^{t} d\,t_1\, \hat{H}(t_1) \right] \tag{1.252}$$

Obviously, (1.232) is recovered if $\hat{H}$ is time independent.

A change in $\hat{U}$ induced by a small variation on $\hat{H}$. If $\hat{H}$ is time independent, then (1.232) gives

$$\delta\hat{U}(t, t') = -\frac{i}{\hbar}(t-t')\,\delta\hat{H}\;e^{-i(t-t')\hat{H}/\hbar}$$
$$= -\frac{i}{\hbar}(t-t')\,\delta\hat{H}\;\hat{U}(t, t') \qquad (1.253a)$$

For time-dependent $\hat{H}$, if the variation occurs only for a small duration Δt around t_2, then (1.253a) can be modified to give, to 1st order in Δt,

$$\delta\hat{U}(\Delta t) = -\frac{i}{\hbar}\Delta t\,\delta\hat{H}(t_2) \qquad (\hat{U}(\Delta t) \approx 1)$$
$$\delta\hat{U}(t, t') = \hat{U}(t, t_2)\left[-\frac{i}{\hbar}\Delta t\,\delta\hat{H}(t_2)\right]\hat{U}(t_2, t')$$

If the variation can occur any time between t' & t, we must sum up contributions from all t_2 so that

$$\delta\hat{U}(t, t') = -\frac{i}{\hbar}\int_{t'}^{t} d\,t_2\,\hat{U}(t, t_2)\,\delta\hat{H}(t_2)\,\hat{U}(t_2, t') \qquad (1.253)$$
$$= -\frac{i}{\hbar}\int_{t'}^{t} d\,t_2\,\hat{T}\exp\left[-\frac{i}{\hbar}\int_{t'}^{t_2} d\,t_1\,\hat{H}(t_1)\right]\delta\hat{H}(t_2)\,\hat{T}\exp\left[-\frac{i}{\hbar}\int_{t_2}^{t} d\,t_1\,\hat{H}(t_1)\right]$$