Unitary Time-Propagation Operator for Time-Dependent Schrödinger Equation

2/11/10

— Consider a time-dependent Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H}(t) |\Psi(t)\rangle, \quad (1)$$

where $\hat{H}(t)$ is a time-dependent operator and the wave vector $|\Psi(t)\rangle$ satisfies the initial condition, $|\Psi(t=t_0)\rangle = |\Psi(t_0)\rangle$.

— The formal solution of Eq. (1) is given by

$$|\Psi(t)\rangle = \hat{U}(t,t_0) |\Psi(t_0)\rangle \quad (2)$$

where the unitary time-propagation operation is defined as

$$\hat{U}(t,t_0) = \sum_{n=0}^{\infty} \left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n \, \hat{H}(t_1)\hat{H}(t_2)\cdots\hat{H}(t_n) \quad (3)$$

$$= 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt_1 \, \hat{H}(t_1) + \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \, \hat{H}(t_1)\hat{H}(t_2) + \cdots \quad (4)$$

☹

$\hat{U}(t\to t_0, t_0) = 1 \Rightarrow$ satisfies the initial condition

$$\frac{d}{dt}\hat{U}(t,t_0) = -\frac{i}{\hbar}\left\{ \hat{H}(t) + \left(-\frac{i}{\hbar}\right)\hat{H}(t)\int_{t_0}^{t} dt_2 \, \hat{H}(t_2) + \cdots \right.$$

$$\left. + \left(-\frac{i}{\hbar}\right)^{n-1}\hat{H}(t)\int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n \, \hat{H}(t_2)\cdots\hat{H}(t_n) + \cdots \right\}$$

$$= -\frac{i}{\hbar}\hat{H}(t)\hat{U}(t,t_0)$$ $\Rightarrow$ statisfies the differential equation. //

– Time-ordered product.

Let T denote a time-ordered product of operators, such that the operators are sorted in the descending order of time from the left to right. Then,

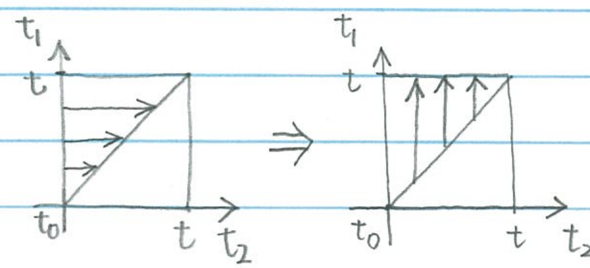
$$\hat{U}(t,t_0) \equiv \sum_{n=0}^{\infty}\left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n\, \hat{H}(t_1)\hat{H}(t_2)\cdots\hat{H}(t_n) \qquad (3)$$

$$= \sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t} dt_n\, T\left[\hat{H}(t_1)\cdots\hat{H}(t_n)\right] \qquad (5)$$

$$\equiv T\exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} dt'\,\hat{H}(t')\right) \qquad (6)$$

∵ Eq. (5)

$(n=2)$



$$\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2\, \hat{H}(t_1)\hat{H}(t_2)$$

$$= \frac{1}{2}\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2\, \hat{H}(t_1)\hat{H}(t_2)$$

$$+ \underbrace{\frac{1}{2}\int_{t_0}^{t} dt_2 \int_{t_2}^{t} dt_1\, \hat{H}(t_1)\hat{H}(t_2)}_{\frac{1}{2}\int_{t_0}^{t} dt_1 \int_{t_1}^{t} dt_2\, \hat{H}(t_2)\hat{H}(t_1)}$$

$t_1 \leftrightarrow t_2$

$$= \frac{1}{2}\underbrace{\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2}_{\text{entire integration range}} \Big[\underbrace{\hat{H}(t_1)\hat{H}(t_2)\Theta(t_1>t_2) + \underbrace{\hat{H}(t_2)\hat{H}(t_1)}_{\text{permutation}}\Theta(t_2>t_1)}_{T[\hat{H}(t_1)\hat{H}(t_2)]}\Big]$$

proper time order

(General n)

$$\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n \, \hat{H}(t_1)\hat{H}(t_2)\cdots\hat{H}(t_n)$$

entire integration range & proper time order

$$= \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n \, \hat{H}(t_1)\hat{H}(t_2)\cdots\hat{H}(t_n)\, \Theta(t_1 > t_2 > \cdots > t_n)$$

$\downarrow$ permutation

$$= \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n \, \hat{H}(t_{p(1)})\hat{H}(t_{p(2)})\cdots\hat{H}(t_{p(n)})\, \Theta(t_{p(1)} > t_{p(2)} > \cdots t_{p(n)})$$

$\downarrow$ sum $\forall$ permutations

$$= \frac{1}{n!}\int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t} dt_n \underbrace{\sum_{p} \hat{H}(t_{p(1)})\cdots\hat{H}(t_{p(n)})\, \Theta(t_{p(1)} > \cdots > t_{p(n)})}_{T[\hat{H}(t_1)\cdots\hat{H}(t_n)]}$$

$\because$ For $\forall (t_1, t_2, \ldots, t_n)$, $\exists p \, (t_{p(1)} > \cdots > t_{p(n)})$

for which add $\hat{H}(t_{p(1)})\cdots\hat{H}(t_{p(n)})\, dt_1 \cdots dt_n$.

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