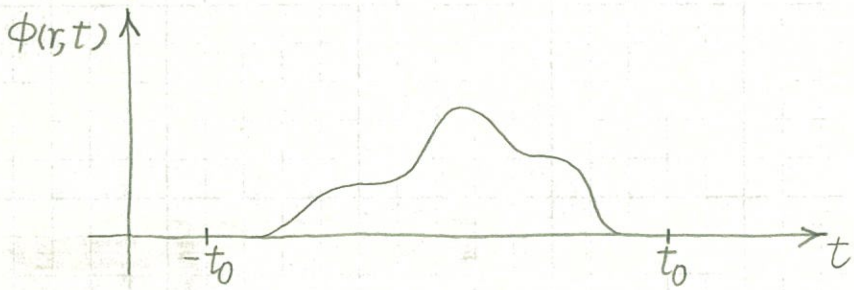
Closed Time Path Formulation of Dynamic Correlations: Basic Relations

9/26/89

§. System

$$\mathcal{H}(t) = H + V(t) = T + U + V(t) \tag{1}$$

$$\begin{cases} T = \sum_{\sigma} \int d^3r\, \psi_\sigma^\dagger(r) \left(-\frac{\hbar^2}{2m}\nabla^2\right) \psi_\sigma(r) & (2) \\ U = \sum_{\sigma\sigma'} \int d^3r \int d^3r'\, \psi_\sigma^\dagger(r)\, \psi_{\sigma'}^\dagger(r')\, v(r-r')\, \psi_{\sigma'}(r')\, \psi_\sigma(r) & (3) \\ V(t) = \int d^3r\, \rho(r)\, \phi(r,t) & (4) \end{cases}$$



We specify an initial state at time $-t_0$. An external field $\phi(r,t)$ is then tured on and off before time t_0.

§. Schrödinger Picture

$$\boxed{\begin{aligned} &|\psi_S(t)\rangle = \mathcal{U}_\pm(t,t_0)\, |\psi_S(t_0)\rangle \quad \text{according to } t \gtrless t_0 && (5) \\ &\text{where} \\ &\mathcal{U}_\pm(t,t_0) = T_\pm \exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} dt_1\, \mathcal{H}(t_1)\right] && (6) \end{aligned}}$$

∵ Noting that

$$\mathcal{U}_\pm(t_0,t_0) = 1 \tag{7}$$

we have only to prove that

$$i\hbar \frac{\partial}{\partial t} \mathcal{U}_\pm(t,t_0) = \mathcal{H}(t)\, \mathcal{U}_\pm(t,t_0) \tag{8}$$

(i) $t > t_0$

$$i\hbar\frac{\partial}{\partial t}\mathcal{U}_+(t,t_0) = \sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n \underbrace{i\hbar\frac{\partial}{\partial t}\int_{t_0}^{t}dt_1\cdots\int_{t_0}^{t}dt_n\, T_+[\mathcal{H}(t_1)\cdots\mathcal{H}(t_n)]}_{\mathcal{H}(t)\, i\hbar n\int_{t_0}^{t}dt_1\cdots\int_{t_0}^{t}dt_{n-1}\, T_+[\mathcal{H}(t_1)\cdots\mathcal{H}(t_{n-1})]}$$

$$= \mathcal{H}(t)\sum_{n=1}^{\infty}\frac{1}{(n-1)!}\left(-\frac{i}{\hbar}\right)^{n-1}\int_{t_0}^{t}dt_1\cdots\int_{t_0}^{t}dt_{n-1}\, T_+[\mathcal{H}(t_1)\cdots\mathcal{H}(t_{n-1})]$$

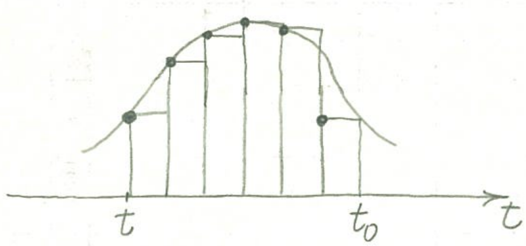
$$= \mathcal{H}(t)\,\mathcal{U}_+(t,t_0)$$

(ii) $t < t_0$

$$i\hbar\frac{\partial}{\partial t}\mathcal{U}_-(t,t_0) = \sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n i\hbar\frac{\partial}{\partial t}\int_{t_0}^{t}dt_1\cdots\int_{t_0}^{t}dt_n\, T_-[\mathcal{H}(t_1)\cdots\mathcal{H}(t_n)]$$

$$= \mathcal{H}(t)\,\mathcal{U}_-(t,t_0) \quad //$$

※



$$F(t) = \int_{t_0}^{t}dt\, f(t) = \sum_{i=1}^{n}\frac{t-t_0}{n} f\left(t_0 + \frac{t-t_0}{n} i\right)$$

$$\frac{dF}{dt} = \frac{F\left(t+\frac{t_0-t}{n}\right) - F(t)}{\frac{t_0-t}{n}}$$

$$= \frac{\sum_{i=1}^{n-1}\frac{t-t_0}{n} f\left(t_0+\frac{t-t_0}{n}i\right) - \sum_{i=1}^{n}\frac{t-t_0}{n} f\left(t_0+\frac{t-t_0}{n}i\right)}{\frac{t_0-t}{n}} \quad \text{num.} = -\frac{t-t_0}{n} f(t)$$

$$= f(t)$$

$$\therefore \quad \boxed{\frac{d}{dt}\int_{t_0}^{t}dt' f(t') = f(t) \quad \text{regardless of} \quad t \gtrless t_0}$$

(Some Relations)

① $\mathcal{U}_\pm(t_1,t_2)\,\mathcal{U}_\pm(t_2,t_3) = \mathcal{U}_\pm(t_1,t_3)$ (9)

with signs $\pm$ according to $t_{left} \gtrless t_{right}$

② $\mathcal{U}_\pm^{-1}(t,t_0) = \mathcal{U}_\pm^\dagger(t,t_0) = \mathcal{U}_\mp(t_0,t)$ (10)

∵ ① $|\psi_S(t_1)\rangle = \mathcal{U}_\pm(t_1,t_2)\underbrace{|\psi_S(t_2)\rangle}_{\mathcal{U}_\pm(t_2,t_3)\,|\psi_S(t_3)\rangle}$

② (i)
$$\mathcal{U}_\pm^\dagger(t,t_0) = \left(\sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n\int_{t_0}^{t}dt_1\cdots\int_{t_0}^{t}dt_n\, T_\pm[\mathcal{H}(t_1)\cdots\mathcal{H}(t_n)]\right)^\dagger$$
$$= \sum_{n=0}^{\infty}\frac{1}{n!}\underbrace{\left(\frac{i}{\hbar}\right)^n\int_{t_0}^{t}dt_1\cdots\int_{t_0}^{t}dt_n}_{\left(-\frac{i}{\hbar}\right)^n\int_{t}^{t_0}dt_1\cdots\int_{t}^{t_0}dt_n}\, T_\mp[\mathcal{H}(t_1)\cdots\mathcal{H}(t_n)]$$
$$= \mathcal{U}_\mp(t_0,t)$$

(ii) $\mathcal{U}_\pm(t,t_0)\,\mathcal{U}_\mp(t_0,t) = 1 \quad \therefore\ \mathcal{U}_\pm^{-1}(t,t_0) = \mathcal{U}_\mp(t_0,t)$ //

§. Heisenberg Picture

$|\psi_{\mathcal{H}}\rangle \equiv |\psi_S(-t_0)\rangle$ (11)

$\mathcal{O}_{\mathcal{H}}(t) \equiv \mathcal{U}_-(-t_0,t)\,\mathcal{O}_S\,\mathcal{U}_+(t,-t_0)$ (12)

then

$\langle\psi_S(t_1)|\,\mathcal{O}_S\,\mathcal{U}_\pm(t_1,t_2)\,\mathcal{O}_S\,|\psi_S(t_2)\rangle = \langle\psi_{\mathcal{H}}|\,\mathcal{O}_{\mathcal{H}}(t_1)\,\mathcal{O}_{\mathcal{H}}(t_2)\,|\psi_{\mathcal{H}}\rangle$ (13)

∵ $(\text{lhs}) = \langle\psi_{\mathcal{H}}|\underbrace{\mathcal{U}_-(-t_0,t_1)\,\mathcal{O}_S\,\mathcal{U}_+(t_1,-t_0)}_{\mathcal{O}_{\mathcal{H}}(t_1)}\underbrace{\mathcal{U}_-(-t_0,t_2)\,\mathcal{O}_S\,\mathcal{U}_+(t_2,-t_0)}_{\mathcal{O}_{\mathcal{H}}(t_2)}|\psi_{\mathcal{H}}\rangle$ //

§. Interaction Picture

$$|\psi_H(t)\rangle \equiv e^{iH(t+t_0)/\hbar}|\psi_S(t)\rangle \tag{14}$$
$$\mathcal{O}_H(t) \equiv e^{iH(t+t_0)/\hbar}\mathcal{O}_S\, e^{-iH(t+t_0)/\hbar} \tag{15}$$

Then,

$$i\hbar\frac{\partial}{\partial t}|\psi_H(t)\rangle = V_H(t)\,|\psi_H(t)\rangle \tag{16}$$

$$\left(\because\ i\hbar\frac{\partial}{\partial t}|\psi_H(t)\rangle = -\cancel{H}\,e^{iH(t+t_0)/\hbar}|\psi_S(t)\rangle + e^{iH(t+t_0)/\hbar}\underbrace{[\cancel{H}+V(t)]\,}_{(e^{-iH(t+t_0)/\hbar}e^{iH(t+t_0)/\hbar})}|\psi_S(t)\rangle \\ = V_H(t)\,|\psi_H(t)\rangle \ //\right)$$

$$|\psi_H(t)\rangle = S_\pm(t,t_0)\,|\psi_H(t_0)\rangle \quad \text{according to} \quad t \gtrless t_0 \tag{17}$$

where

$$S_\pm(t,t_0) = T_\pm \exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} dt_1\, V_H(t_1)\right) \tag{18}$$

($\because$ The same proof as leads to Eqs. (5) and (6).)

(Some Relations)

① $S_\pm(t_1,t_2)S_\pm(t_2,t_3) = S_\pm(t_1,t_3)$ with signs $\pm$ according to $t_{left} \gtrless t_{right}$ (19)

② $S_\pm^{-1}(t,t_0) = S_\pm^{\dagger}(t,t_0) = S_\mp(t_0,t)$ (20)

③ $\langle\psi_{\mathcal{H}}|\,\mathcal{O}_{\mathcal{H}}(t_1)\,\mathcal{O}_{\mathcal{H}}(t_2)\,|\psi_{\mathcal{H}}\rangle$

$$= \langle\psi_{\mathcal{H}}|S_-(-\infty,t_1)\,\mathcal{O}_H(t_1)\,S_\pm(t_1,t_2)\,\mathcal{O}_H(t_2)\,S_+(t_2,-\infty)\,|\psi_{\mathcal{H}}\rangle \tag{21}$$

∵ ③

(i) $$|\psi_S(t)\rangle = \underbrace{e^{-iH(t+t_0)/\hbar}\ \underbrace{|\psi_H(t)\rangle}_{S_\pm(t,t')\, e^{iH(t'+t_0)/\hbar}}}_{\mathcal{U}_\pm(t,t') = e^{-iH(t+t_0)/\hbar} S_\pm(t,t')\, e^{iH(t'+t_0)/\hbar}} |\psi_S(t')\rangle$$

Setting $t' = -t_0$,

$$|\psi_S(t)\rangle = e^{-iH(t+t_0)/\hbar} S_+(t,-\infty)\, |\psi_{\mathcal{H}}\rangle$$

(ii) $\langle\psi_S(t_1)|\mathcal{O}_S\, \mathcal{U}_\pm(t_1,t_2)\, \mathcal{O}_S|\psi_S(t_2)\rangle$

$$= \langle\psi_{\mathcal{H}}|S_-(-\infty,t_1)\underbrace{e^{iH(t_1+t_0)/\hbar}\mathcal{O}_S\, e^{-iH(t_1+t_0)/\hbar}}_{\mathcal{O}_H(t_1)} S_\pm(t_1,t_2)\underbrace{e^{iH(t_2+t_0)/\hbar}\mathcal{O}_S\, e^{-iH(t_2+t_0)/\hbar}}_{\mathcal{O}_H(t_2)} \times S_+(t_2,-\infty)|\psi_{\mathcal{H}}\rangle$$

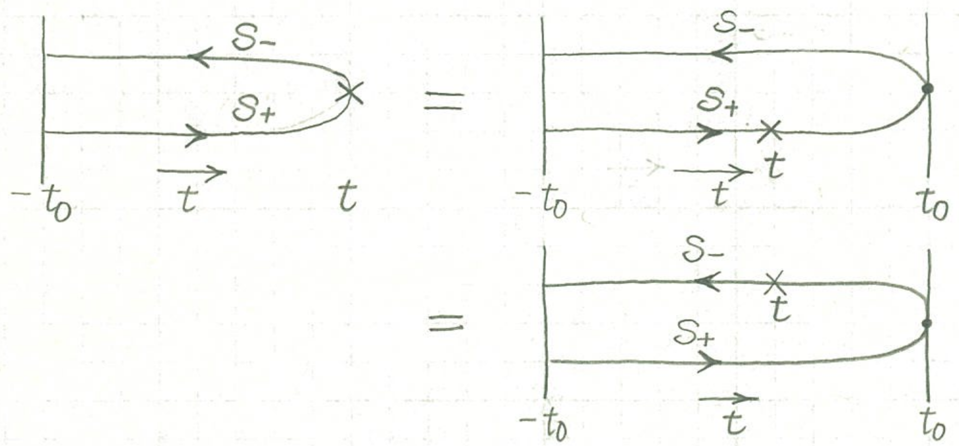
$$= \langle\psi_{\mathcal{H}}|S_-(-\infty,t_1)\, \mathcal{O}_H(t_1)\, S_\pm(t_1,t_2)\, \mathcal{O}_H(t_2)\, S_+(t_2,-\infty)\, |\psi_{\mathcal{H}}\rangle \qquad //$$

※ Single-time average may be written either in the following forms:

$$\langle\psi_{\mathcal{H}}|\, \mathcal{O}_{\mathcal{H}}(t)\, |\psi_{\mathcal{H}}\rangle$$

$$= \langle\psi_{\mathcal{H}}|\, S_-\, T_+[\mathcal{O}_H(t) S_+]\, |\psi_{\mathcal{H}}\rangle \tag{22a}$$

$$= \langle\psi_{\mathcal{H}}|\, T_-[S_-\mathcal{O}_H(t)] S_+\, |\psi_{\mathcal{H}}\rangle \tag{22b}$$



∵ Because of unitarity, $S_\pm^\dagger(t,t_0)\, S_\mp(t_0,t) = 1$,

$$S_-(-\infty,t)\ \underbrace{\ }_{S_-(t,\infty)\, S_+(\infty,t)}\ \mathcal{O}_H(t)\ \underbrace{\ }_{\text{or } S_-(t,\infty)\, S_+(\infty,t)}\ S_+(t,-\infty) \qquad //$$

§. Response Theorem

$$\boxed{\frac{\delta S_\pm(t,t_0)}{\delta\phi(1)} = \mp\frac{i}{\hbar}\Theta_\pm(t,t_1,t_0)\,T_\pm[\rho_H(1)S_\pm(t,t_0)]} \tag{23}$$

where

$$\Theta_+(t_1,t_2,\cdots,t_n) = \Theta(t_1-t_2)\cdots\Theta(t_{n-1}-t_n) \tag{24a}$$

$$\Theta_-(t_1,t_2,\cdots,t_n) = \Theta(t_n-t_{n-1})\cdots\Theta(t_2-t_1) \tag{24b}$$

$$\because \frac{\delta}{\delta\phi(1)}\sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n \underbrace{\int_{t_0}^{t}d1\cdots\int_{t_0}^{t}dn\,\phi(1)\cdots\phi(n)\,T_\pm[\rho_H(1)\cdots\rho_H(n)]}$$

$$(\pm)n\int_{t_0}^{t}d2\cdots\int_{t_0}^{t}dn\,\phi(2)\cdots\phi(n)\,T_\pm[\rho_H(1)\rho_H(2)\cdots\rho_H(n)]$$

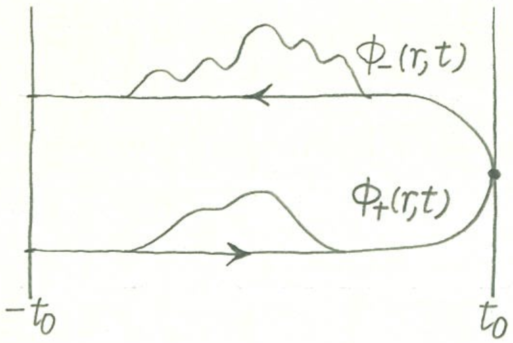
※ Functional derivative is defined such that

$$\delta f(t) = \int_{-\infty}^{\infty}dt'\frac{\delta f(t)}{\delta g(t')}\delta g(t')$$

$$\therefore \int_{t_0}^{t}d1\,\rho_H(1)\,\delta\phi(1)\underset{(t<t_0)}{} = -\int_{t}^{t_0}d1\,\rho_H(1)\,\delta\phi(1)$$

$$= \mp\frac{i}{\hbar}T_\pm[\rho_H(1)S_\pm(t,t_0)] \quad \text{if} \quad t \gtrless t_1 \gtrless t_0 \qquad //$$

§. Closed Time Path



§. Scattering Matrix on the Closed Time Path

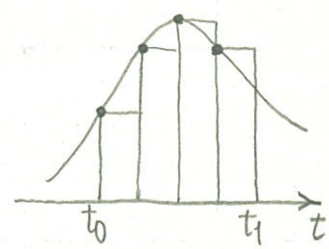
$$S = T\exp\left[-\frac{i}{\hbar}\int d^3r\int_P dt\ \rho_H(r,t)\phi(r,t)\right] \tag{25a}$$

$$\equiv T_-\exp\left[-\frac{i}{\hbar}\int d^3r\int_{\infty}^{-\infty} dt\ \rho_H(r,t)\phi_-(r,t)\right] T_+\exp\left[-\frac{i}{\hbar}\int d^3r\int_{-\infty}^{\infty} dt\ \rho_H(r,t)\phi_+(r,t)\right] \tag{25b}$$

$$= S_- S_+ \tag{25c}$$

Note that $\int_P dt = \int_{-\infty}^{\infty} dt_+ - \int_{-\infty}^{\infty} dt_-$.

$$\left(\because\ \begin{aligned}\int_{t_1}^{t_0} dt\, f(t) &\equiv \frac{t_0-t_1}{N}\sum_{i=1}^{N} f\left(t_1+\frac{t_0-t_1}{N}\,i\right) \quad \Big\}\ i+j=N \\ &= -\frac{t_1-t_0}{N}\sum_{j=0}^{N-1} f\left(t_0+\frac{t_1-t_0}{N}\,j\right) \\ &\equiv -\int_{t_0}^{t_1} dt\, f(t) \qquad //\end{aligned}\right)$$



§. Equation of Motion for S Matrix

$$\boxed{\begin{aligned} i\hbar\frac{\partial}{\partial t}S(t,t') &= V_H(t)\,S(t,t') &(26)\\ i\hbar\frac{\partial}{\partial t'}S(t,t') &= -S(t,t')\,V_H(t') &(27)\end{aligned}}$$

∵ (26) $S(t,t') = \begin{cases} S_+(t,t') & \text{for } (t>t') \in (+,+) \\ S_-(t,\infty)\,S_+(\infty,t') & (-,+) \\ S_-(t,t') & (-,-), \end{cases}$

and $S_\pm(t,t')$ satisfy Eq. (26) by their definitions.

(27) $i\hbar\frac{\partial}{\partial t'}S_\pm(t,t') = \sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n \underbrace{i\hbar\frac{\partial}{\partial t'}\int_{t'}^{t}dt_1\cdots\int_{t'}^{t}dt_n\, T_\pm[V_H(t_1)\cdots V_H(t_n)]}_{-n i\hbar\int_{t'}^{t}dt_1\cdots\int_{t'}^{t}dt_{n-1}\,T_\pm[V_H(t_1)\cdots V_H(t_{n-1})]\,V_H(t')}$

$$= -S_\pm(t,t')\,V_H(t') \qquad //$$

§. Generating Theorem for S Matrix

$$\boxed{\frac{\delta S(t,t')}{\delta\phi(1)} = -\frac{i}{\hbar}\Theta(t,t_1,t')\,T[\rho_H(1)S(t,t')] \qquad (28)}$$

where $\Theta(t,t_1,t') = 1$ for $t \underset{p}{>} t_1 \underset{p}{>} t'$ and $=0$ otherwise; $t \underset{p}{>} t_1$ means that t is later than t_1 on the closed time path.

∵ $\frac{\delta}{\delta\phi(1)}S(t,t')$

$$= \sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n\frac{\delta}{\delta\phi(1)}\int_p d1\cdots\int_p dn\,\phi(1)\cdots\phi(n)\,T[\rho_H(1)\cdots\rho_H(n)]$$

$$= \sum_{n=1}^{\infty}\frac{1}{(n-1)!}\left(-\frac{i}{\hbar}\right)^n\int_p d2\cdots\int_p dn\,\phi(2)\cdots\phi(n)\,T[\rho_H(1)\rho_H(2)\cdots\rho_H(n)] \quad (\text{for } t>t_1>t')$$

$$= -\frac{i}{\hbar}T[\rho_H(1)S] \qquad //$$

※ Note that the functional derivatives in the closed time path formalism is defined so that

$$\delta f = \int_p \frac{\delta f}{\delta g(t)} \delta g(t)\, dt$$

$$= \int_{-\infty}^{\infty} \frac{\delta f}{\delta g(t)} \delta g(t)\, dt + \int_{\infty}^{-\infty} \frac{\delta f}{\delta g(t)} \delta g(t) dt \qquad (29)$$

In the "single-time representation", on the other hand,

$$\delta f = \int_{-\infty}^{\infty} \frac{\delta f}{g(t_+)} \delta g(t_+) dt_+ + \int_{-\infty}^{\infty} \frac{\delta f}{\delta g(t_-)} \delta g(t_-) dt_- \qquad (30)$$

so that the sign on the minus path is opposite to that in Eq. (29).

§. Generating Theorem

$$\langle \theta(t) \rangle \equiv \frac{\mathrm{tr}\{T[\theta_H(t) S] \rho\}}{\mathrm{tr}[S\rho]} \tag{31}$$

where

$$\rho = \sum_n |\psi_{\mathcal{H}}^{(n)}\rangle P_n \langle \psi_{\mathcal{H}}^{(n)}| \tag{32}$$

with $|\psi_{\mathcal{H}}^{(n)}\rangle$ the nth eigenstate of the Hamiltonian H and P_n its probability.

We likewise define the averages of $\theta(t)$ separately on the plus and minus paths as follows:

$$\begin{cases} \langle \theta_+(t) \rangle \equiv \mathrm{tr}\{S_- T_+[\theta_H(t) S_+] \rho\} / \mathrm{tr}[S\rho] & (33a) \\ \langle \theta_-(t) \rangle \equiv \mathrm{tr}\{T_-[\theta_H(t) S_-] S_+ \rho\} / \mathrm{tr}[S\rho] & (33b) \end{cases}$$

Generating theorem is stated as

$$\frac{\delta \langle T[\theta(1)\cdots] \rangle}{\delta\phi(\nu)} = -\frac{i}{\hbar} \langle T[\delta P(\nu)\, \theta(1)\cdots] \rangle \tag{34}$$

where

$$\delta P(\nu) = P(\nu) - \langle P(\nu) \rangle \tag{35}$$

$$\because \frac{\delta}{\delta\phi(\nu)} \frac{\mathrm{tr}\{T[\theta_H(1)\cdots S] \rho\}}{\mathrm{tr}[S\rho]}$$

$$= -\frac{i}{\hbar}\left[\frac{\mathrm{tr}\{T[P_H(\nu)\theta_H(1)\cdots S]\rho\}}{\mathrm{tr}[S\rho]} - \frac{\mathrm{tr}\{T[\theta_H(1)\cdots S]\rho\}\,\mathrm{tr}\{T[P(\nu) S]\rho\}}{\{\mathrm{tr}[S\rho]\}^2} \right]$$

$$= -\frac{i}{\hbar}\left[\langle T[P(\nu)\theta(1)\cdots] \rangle - \langle T[\theta(1)\cdots] \rangle \langle P(\nu) \rangle \right] \quad //$$

※On the Generating Average

In the case $\Phi_-(1) = \Phi_+(1)$, $S = S_-(-\infty,\infty)\, S_+(\infty,-\infty) = 1$,

so that

$$\frac{\mathrm{tr}\{T[\theta_H(t) S]\rho\}}{\mathrm{tr}[S\rho]} \xrightarrow[\Phi_+=\Phi_-]{} \mathrm{tr}[S_-(-\infty,t)\,\theta_H(t)\,S_+(t,-\infty)\,\rho],$$

i.e., the generating average reduces to the physical average. Here, we have used the identity $\mathrm{tr}\,\rho = 1$.