The Generalized Master Equation within the Nakajima-Zwanzig Formalism (Following F. Haake, Springer tracts in Modern Physics, 66 98 (1973))

Consider an extended system S+B consisting of a system S and a bath B, each of which with a distinct Hilbert space ($\mathcal{H}_{S+B} = \mathcal{H}_S \otimes \mathcal{H}_B$).

Let $W(t)$ be the density operator of S+B and H its Hamiltonian such that:

$$\boxed{\dot{W} = -\frac{i}{\hbar}[H,W] = -i\mathcal{L}W \quad ; \quad \mathcal{L} = \frac{1}{\hbar}[H,\cdot\,]}$$

Assume that

$$\boxed{H = \underbrace{H_S}_{\text{free } S} + \underbrace{H_B}_{\text{free } B} + \underbrace{H_{SB}}_{SB \text{ interaction}}}$$

Let $\boxed{\rho(t) = \operatorname{tr}_B(W(t))}$ be the reduced density operator of S.

Definition of projector operator ($\mathcal{B}$):

$$W(t) = \mathcal{B}W(t) + (1-\mathcal{B})W(t) \quad , \quad \mathcal{B}^2 = \mathcal{B}$$

$$\mathcal{B} = B_{ref} \otimes \operatorname{tr}_B \quad ; \quad \operatorname{tr}_B(B_{ref}) = 1 \quad (B_{ref} \text{ a bath operator})$$

$$\Rightarrow \mathcal{B}W(t) = B_{ref} \otimes \operatorname{tr}_B(W) = B_{ref} \otimes \rho(t)$$

Remarks
- $(1-\mathcal{B})W(t)$ contains information on bath dynamics and bath-system correlations.
- B_{ref} is chosen arbitrarily by convinience (as long as $\operatorname{tr}_B(B_{ref}) = 1$

$$\dot W = \mathcal{B}\dot W + (1-\mathcal{B})\dot W = -i\mathcal{L}W = -i\mathcal{L}\mathcal{B}W - i\mathcal{L}(1-\mathcal{B})W$$

Operate on this Eq. with $\mathcal{B}$ from left $(\mathcal{B}(1-\mathcal{B})=0)$

$$\mathcal{B}^2\dot W + \cancel{\mathcal{B}(1-\mathcal{B})}\dot W = -i\mathcal{B}\mathcal{L}\mathcal{B}W - i\mathcal{B}\mathcal{L}(1-\mathcal{B})W$$

$$\Rightarrow \boxed{\mathcal{B}\dot W = -i\mathcal{B}\mathcal{L}\mathcal{B}W - i\mathcal{B}\mathcal{L}(1-\mathcal{B})W}$$

Operate on this Eq. with $1-\mathcal{B}$ from left:

$$\boxed{(1-\mathcal{B})\dot W = -i(1-\mathcal{B})\mathcal{L}\mathcal{B}W - i(1-\mathcal{B})\mathcal{L}(1-\mathcal{B})W}$$

~~The last equation has the following form:~~

$$\cancel{\dot y + py = Q(t)}, \text{ ~~where:~~}$$

$$\cancel{y \leftrightarrow (1-\mathcal{B})W}$$

$$\cancel{Q(t) \leftrightarrow -i(1-\mathcal{B})\mathcal{L}\mathcal{B}W(t)}$$

$$\cancel{p \leftrightarrow +i(1-\mathcal{B})\mathcal{L}}$$

~~The solution (1-st order differential Eq.):~~

$$\cancel{y(t) = e^{-pt}\left\{\int_0^t Q(t')e^{pt'}dt' + y(0)\right\}}$$

$$\cancel{\Rightarrow (1-\mathcal{B})W(t) = e^{-i(1-\mathcal{B})\mathcal{L}t}(1-\mathcal{B})W(0) - i\int_0^t dt'(1-\mathcal{B})\mathcal{L}\mathcal{B}W(t')}$$

Consider an operator Equation :

$$\boxed{\frac{dy}{dt} + Py = Q(t)}$$

where y $Q(t)$ are operators and P a super-operator.

Operate with the yet undefined operator z from the left :

$$z\frac{dy}{dt} + zPy = zQ(t)$$

Define z such that $\frac{dz}{dt} = zP$. Operate with z^{-1} on both sides: $z^{-1}dz = Pdt \Rightarrow z(t) = e^{Pt}$ (we chose $z(0) = I$ so it doesn't matter from which side it appears).

$$\Rightarrow z\frac{dy}{dt} + zPy = z\frac{dy}{dt} + \frac{dz}{dt}y = \frac{d}{dt}(zy) = \frac{d}{dt}(e^{Pt}y) = e^{Pt}Q(t$$

$$\Rightarrow e^{Pt}y(t) - y(0) = \int_0^t e^{Pt'}Q(t')dt'$$

$$\Rightarrow y(t) = e^{-Pt}y(0) + \int_0^t dt' e^{-P(t-t')} Q(t')dt'$$

$$\tau = t - t' \Rightarrow dt' = -d\tau$$

$$t' = 0 \Rightarrow \tau = t$$

$$t' = t \Rightarrow \tau = 0$$

$$\Rightarrow y(t) = e^{-Pt}y(0) + \int_0^t d\tau\, e^{-P\tau} Q(t-\tau)$$

$$\Rightarrow \boxed{y(t) = e^{-Pt}y(0) + \int_0^t dt' e^{-Pt'} Q(t-t')}$$

In our case:

$$y \leftrightarrow (1-\mathfrak{B})W$$

$$P \leftrightarrow i(1-\mathfrak{B})\mathcal{L}$$

$$Q(t) \leftrightarrow -i(1-\mathfrak{B})\mathcal{L}\mathfrak{B}W(t)$$

$$\Rightarrow \boxed{\begin{aligned} &(1-\mathfrak{B})W(t) = e^{-i(1-\mathfrak{B})\mathcal{L}t}\, W(0) \\ &-i\int_0^t dt'\, e^{-i(1-\mathfrak{B})\mathcal{L}t'} (1-\mathfrak{B})\mathcal{L}\mathfrak{B}W(t-t') \end{aligned}}$$

We substitute this expression for $(1-\mathcal{B})W(t)$ in the first equation (that for $\mathcal{B}\dot{W}(t)$):

$$\mathcal{B}\dot{W} = -i\mathcal{B}\mathcal{L}\mathcal{B}W - i\mathcal{B}\mathcal{L}\Big\{ e^{-i(1-\mathcal{B})\mathcal{L}t}(1-\mathcal{B})W(0) - i\int_0^t dt'\, e^{-i(1-\mathcal{B})\mathcal{L}t'}(1-\mathcal{B})\mathcal{L}\mathcal{B}W(t-t') \Big\}$$

We now operate with tr_B on each of the terms and expand them:

- $\mathrm{tr}_B(\mathcal{B}\dot{W}) = \frac{d}{dt}\mathrm{tr}_B\{B_{ref}\,\mathrm{tr}_B(W)\} = \mathrm{tr}_B(B_{ref})\dot{\rho} = \dot{\rho}$

$$\Rightarrow \boxed{\mathrm{tr}_B(\mathcal{B}\dot{W}) = \dot{\rho}}$$

- $-i\,\mathrm{tr}_B(\mathcal{B}\mathcal{L}\mathcal{B}W) = -i\,\mathrm{tr}_B\{B_{ref}\otimes \mathrm{tr}_B\,\mathcal{L}\mathcal{B}W\} = -i\,\mathrm{tr}_B(\mathcal{L}\mathcal{B}W)$

$$= -i\,\mathrm{tr}_B(\mathcal{L}(B_{ref}\otimes\rho(t)) = -i\,\mathrm{tr}_B(\mathcal{L}B_{ref})\rho(t)$$

$$\mathrm{tr}_B(\mathcal{L}B_{ref}\rho) = \underbrace{\frac{1}{\hbar}\mathrm{tr}_B[H_S, B_{ref}\rho]}_{I} + \underbrace{\frac{1}{\hbar}\mathrm{tr}_B[H_b, B_{ref}\rho]}_{II} + \underbrace{\frac{1}{\hbar}\mathrm{tr}_B(H_{BS}, B_{ref}}_{III}$$

$$I = \frac{1}{\hbar}\mathrm{tr}_B(B_{ref})[H_S,\rho] = \frac{1}{\hbar}[H_S,\rho] = \mathcal{L}_S(\rho)$$

$$II = \frac{1}{\hbar}\left(\mathrm{tr}_B[H_B, B_{ref}]\right)\rho = 0$$

$$III = \frac{1}{\hbar}\mathrm{tr}_B(H_{BS}, B_{ref}\rho) = \left(\mathrm{tr}_B(\mathcal{L}_{BS}B_{ref})\right)\rho$$

$$\Rightarrow \boxed{-i\,\mathrm{tr}_B(\mathcal{B}\mathcal{L}\mathcal{B}W) = -i\mathcal{L}_{eff}(\rho) = -i\mathcal{L}_S(\rho) - i\left(\mathrm{tr}_B(\mathcal{L}_{BS}B_{ref})\right)\rho}$$

$$\cdot \operatorname{tr}_B \mathcal{B}\mathcal{L}\int_0^t dt'\, e^{-i(1-\mathcal{B})\mathcal{L}t'}(1-\mathcal{B})\mathcal{L}\,\mathcal{B}\,W(t-t')$$

$$= -\int_0^t dt' \operatorname{tr}_B\left\{\mathcal{L}\, e^{-i(1-\mathcal{B})\mathcal{L}t'}(1-\mathcal{B})\mathcal{L}\, B_{ref}\right\}\rho(t-t')$$

$$\equiv \int_0^t dt'\, K(t')\,\rho(t-t') \quad , \text{ where}$$

$$K(t) = -\operatorname{tr}_B\left\{\mathcal{L}\, e^{-i(1-\mathcal{B})\mathcal{L}t'}(1-\mathcal{B})\mathcal{L}\, B_{ref}\right\}$$

$$*\;(1-\mathcal{B})\mathcal{L}_s B_{ref}\,\rho = \mathcal{L}_s B_{ref}\,\rho - \underbrace{\mathcal{B}\mathcal{L}_s B_{ref}\,\rho}_{B_{ref}\left(\operatorname{tr}_B B_{ref}\right)\mathcal{L}_s\rho \,=\, B_{ref}\,\mathcal{L}_s\rho \,=\, \mathcal{L}_s B_{ref}\,\rho} = 0$$

$$\Rightarrow \quad (1-\mathcal{B})\mathcal{L}\, B_{ref} = (1-\mathcal{B})(\mathcal{L}_b + \mathcal{L}_{sb})B_{ref}$$

$$*\;\operatorname{tr}_B(\mathcal{L}_B A) = \operatorname{tr}_B\Big(H_B, \sum_{i,j} a_{ij}\, B_i\otimes S_j\Big) = \sum_{i,j} a_{ij}\, S_j \overbrace{\operatorname{tr}_B\left(H_B, B_i\right)}^{0} = 0$$

$$*\;\operatorname{tr}_b\left(\mathcal{L}_s\, e^{-i(1-\mathcal{B})\mathcal{L}t'}(1-\mathcal{B})\mathcal{L}\, B_{ref}\right)$$

$$= \mathcal{L}_s \operatorname{tr}_b\left(e^{-i(1-\mathcal{B})\mathcal{L}t'}(1-\mathcal{B})\mathcal{L}\, B_{ref}\right)$$

$$= \mathcal{L}_s \operatorname{tr}_b\left((1-\mathcal{B})\mathcal{L}\, e^{-i(1-\mathcal{B})\mathcal{L}t'} B_{ref}\right) \leftarrow$$ unnecessary - see remark in next page.

Now, $\operatorname{tr}_B[(1-\mathcal{B})A] = \operatorname{tr}_B(A) - \operatorname{tr}_B(\mathcal{B}A) = \operatorname{tr}_B(A) - \operatorname{tr}_B\left(B_{ref}\operatorname{tr}_B(A)\right)$

$$= \operatorname{tr}_B(A) - \operatorname{tr}_B(A) = 0 .$$

where did the $\mathcal{L}_S$ go?

$$\Rightarrow \boxed{K(t) = -\operatorname{tr}_B\left\{(\mathcal{L}_{sB}\, e^{-i(1-\mathcal{B})\mathcal{L}t'}(1-\mathcal{B})(\mathcal{L}_B + \mathcal{L}_{sB})B_{ref}\right\}}$$

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$$\bullet\ -i\,\mathrm{tr}_B\left\{\mathcal{B}\mathcal{L}e^{-i(1-\mathcal{B})\mathcal{L}t}(1-\mathcal{B})W(0)\right\} = I(t)$$

$$= -i\,\mathrm{tr}_B\left\{\mathcal{L}e^{-i(1-\mathcal{B})\mathcal{L}t}(1-\mathcal{B})W(0)\right\}$$

$$*\ \mathrm{tr}_B(\mathcal{L}_B A) = 0$$

$$*\ \mathrm{tr}_B\,\mathcal{L}_S e^{-i(1-\mathcal{B})\mathcal{L}t}(1-\mathcal{B})W(0)$$

$$= \mathcal{L}_S\,\mathrm{tr}_B\left(e^{-i(1-\mathcal{B})\mathcal{L}t}(1-\mathcal{B})W(0)\right)$$

(* see remark below)

$$= \mathcal{L}_S\,\mathrm{tr}_B\left((1-\mathcal{B})\mathcal{L}e^{-i(1-\mathcal{B})\mathcal{L}t}\mathcal{L}^{-1}W(0)\right) = 0 \quad (\text{as for } K(t))$$

$$\Rightarrow \boxed{I(t) = -i\,\mathrm{tr}_B\,\mathcal{L}_{SB}\,e^{-i(1-\mathcal{B})\mathcal{L}t}(1-\mathcal{B})W(0)}$$

Remark:

We don't have to assume the existance of $\mathcal{L}^{-1}$:

$$e^{-i(1-\mathcal{B})\mathcal{L}t}(1-\mathcal{B})W(0)$$

$$= \sum_{n=0}^{\infty}\frac{1}{n!}(-i)^n[(1-\mathcal{B})\mathcal{L}t]^n(1-\mathcal{B})W(0)$$

This is a sum of terms, each of which has the form

$$(1-\mathcal{B})A$$

Since $\mathrm{tr}_B[(1-\mathcal{B})A] = 0$, whatever A is (see above in the proof for $K(t)$) $\mathrm{tr}_B\left(e^{-i(1-\mathcal{B})\mathcal{L}t}(1-\mathcal{B})W(0)\right) = 0$.

Let $B_{ref} = \rho_b^{eq} = e^{-\beta H_b} / \mathrm{Tr}_b (e^{-\beta H_b})$

$\mathcal{L}_B B_{ref} = [H_B, \rho_b^{eq}] = 0$

$$\Rightarrow K(t) = -\mathrm{tr}_B \, \mathcal{L}_{sb} \, e^{-i(1-\mathcal{B})\mathcal{L}t} (1-\mathcal{B}) \mathcal{L}_{sb} \rho_b^{eq}$$

$$I(t) = -i \, \mathrm{tr}_B \, \mathcal{L}_{sb} \, e^{-i(1-\mathcal{B})\mathcal{L}t} (1-\mathcal{B}) \, W(0)$$

Make a second order perturbation expansion approx:

$$e^{-i(1-\mathcal{B})\mathcal{L}t} \to e^{-i(1-\mathcal{B})(\mathcal{L}_s + \mathcal{L}_b)t} \equiv e^{-i(1-\mathcal{B})\mathcal{L}_0 t}$$

$$\Rightarrow K(t) \simeq -\mathrm{tr}_B \, \mathcal{L}_{sb} \, e^{-i(1-\mathcal{B})\mathcal{L}_0 t} (1-\mathcal{B}) \mathcal{L}_{sb} \rho_b^{eq}$$

$$I(t) = -i \, \mathrm{tr}_B \, \mathcal{L}_{sb} \, e^{-i(1-\mathcal{B})\mathcal{L}_0 t} (1-\mathcal{B}) \, W(0)$$

Now, for a projection operator $\mathcal{P}$ ($\mathcal{P}^2 = \mathcal{P}$):

$$\mathcal{P} F(A) \mathcal{P} = \mathcal{P} F(A\mathcal{P}) = F(\mathcal{P}A)\mathcal{P} = F(\mathcal{P}A\mathcal{P})$$

Proof:

$$F(\mathcal{P}A\mathcal{P}) = \sum_{n=0}^{\infty} a_n (\mathcal{P}A\mathcal{P})^n = \sum_n a_n (\mathcal{P}A\mathcal{P})^n = \sum_n a_n \mathcal{P}^n A^n \mathcal{P}^n$$

$$= \underbrace{\mathcal{P} \sum_n a_n A^n \mathcal{P}^n}_{\mathcal{P} F(A\mathcal{P})} = \underbrace{\left(\sum_n a_n \mathcal{P}^n A^n\right) \mathcal{P}}_{F(\mathcal{P}A)\mathcal{P}} = \underbrace{\mathcal{P} \left(\sum_n a_n A^n\right) \mathcal{P}}_{\mathcal{P} F(A) \mathcal{P}}$$

Hence

$$e^{-i(1-\mathcal{B})\mathcal{L}_0 t} (1-\mathcal{B}) = e^{-i(1-\mathcal{B})\mathcal{L}_0 (1-\mathcal{B}) t}$$

$$\bullet\ \mathcal{B}\mathcal{L}_{sb}\rho_b^{eq} = \rho_b^{eq}\,\mathrm{tr}_B\,[H_{sb},\rho_b^{eq}]$$

Let $H_{sb} = \sum_{i,j} a_{ij}\, S_i B_j$

$$\Rightarrow \mathcal{B}\mathcal{L}_{sb}\rho_b^{eq} = \sum_{i,j} a_{ij}\,\rho_b^{eq}\,\underbrace{\mathrm{tr}_B[B_j,\rho_b^{eq}]}_{=0}\, S_i = 0$$

$$\Rightarrow \boxed{\mathcal{B}\mathcal{L}_{sb}\rho_b^{eq} = 0}$$

$$\bullet\ \mathcal{L}_0\mathcal{B}A = \mathcal{L}_0\rho_b^{eq}\,\mathrm{tr}_B(A) = [H_s + H_b,\ \rho_b^{eq}\,\mathrm{tr}_B(A)]$$

$$= \rho_b^{eq}[H_s, \mathrm{tr}_B(A)] + \underbrace{[H_b, \rho_b^{eq}]}_{=0}\,\mathrm{tr}_B(A) = \mathcal{L}_s\mathcal{B}A$$

$$\Rightarrow \boxed{\mathcal{L}_0\mathcal{B} = \mathcal{L}_s\mathcal{B}}$$

$$\Rightarrow \mathcal{B}\mathcal{L}_0\mathcal{B} = \mathcal{B}\mathcal{L}_s\mathcal{B} = \rho_b^{eq}\,\mathrm{tr}_B\,[H_s, \rho_b^{eq}\,\mathrm{tr}_B(A)]$$

$$= \rho_b^{eq}\,\underbrace{\mathrm{tr}_B(\rho_b^{eq})}_{=1}\,[H_s, \mathrm{tr}_B(A)] = \mathcal{L}_s\mathcal{B} = \mathcal{L}_0\mathcal{B}$$

$$\Rightarrow \mathcal{B}\mathcal{L}_0\mathcal{B} = \mathcal{L}_0\mathcal{B} \Rightarrow (1-\mathcal{B})\mathcal{L}_0\mathcal{B} = 0 \Rightarrow \boxed{(1-\mathcal{B})\mathcal{L}_0(1-\mathcal{B}) = (1-\mathcal{B})\mathcal{L}_0}$$

$$\bullet\ e^{-i(1-\mathcal{B})\mathcal{L}_0 t} = 1 - it(1-\mathcal{B})\mathcal{L}_0 - \frac{1}{2}t^2(1-\mathcal{B})\mathcal{L}_0(1-\mathcal{B})\mathcal{L}_0$$

$$+ i\frac{1}{3!}(1-\mathcal{B})\mathcal{L}_0(1-\mathcal{B})\mathcal{L}_0(1-\mathcal{B})\mathcal{L}_0 + \frac{1}{4!}(1-\mathcal{B})\mathcal{L}_0(1-\mathcal{B})\mathcal{L}_0(1-\mathcal{B})\mathcal{L}_0(1-\mathcal{B})\mathcal{L}_0$$

$$+ \dots$$

$$= 1 - it(1-\mathcal{B})\mathcal{L}_0 - \frac{1}{2}t^2(1-\mathcal{B})\mathcal{L}_0^2 + i\frac{1}{3!}(1-\mathcal{B})\mathcal{L}_0^3 + \dots$$

$$= \mathcal{B} + (1-\mathcal{B})e^{-i\mathcal{L}_0 t}$$

$$\Rightarrow \boxed{e^{-i(1-\mathcal{B})\mathcal{L}_0 t} = \mathcal{B} + (1-\mathcal{B})e^{-i\mathcal{L}_0 t}}$$

$$\bullet\ \mathrm{tr}_B(\mathcal{L}_{SB}\,\mathcal{B}A) = \mathrm{tr}_B\left\{\left[H_{SB}, \rho_b^{eq}\,\mathrm{tr}_B(A)\right]\right\}$$

$$= \sum_{i,j} a_{ij}\,\mathrm{tr}_B\left[S_i B_j, \rho_b^{eq}\,\mathrm{tr}_B(A)\right]$$

$$= \sum_{i,j} a_{ij}\,\underbrace{\mathrm{tr}_B(B_j\rho_b^{eq})}_{\langle B_j\rangle_{eq}=0}\left[S_i, \mathrm{tr}_B(A)\right] = 0$$

$$\Rightarrow \boxed{\text{If } \mathrm{tr}_B(B_j\rho_b^{eq}) = 0 \Rightarrow \mathrm{tr}_B(\mathcal{L}_{SB}\,\mathcal{B}A) = 0}$$

$$\Rightarrow \boxed{\begin{aligned} K(t) &= -\mathrm{tr}_B\,\mathcal{L}_{SB}\,e^{-i\mathcal{L}_0 t}\,\mathcal{L}_{SB}\,\rho_B^{eq} \\ I(t) &= -i\,\mathrm{tr}_B\,\mathcal{L}_{SB}\,e^{-i\mathcal{L}_0 t}(1-\mathcal{B})\,W(0) \end{aligned}}$$

<u>Summary</u>

$$\boxed{\begin{aligned} \dot{\rho}(t) &= -i\mathcal{L}_{eff}\,\rho(t) + \int_0^t dt'\,K(t')\,\rho(t-t') + I(t) \\ \mathcal{L}_{eff} &= \mathcal{L}_S + \mathrm{tr}_B(\mathcal{L}_{SB}\,\rho_B^{eq}) \\ K(t) &= -\mathrm{tr}_B(\mathcal{L}_{SB}\,e^{-i\mathcal{L}_0 t}\,\mathcal{L}_{SB}\,\rho_B^{eq}) \\ I(t) &= -i\,\mathrm{tr}_B\,\mathcal{L}_{SB}\,e^{-i\mathcal{L}_0 t}(1-\mathcal{B})\,W(0) \end{aligned}}$$

$K(t) = ?$

Let σ be an operator in $\mathcal{H}_S$.

* x does not have to be the coordinate - It can be any system operator !

$$K(t)\sigma = -\mathrm{tr}_B\left(\mathcal{L}_{SB}\, e^{-i\mathcal{L}_0 t}\mathcal{L}_{SB}\,\rho_b^{eq}\sigma\right)$$

$$H_{sb} = -\sum_i c_i x_i\, x \equiv \Lambda x\,; \quad \Lambda = -\sum_i c_i x_i$$

- $\mathcal{L}_{SB}\rho_b^{eq}\sigma = \frac{1}{\hbar}[\Lambda x, \rho_b^{eq}\sigma] = \frac{1}{\hbar}\left(\Lambda\rho_b^{eq}\otimes x\sigma - \rho_b^{eq}\Lambda\otimes\sigma x\right)$

- $e^{-i\mathcal{L}_0 t}\mathcal{L}_{SB}\rho_b^{eq}\sigma = \frac{1}{\hbar}\Big\{e^{-i\mathcal{L}_b t}\Lambda\rho_b^{eq}\otimes e^{-i\mathcal{L}_s t}x\sigma$

$$- e^{-i\mathcal{L}_b t}\rho_b^{eq}\Lambda\otimes e^{-i\mathcal{L}_s t}\sigma x\Big\}$$

* $\dot{\Lambda} = i\mathcal{L}_B\Lambda \Rightarrow e^{-i\mathcal{L}_B t}\Lambda = \Lambda(-t)$

$$= \frac{1}{\hbar}\left\{\Lambda(-t)\rho_b^{eq}\otimes e^{-i\mathcal{L}_s t}x\sigma - \rho_b^{eq}\Lambda(-t)\otimes e^{-i\mathcal{L}_s t}\sigma x\right\}$$

- $-\mathrm{tr}_B\left(\mathcal{L}_{SB}\, e^{-i\mathcal{L}_0 t}\mathcal{L}_{SB}\,\rho_b^{eq}\sigma\right)$

$$= -\frac{1}{\hbar^2}\mathrm{tr}_B\left\{\left[\Lambda x, \Lambda(-t)\rho_b^{eq}\otimes e^{-i\mathcal{L}_s t}x\sigma - \rho_b^{eq}\Lambda(-t)\otimes e^{-i\mathcal{L}_s t}\sigma x\right]\right\}$$

$$= -\frac{1}{\hbar^2}\Big[x, \Big\{\mathrm{tr}_B(\Lambda\Lambda(-t)\rho_b^{eq})\, e^{-i\mathcal{L}_s t}x\sigma$$

$$- \mathrm{tr}_B(\Lambda(-t)\Lambda\rho_b^{eq})\, e^{-i\mathcal{L}_s t}\sigma x\Big\}$$

proof?

* $\mathrm{tr}_B(\Lambda\Lambda(-t)\rho_b^{eq}) = \mathrm{tr}_B(\Lambda(t)\Lambda\rho_b^{eq}) = c(t)$

$\mathrm{tr}_B(\Lambda(-t)\Lambda\rho_b^{eq}) = \left(\mathrm{tr}_B(\rho_b^{eq}\Lambda\Lambda(-t))\right)^* = c^*(t)$

$$= -\frac{1}{\hbar^2}\left[x, c(t)e^{-i\mathcal{L}_s t}x\sigma - c^*(t)e^{-i\mathcal{L}_s t}\sigma x\right]$$

Let $c(t) = a(t) + ib(t)$ (12)

$$\Rightarrow -\operatorname{tr}_B \left(\mathcal{L}_{sb} e^{-i\mathcal{L}_0 t} \mathcal{L}_{sb} \rho_b^{eq} \sigma \right)$$

$$= -\frac{1}{\hbar^2} \left[x, (a(t) + ib(t)) e^{-i\mathcal{L}_s t} x\sigma - (a(t) - ib(t)) e^{-i\mathcal{L}_s t} \sigma x \right]$$

$$= -\frac{1}{\hbar^2} \left\{ [x, a(t) e^{-i\mathcal{L}_s t} \underset{\substack{\uparrow \\ i\mathcal{L}_-}}{[x,\sigma]} + ib(t) e^{-i\mathcal{L}_s t} [x,\sigma]_+ \right\}$$

Let $\mathcal{L}_+ = [x, \cdot]_+ = x \cdot - \cdot x$

$\mathcal{L}_- = -i[x, \cdot]$

$$= +\frac{1}{\hbar^2} \mathcal{L}_- \left(a(t) e^{-i\mathcal{L}_s t} \mathcal{L}_- + b(t) e^{-i\mathcal{L}_s t} \mathcal{L}_+ \right) \sigma$$

$\underline{I(t) = ?}$

$$I(t) = -i\lambda \operatorname{tr}_B \mathcal{L}_{SB}^{(1)} e^{-i\mathcal{L}_0 t} (1 - \mathcal{P}) W(0)$$

$$= -i\lambda \operatorname{tr}_B \mathcal{L}_{SB}^{(1)} e^{-i\mathcal{L}_0 t} \left(\rho_T(0) - \rho_b^{eq} \operatorname{tr}_b(\rho_T(0))\right)$$

$$\cong +i\lambda^2 \operatorname{tr}_B \mathcal{L}_{SB}^{(1)} e^{-i\mathcal{L}_0 t} \frac{1}{Z_s Z_b} \int_0^\beta d\beta' e^{(\beta'-\beta)(H_b+H_s)} H_{bs}^{(1)} e^{-\beta'(H_b+H_s)}$$

$$= \frac{i\lambda^2}{Z_s Z_b} \int_0^\beta d\beta' \operatorname{tr}_B \mathcal{L}_{SB}^{(1)} e^{-i\mathcal{L}_0 t} e^{(\beta'-\beta)(H_b+H_s)} H_{bs}^{(1)} e^{-\beta'(H_b+H_s)}$$

• $e^{(\beta'-\beta)(H_b+H_s)} H_{bs}^{(1)} e^{-\beta'(H_b+H_s)} =$

$$= e^{(\beta'-\beta)H_b} \Lambda e^{-\beta' H_b} \otimes e^{(\beta'-\beta)H_s} \times e^{-\beta' H_s}$$

• $e^{-i\mathcal{L}_0 t} e^{(\beta'-\beta)(H_b+H_s)} H_{bs}^{(1)} e^{-\beta'(H_b+H_s)}$

$$= e^{(\beta'-\beta)H_b} e^{-i\mathcal{L}_b t} \Lambda e^{-\beta' H_b} \otimes e^{(\beta'-\beta)H_s} e^{-i\mathcal{L}_s t} \times e^{-\beta' H_s}$$

$$= e^{(\beta'-\beta)H_b} \Lambda(-t) e^{-\beta' H_b} \otimes e^{(\beta'-\beta)H_s} e^{-i\mathcal{L}_s t} \times e^{-\beta' H_s}$$

Switching the order of these two operators is not allowed in the time-dependent case. But it is not necessary for the final result (we switch again at the end).

• $\operatorname{tr}_B \mathcal{L}_{SB}^{(1)} e^{-i\mathcal{L}_0 t} e^{(\beta'-\beta)(H_b+H_s)} H_{bs}^{(1)} e^{-\beta'(H_b+H_s)}$

$$= \frac{1}{\hbar}\left[x, \operatorname{tr}_B\left(\Lambda e^{(\beta'-\beta)H_b} \Lambda(-t) e^{-\beta' H_b}\right) e^{(\beta'-\beta)H_s} e^{-i\mathcal{L}_s t} \times e^{-\beta' H_s}\right]$$

$$= \frac{1}{\hbar}\Big[x, \operatorname{tr}_B\Big(\underbrace{e^{-\beta' H_b} \Lambda e^{\beta' H_b}}_{\substack{e^{i(i\beta')H_b} \Lambda e^{-i(i\beta')H_b} \\ = \Lambda(i\beta'\hbar)}} e^{-\beta H_b} \Lambda(-t)\Big) e^{(\beta'-\beta)H_s} e^{-i\mathcal{L}_s t} \times e^{-\beta' H_s}\Big]$$

$$= \frac{1}{\hbar}\left[x, \operatorname{tr}_B\left(e^{-\beta H_b} \Lambda(-t) \Lambda(i\beta'\hbar)\right) e^{(\beta'-\beta)H_s} e^{-i\mathcal{L}_s t} \times e^{-\beta' H_s}\right]$$

$$= \frac{1}{\hbar} Z_B \left[x, C(-i\hbar\beta' - t) e^{(\beta'-\beta)H_s} e^{-i\mathcal{L}_s t} \times e^{-\beta' H_s}\right.$$

$$\Rightarrow I(t) = \frac{i\lambda^2}{\hbar Z_s} \int_0^\beta d\beta' \left[x, c(-i\hbar\beta' - t) e^{(\beta'-\beta)H_s} e^{-i\mathcal{L}_s t} \times e^{-\beta' H_s} \right]$$

Let $\mathcal{L}_- = -i[x, \cdot]$

$$\Rightarrow I(t) = -\frac{\lambda^2}{\hbar Z_s} \mathcal{L}_- e^{-i\mathcal{L}_s t} \int_0^\beta d\beta' \underbrace{c(-i\hbar\beta' - t)}_{\shortparallel} e^{(\beta'-\beta)H_s} \times e^{-\beta' H_s}$$

$$\int_{-\infty}^{\infty} \frac{d\omega}{\pi} J(\omega) \frac{e^{-i\omega(-i\hbar\beta' - t)}}{1 - e^{-\beta\hbar\omega}}$$

$$= \int_{-\infty}^{\infty} \frac{d\omega}{\pi} J(\omega) \frac{e^{i\omega t - \hbar\beta'\omega}}{1 - e^{-\hbar\beta\omega}}$$

$$\Rightarrow \boxed{I(t) = -\frac{\lambda^2}{\hbar Z_s} \mathcal{L}_- e^{-i\mathcal{L}_s t} \int_0^\beta d\beta' c(-i\hbar\beta' - t) e^{(\beta'-\beta)H_s} \times e^{-\beta' H_s}}$$

Appendix to 22.2.98 version

Consider the expression:

$$\mathcal{G}(\beta,t) =$$

$$\lim_{T\to\infty} \int_0^T dt' \int_0^\beta d\beta' \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{J(\omega)}{1-e^{-\beta\hbar\omega}} (-i\mathcal{L}_s^0 + i\omega)\, e^{(-i\mathcal{L}_s^0+i\omega)t'}\, e^{i\omega t}$$

$$\times e^{-(\beta-\beta')H_s^0} \times e^{-\beta'(H_s^0+\hbar\omega)}$$

The integration with respect to t' can be carried out analytically

$$\int_0^T dt'\, e^{(-i\mathcal{L}_s^0+i\omega)t'} = (-i\mathcal{L}_s^0+i\omega)^{-1}\left(e^{(-i\mathcal{L}_s^0+i\omega)T} - 1\right)$$

$$\Rightarrow \mathcal{G}(\beta,t) = \lim_{T\to\infty}\Bigg\{ \int_0^\beta d\beta' \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{J(\omega)}{1-e^{-\beta\hbar\omega}} e^{(-i\mathcal{L}_s^0+i\omega)T}\, e^{i\omega t}$$

$$e^{-(\beta-\beta')H_s^0} \times e^{-\beta'(H_s^0+\hbar\omega)}$$

$$- \int_0^\beta d\beta' \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{J(\omega)}{1-e^{-\beta\hbar\omega}} e^{i\omega t} e^{-(\beta-\beta')H_s^0}$$

$$\times e^{-\beta'(H_s^0+\hbar\omega)} \Bigg\}$$

The integral in ω in the first term vanishes at $T\to\infty$:

$$\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{J(\omega)}{1-e^{-\beta\hbar\omega}} e^{i\omega(T+t+i\hbar\beta'\omega)} = C(-T-t-i\hbar\beta'\omega)$$

$$= C^*(T+t+i\hbar\beta'\omega) \xrightarrow{T\to\infty} 0$$

Hence the first term vanishes.

$$\Rightarrow \mathcal{G}(\beta,t) = -\int_0^\beta d\beta' \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{J(\omega)}{1-e^{-\beta\hbar\omega}} e^{i\omega t} e^{-(\beta-\beta')H_s^0} \times e^{-\beta'(H_s^0+\hbar\omega)}$$

(15)

$$= -\int_0^\beta d\beta' \left\{ \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{J(\omega)}{1-e^{-\beta\hbar\omega}} e^{i\omega(t+i\beta\hbar)} \right\} e^{-(\beta-\beta')H_S^0} \times e^{-\beta' H_S^0}$$

$$= -\int_0^\beta d\beta' < (-t - i\beta\hbar) \, e^{(\beta'-\beta)H_S^0} \times e^{-\beta' H_S^0}$$

which is the integral in $I(t)$.

On the other hand:

$$g(\beta,t) = \lim_{T\to\infty} \int_0^T dt' \int_0^\beta d\beta' \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{J(\omega)}{1-e^{-\beta\hbar\omega}} e^{(-i\mathcal{L}_S^0 + i\omega)t'} e^{i\omega(t+i\beta'\hbar)}$$

$$\underbrace{(-i\mathcal{L}_S^0 + i\omega) \cdot e^{-(\beta-\beta')H_S^0} \times e^{-\beta' H_S^0}}$$

$$e^{-(\beta-\beta')H_S^0} \underbrace{(-i\mathcal{L}_S^0 + i\omega) \times e^{-\beta' H_S^0}}$$

$$\mathcal{L}_S^0 \times e^{-\beta' H_S^0} = \frac{1}{\hbar}\left[H_S^0, x e^{-\beta' H_S^0}\right]$$

$$= \frac{1}{\hbar}[H_S^0, x] e^{-\beta' H_S^0} + \frac{1}{\hbar} x \left(H_S^0, e^{-\beta' H_S^0} \right)$$

$$\Rightarrow (-i\mathcal{L}_S^0 + i\omega) e^{-(\beta-\beta')H_S^0} \times e^{-\beta' H_S^0}$$

$$= e^{-(\beta-\beta')H_S^0} \left\{ -\frac{i}{\hbar}(H_S^0, x) e^{-\beta' H_S^0} + i\omega x e^{-\beta' H_S^0} \right\}$$

On the other hand:

$$\mathcal{G}(\beta,t) =$$

$$\lim_{T\to\infty} \int_0^T dt' \int_0^\beta d\beta' \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{J(\omega)}{1-e^{-\beta\hbar\omega}} e^{(-i\mathcal{L}_s^\circ + i\omega)t'} e^{i\omega t}$$

$$\underbrace{\times (-i\mathcal{L}_s^\circ + i\omega) e^{-(\beta-\beta')H_s^\circ} \times e^{-\beta'(H_s^\circ+\hbar\omega)}}$$

$$-\frac{i}{\hbar} e^{-(\beta-\beta')H_s^\circ} [H_s, X] e^{-\beta'(H_s^\circ+\hbar\omega)} + i\omega e^{-(\beta-\beta')H_s^\circ} \times e^{-\beta'(H_s^\circ+\hbar\omega)}$$

$$= -i\left\{ \underbrace{e^{-(\beta-\beta')H_s^\circ}[H_s, X] e^{-\beta' H_s^\circ}}_{\frac{d}{d\beta'}\left\{e^{-(\beta-\beta')H_s^\circ} \times e^{-\beta' H_s^\circ}\right\}} \frac{1}{\hbar} e^{-\beta'\hbar\omega} + \underbrace{\frac{1}{\hbar}\left(-\hbar\omega e^{-\beta'\hbar\omega}\right)}_{\frac{d}{d\beta'}\left(\frac{1}{\hbar} e^{-\beta'\hbar\omega}\right)} e^{-(\beta-\beta')H_s^\circ} \times e^{-\beta' H_s^\circ} \right\}$$

$$= e^{-(\beta-\beta')H_s^\circ} (H_s^\circ X - X H_s^\circ) e^{-\beta' H_s^\circ}$$

$$= e^{-(\beta-\beta')H_s^\circ} [H_s^\circ, X] e^{-\beta' H_s^\circ}$$

$$\Rightarrow \mathcal{G}(\beta,t) =$$

$$-i \lim_{T\to\infty} \int_0^T dt' \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{J(\omega)}{1-e^{-\beta\hbar\omega}} e^{-i(\mathcal{L}_s^\circ + i\omega)t'} e^{i\omega t}$$

$$\times \frac{1}{\hbar} e^{-\beta'\hbar\omega} e^{-(\beta-\beta')H_s^\circ} \times e^{-\beta' H_s^\circ} \Big|_0^\beta$$

$$= -i \lim_{T\to\infty} \int_0^T dt' \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{J(\omega)}{1-e^{-\beta\hbar\omega}} e^{(-i\mathcal{L}_s^\circ + i\omega)t'} e^{i\omega t}$$

$$\times \frac{1}{\hbar}\left(e^{-\beta\hbar\omega} X e^{-\beta H_s^\circ} - e^{-\beta H_s^\circ} X \right)$$

$$= -i\frac{1}{\hbar}\lim_{T\to\infty}\int_0^T dt'\left(\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{J(\omega)}{1-e^{-\beta\hbar\omega}}e^{-\beta\hbar\omega}\,e^{i\omega(t+t')}\right)e^{-i\mathcal{L}_s^0 t'}\times e^{-\beta H_s^0}$$

$$+ i\frac{1}{\hbar}\lim_{T\to\infty}\int_0^T dt'\left(\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{J(\omega)}{1-e^{-\beta\hbar\omega}}\,e^{i\omega(t+t')}\right)e^{-i\mathcal{L}_s^0 t'}e^{-\beta H_s^0}\times$$

$$= -\frac{i}{\hbar}\int_0^\infty dt'\left(c(t+t')\,e^{-i\mathcal{L}_s^0 t'}\times e^{-\beta H_s^0} - c^*(t+t')\,e^{-i\mathcal{L}_s^0 t'}e^{-\beta H_s^0}\times\right)$$

$$* \int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{J(\omega)}{1-e^{-\beta\hbar\omega}}e^{-\beta\hbar\omega}\,e^{i\omega t} = \int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{J(\omega)}{e^{\beta\hbar\omega}-1}e^{i\omega t}$$

$$\overset{\omega\to-\omega}{=}\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{J(-\omega)}{e^{-\beta\hbar\omega}-1}e^{-i\omega t} \overset{J(-\omega)=-J(\omega)}{=} \int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{J(\omega)}{1-e^{-\beta\hbar\omega}}e^{-i\omega t} = c(t)$$

$$\Rightarrow\ \mathcal{G}(\beta,t) = -\frac{i}{\hbar}\int_0^\infty dt'\Big\{\underbrace{c(t+t')}_{=\,a+ib}\,e^{-i\mathcal{L}_s^0 t'}\times e^{-\beta H_s^0} - \underbrace{c^*(t+t')}_{=\,a-ib}\,e^{-i\mathcal{L}_s^0 t'}e^{-\beta H_s^0}\times\Big\}$$

$$= -\frac{i}{\hbar}\int_0^\infty dt'\Big\{a(t+t')\left(e^{-i\mathcal{L}_s^0 t'}\times e^{-\beta H_s^0} - e^{-i\mathcal{L}_s^0 t'}e^{-\beta H_s^0}\times\right)$$
$$+ ib(t+t')\left(e^{-i\mathcal{L}_s^0 t'}\times e^{-\beta H_s^0} + e^{-i\mathcal{L}_s^0 t'}e^{-\beta H_s}\times\right)\Big\}$$

$$= -\frac{i}{\hbar}\int_0^\infty dt'\Big\{a(t+t')\,e^{-i\mathcal{L}_s^0 t'}\,i\mathcal{L}_-\,e^{-\beta H_s^0} + ib(t+t')\,e^{-i\mathcal{L}_s^0 t'}\mathcal{L}_+\,e^{-\beta H_s}\Big\}$$

$$= \frac{1}{\hbar}\int_0^\infty dt'\,e^{-i\mathcal{L}_s^0 t'}\left(a(t+t')\mathcal{L}_- + b(t+t')\mathcal{L}_+\right)e^{-\beta H_s^0}$$

$t'\to -t'$

$$= \frac{1}{\hbar}\int_{-\infty}^0 dt'\,e^{i\mathcal{L}_s^0 t'}\left(a(t-t')\mathcal{L}_- + b(t-t')\mathcal{L}_+\right)e^{-\beta H_s^0}$$

$$\Rightarrow I(t) = \frac{\lambda^2}{\hbar Z_s} \mathcal{L}_- e^{-i\mathcal{L}_s t} \, g(\beta, t)$$

$$= \frac{\lambda^2}{\hbar Z_s} \mathcal{L}_- e^{-i\mathcal{L}_s t} \frac{1}{\hbar} \int_{-\infty}^{0} dt' e^{i\mathcal{L}_s^0 t'} \left(a(t-t')\mathcal{L}_- + b(t-t')\mathcal{L}_+ \right) e^{-\beta H_s^0}$$

$$= \frac{1}{\hbar^2} \lambda^2 \mathcal{L}_- \int_{-\infty}^{0} dt' e^{-i\mathcal{L}_s (t-t')} \left(a(t-t')\mathcal{L}_- + b(t-t')\mathcal{L}_+ \right) \frac{e^{-\beta H_s^0}}{Z_s}$$

$$\Rightarrow \boxed{I(t) = \frac{1}{\hbar^2} \lambda^2 \mathcal{L}_- \int_{-\infty}^{0} dt' e^{-i\mathcal{L}_s (t-t')} \left(a(t-t')\mathcal{L}_- + b(t-t')\mathcal{L}_+ \right) \frac{e^{-\beta H_s^0}}{Z_s}}$$