

# 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:

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

Assume that

$$H = H_S + H_B + H_{SB}$$

free  $S$       free  $B$        $S+B$  interaction

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

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

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

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

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

Remarks •  $(1-\mathcal{B})W(t)$  contains information on bath dynamics and bath-system correlations.

•  $\mathcal{B}_{\text{ref}}$  is chosen arbitrarily by convenience (as long as  $\text{tr}_B(\mathcal{B}_{\text{ref}}) = 1$ )

$$\dot{w} = \mathcal{B}\dot{w} + (1-\mathcal{B})\dot{w} = -iLw = -iL\mathcal{B}w - iL(1-\mathcal{B})w$$

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

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

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

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

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

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

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

~~$$y = (1-\mathcal{B})w$$~~

~~$$Q(t) \leftrightarrow i(1-\mathcal{B})L\mathcal{B}w(t)$$~~

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

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

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

~~$$(1-\mathcal{B})w(t) = e^{-i(1-\mathcal{B})Lt} (1-\mathcal{B})w(0) + \int_0^t dt' (1-\mathcal{B})L\mathcal{B}w(t')$$~~

Consider an operator Equation :

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

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 :  $Z^{-1} dz = P dt \Rightarrow Z(t) = e^{Pt}$  (we chose

$Z(0) = I$  so it doesn't matter from which side it appears).

$$\Rightarrow Z \frac{dy}{dt} + ZPy = Z \frac{dy}{dt} + \frac{dz}{dt} y = \frac{d}{dt}(Zy) = \frac{d}{dt}(e^{Pt} y) = e^{Pt} Q(t)$$

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

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

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

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

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

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

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

In our case:

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$$y \leftrightarrow (1-\beta)W$$

$$P \leftrightarrow i(1-\beta)L$$

$$Q(t) \leftrightarrow -i(1-\beta)L\beta W(t)$$

$$\Rightarrow (1-\beta)W(t) = e^{-i(1-\beta)Lt} W(0) + \int_0^t e^{-i(1-\beta)Lt'} (1-\beta)L\beta W(t-t') dt'$$



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$$\textcircled{1} \text{tr}_B \mathcal{B} \int_0^+ dt' e^{-i(1-\mathcal{B})L t'} (1-\mathcal{B}) L \mathcal{B} W(+t')$$

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

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

$$K(t) = - \text{tr}_B \left\{ L e^{-i(1-\mathcal{B})L t} (1-\mathcal{B}) L \mathcal{B} \text{ref} \right\}$$

$$*(1-\mathcal{B}) L_S \mathcal{B} \text{ref} \rho = L_S \mathcal{B} \text{ref} \rho - \mathcal{B} L_S \mathcal{B} \text{ref} \rho = 0$$

$$\downarrow$$

$$\mathcal{B} \text{ref} \left( \text{tr}_B \mathcal{B} \text{ref} \right) L_S \rho = \mathcal{B} \text{ref} L_S \rho = L_S \mathcal{B} \text{ref} \rho$$

$$\rightarrow (1-\mathcal{B}) L \mathcal{B} \text{ref} = (1-\mathcal{B})(L_b + L_{SB}) \mathcal{B} \text{ref}$$

$$* \text{tr}_B (L_B A) = \text{tr}_B \left( H_B, \sum_{i,j} a_{ij} B_i \otimes S_j \right) = \sum_{i,j} a_{ij} S_j \text{tr}_B \left( H_B, B_i \right) = 0$$

$$* \text{tr}_b \left( L_S e^{-i(1-\mathcal{B})L t} (1-\mathcal{B}) L \mathcal{B} \text{ref} \right)$$

$$= L_S \text{tr}_b \left( e^{-i(1-\mathcal{B})L t} (1-\mathcal{B}) L \mathcal{B} \text{ref} \right)$$

$$= L_S \text{tr}_b \left( (1-\mathcal{B}) L e^{-i(1-\mathcal{B})L t} \mathcal{B} \text{ref} \right) \leftarrow \text{unnecessary - see remark in next page.}$$

$$\text{Now, } \text{tr}_B [(1-\mathcal{B})A] = \text{tr}_B (A) - \text{tr}_B (\mathcal{B}A) = \text{tr}_B (A) - \text{tr}_B (\mathcal{B} \text{ref} \text{tr}_B (A))$$

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

*where did it go?*

$$\Rightarrow K(t) = - \text{tr}_B \left\{ L_{SB} e^{-i(1-\mathcal{B})L t} (1-\mathcal{B})(L_B + L_{SB}) \mathcal{B} \text{ref} \right\}$$

$$\bullet -i \text{tr}_B \left\{ 2L e^{-i(1-\beta)Lt} (1-\beta) W(r_0) \right\} = I(t)$$

$$= -i \text{tr}_B \left\{ L e^{-i(1-\beta)Lt} (1-\beta) W(r_0) \right\}$$

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$$\bullet \text{tr}_B(L_B A) = 0$$

$$\bullet \text{tr}_B L_S e^{-i(1-\beta)Lt} (1-\beta) W(r_0)$$

$$= L_S \text{tr}_B \left( e^{-i(1-\beta)Lt} (1-\beta) W(r_0) \right) \quad (* \text{ see remark below})$$

$$= L_S \text{tr}_B \left( (1-\beta) L e^{-i(1-\beta)Lt} L^{-1} W(r_0) \right) = 0 \quad (\text{as for } k(t))$$

$$\Rightarrow I(t) = -i \text{tr}_B L_{SB} e^{-i(1-\beta)Lt} (1-\beta) W(r_0)$$

Remark :

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

$$e^{-i(1-\beta)Lt} (1-\beta) W(r_0)$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} (-i)^n [(1-\beta)Lt]^n (1-\beta) W(r_0)$$

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

$$(1-\beta)A$$

Since  $\text{tr}_B((1-\beta)A) = 0$ , whatever  $A$  is (see above in the

proof for  $k(t)$ )  $\text{tr}_B \left( e^{-i(1-\beta)Lt} (1-\beta) W(r_0) \right) = 0$ .

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

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$$\mathcal{L}_B B_{\text{ref}} = (H_B \rho_b^{\text{eq}}) = 0$$

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

$$I(t) = -i \text{tr}_B \mathcal{L}_{sb} e^{-i(1-\mathcal{B})Lt} (1-\mathcal{B}) \text{ wr } 0$$

Make a second order perturbation expansion approx:

$$e^{-i(1-\mathcal{B})Lt} \rightarrow e^{-i(1-\mathcal{B})(\mathcal{L}_s + \mathcal{L}_b)t} \approx e^{-i(1-\mathcal{B})\mathcal{L}_s t}$$

$$\Rightarrow K(t) \approx -\text{tr}_B \mathcal{L}_{sb} e^{-i(1-\mathcal{B})\mathcal{L}_s t} (1-\mathcal{B}) \mathcal{L}_{sb} \rho_b^{\text{eq}}$$

$$I(t) = -i \text{tr}_B \mathcal{L}_{sb} e^{-i(1-\mathcal{B})\mathcal{L}_s t} (1-\mathcal{B}) \text{ wr } 0$$

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:

$$F(\mathcal{P} A \mathcal{P}) = \sum_{n=0}^{\infty} \frac{1}{n!} a_n (\mathcal{P} A \mathcal{P})^n = \sum_n a_n (\mathcal{P} A \mathcal{P})^n = \sum_n a_n \mathcal{P} A^n \mathcal{P}$$

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

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

Hence:

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



$$\bullet \mathcal{B}L_{sb} \rho_b^{eq} = \rho_b^{eq} \text{tr} [H_{sb}, \rho_b^{eq}]$$

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$$\text{Let } H_{sb} = \sum_{ij} a_{ij} s_i B_j$$

$$\Rightarrow \mathcal{B}L_{sb} \rho_b^{eq} = \sum_{ij} a_{ij} \rho_b^{eq} \text{tr} [B_j, \rho_b^{eq}] s_i = 0$$

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

$$\bullet L_0 \mathcal{B}A = L_0 \rho_b^{eq} \text{tr} (A) = [H_s + H_b, \rho_b^{eq} \text{tr} (A)]$$

$$= \rho_b^{eq} \text{tr} (A) + \underbrace{(H_b, \rho_b^{eq})}_{=0} \text{tr} (A) = L_s \mathcal{B}A$$

$$\Rightarrow \boxed{L_0 \mathcal{B} = L_s \mathcal{B}}$$

$$\Rightarrow \mathcal{B}L_0 \mathcal{B} = \mathcal{B}L_s \mathcal{B} = \rho_b^{eq} \text{tr} [H_s, \rho_b^{eq} \text{tr} (A)]$$

$$= \rho_b^{eq} \text{tr} (\rho_b^{eq}) \text{tr} (A) = L_s \mathcal{B} = L_0 \mathcal{B}$$

$$\Rightarrow \mathcal{B}L_0 \mathcal{B} = L_0 \mathcal{B} \Rightarrow (1 - \mathcal{B}) L_0 \mathcal{B} = 0 \Rightarrow \boxed{(1 - \mathcal{B}) L_0 (1 - \mathcal{B}) = (1 - \mathcal{B}) L_0}$$

$$\bullet e^{-i(1-\mathcal{B})L_0 t} = 1 - it(1-\mathcal{B})L_0 - \frac{1}{2}t^2(1-\mathcal{B})L_0(1-\mathcal{B})L_0 + i\frac{1}{3!}(1-\mathcal{B})L_0(1-\mathcal{B})L_0(1-\mathcal{B})L_0 + \frac{1}{4!}(1-\mathcal{B})L_0(1-\mathcal{B})L_0(1-\mathcal{B})L_0(1-\mathcal{B})L_0 + \dots$$

$$= 1 - it(1-\mathcal{B})L_0 - \frac{1}{2}t^2(1-\mathcal{B})L_0^2 + i\frac{1}{3!}(1-\mathcal{B})L_0^3 + \dots$$

$$= \mathcal{B} + (1-\mathcal{B})e^{-iL_0 t}$$

$$\Rightarrow \boxed{e^{-i(1-\mathcal{B})L_0 t} = \mathcal{B} + (1-\mathcal{B})e^{-iL_0 t}}$$

