

# The Mother of all Master Equations

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## I. THE HAMILTONIAN

We start with a time-dependent Hamiltonian of the form:

$$H_T(t) = H_S(t) + H_I + H_B, \quad (1)$$

$$H_S(t) = \sum_i \varepsilon_i(t) |i\rangle\langle i| + \sum_{i \neq j} V_{ij}(t) |i\rangle\langle j|, \quad (2)$$

$$H_I = \sum_i |i\rangle\langle i| \sum_{\mathbf{k}} \left( g_{i\mathbf{k}} b_{\mathbf{k}}^\dagger + g_{i\mathbf{k}}^* b_{\mathbf{k}} \right), \quad (3)$$

$$H_B = \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}}. \quad (4)$$

## II. UNITARY TRANSFORMATION INTO THE VARIATIONALLY OPTIMIZABLE FRAME

We will apply to  $H(t)$ , the unitary transformation defined by  $e^{\pm V(t)}$ , where  $V(t)$  is the variationally optimizable anti-Hermitian operator:

$$V(t) \equiv \sum_i |i\rangle\langle i| \sum_{\mathbf{k}} \left( \frac{v_{i\mathbf{k}}(t)}{\omega_{\mathbf{k}}} b_{\mathbf{k}}^\dagger - \frac{v_{i\mathbf{k}}^*(t)}{\omega_{\mathbf{k}}} b_{\mathbf{k}} \right) \quad (5)$$

in terms of the variational scalar parameters  $\{v_{\mathbf{k}}\}$ , which will soon be optimized in order to give the most accurate possible master equation for the system's dynamics in the presence of this bath. Operators  $O(t)$  in the variational frame will be written as:

$$\overline{O}(t) \equiv e^{V(t)} O(t) e^{-V(t)}. \quad (6)$$

We assume that the bath starts equilibrium with inverse temperature  $\beta = 1/k_B T$ :

$$\rho_B \equiv \rho_B(0) \quad (7)$$

$$= \frac{e^{-\beta H_B}}{\text{Tr}(e^{-\beta H_B})} \quad (8)$$

With the following definitions:

$$\begin{pmatrix} B_{iz}(t) & B_i^\pm(t) \\ B_x(t) & B_i(t) \\ B_y(t) & B_{ij}(t) \end{pmatrix} \equiv \begin{pmatrix} \sum_{\mathbf{k}} \left( (g_{i\mathbf{k}} - v_{i\mathbf{k}}(t)) b_{\mathbf{k}}^\dagger + (g_{i\mathbf{k}} - v_{i\mathbf{k}}(t))^* b_{\mathbf{k}} \right) & e^{\pm \sum_{\mathbf{k}} \left( \frac{v_{i\mathbf{k}}(t)}{\omega_{\mathbf{k}}} b_{\mathbf{k}}^\dagger - \frac{v_{i\mathbf{k}}^*(t)}{\omega_{\mathbf{k}}} b_{\mathbf{k}} \right)} \\ \frac{B_0^+(t) B_0^-(t) + B_0^+(t) B_1^-(t) - B_{10}(t) - B_{01}(t)}{2} & e^{-\frac{1}{2} \sum_{\mathbf{k}} \left| \frac{v_{i\mathbf{k}}(t)}{\omega_{\mathbf{k}}} \right|^2 \coth(\beta \omega_{\mathbf{k}}/2)} \\ \frac{B_0^+(t) B_1^-(t) - B_1^+(t) B_0^-(t) + B_{10}(t) - B_{01}(t)}{2i} & e^{-\frac{1}{2} \sum_{\mathbf{k}} \left| \frac{v_{i\mathbf{k}}(t) - v_{j\mathbf{k}}(t)}{\omega_{\mathbf{k}}} \right|^2 \coth(\frac{\beta \omega_{\mathbf{k}}}{2})} e^{\chi_{ij}(t)} \end{pmatrix}, \quad (9)$$

$$R_i(t) \equiv \sum_{\mathbf{k}} \left( \frac{|v_{i\mathbf{k}}(t)|^2}{\omega_{\mathbf{k}}} - \left( g_{i\mathbf{k}} \frac{v_{i\mathbf{k}}^*(t)}{\omega_{\mathbf{k}}} + g_{i\mathbf{k}}^* \frac{v_{i\mathbf{k}}(t)}{\omega_{\mathbf{k}}} \right) \right), \quad (10)$$

$$\chi_{ij}(t) \equiv \sum_{\mathbf{k}} \left( \frac{v_{i\mathbf{k}}^*(t) v_{j\mathbf{k}}(t) - v_{i\mathbf{k}}(t) v_{j\mathbf{k}}^*(t)}{2\omega_{\mathbf{k}}^2} \right), \quad (11)$$

$$(\cdot)^{\Re} \equiv \Re(\cdot), \quad (12)$$

$$(\cdot)^{\Im} \equiv \Im(\cdot). \quad (13)$$

we may write the transformed Hamiltonian as a sum of the form:

$$\overline{H}_T(t) \equiv \overline{H}_{\bar{S}}(t) + \overline{H}_{\bar{I}}(t) + \overline{H}_{\bar{B}} \quad (14)$$

$$\overline{H}_{\bar{S}}(t) \equiv \sum_i (\varepsilon_i(t) + R_i(t)) |i\rangle\langle i| + \sigma_x (B_{10}^{\Re}(t) V_{10}^{\Re}(t) - B_{10}^{\Im}(t) V_{10}^{\Im}(t)) - \sigma_y (B_{10}^{\Re}(t) V_{10}^{\Im}(t) + B_{10}^{\Im}(t) V_{10}^{\Re}(t)) \quad (15)$$

$$\overline{H}_{\bar{I}}(t) \equiv \sum_i B_{iz}(t) |i\rangle\langle i| + V_{10}^{\Re}(t) (B_x(t) \sigma_x + B_y(t) \sigma_y) - V_{10}^{\Im}(t) (B_x(t) \sigma_y - B_y(t) \sigma_x) \quad (16)$$

$$\overline{H}_{\bar{B}} \equiv \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} \quad (17)$$

$$= H_B \quad (18)$$

### III. FREE-ENERGY MINIMIZATION

The true free energy  $A(t)$  is bounded by the Bogoliubov inequality:

$$A(t) \leq A_B(t) \equiv -\frac{1}{\beta} \ln \left( \text{Tr} \left( e^{-\beta \overline{H}_{\bar{S}}(t) + \overline{H}_{\bar{B}}} \right) \right) + \langle \overline{H}_{\bar{I}}(t) \rangle_{\overline{H}_{\bar{S}}(t) + \overline{H}_{\bar{B}}} + O \left( \langle \overline{H}_{\bar{I}}(t) \rangle_{\overline{H}_{\bar{S}}(t) + \overline{H}_{\bar{B}}} \right) \quad (19)$$

We will optimize the set of variational parameters  $\{v_{\mathbf{k}}(t)\}$  in order to minimize  $A_B(t)$  (i.e. to make it as close to the true free energy  $A(t)$  as possible). Neglecting the higher order terms and using  $\langle \overline{H}_{\bar{I}}(t) \rangle_{\overline{H}_{\bar{S}}(t) + \overline{H}_{\bar{B}}} = 0$  we can obtain the following condition to obtain the set  $\{v_{\mathbf{k}}(t)\}$ :

$$\frac{\partial A_B(\{v_{\mathbf{k}}(t)\}; t)}{\partial v_{i\mathbf{k}}(t)} = 0. \quad (20)$$

This leads us to:

$$v_{i\mathbf{k}}(\omega_{\mathbf{k}}, t) = \frac{g_i(\omega_{\mathbf{k}}) \left( 1 - \frac{\tanh(\frac{\beta\eta(t)}{2})}{\eta(t)} (2\varepsilon_i(t) + 2R_i(t) - \varepsilon(t)) \right) + 2 \frac{\tanh(\frac{\beta\eta(t)}{2})}{\eta(t)} \frac{v_{i'\mathbf{k}}(\omega_{\mathbf{k}}, t)}{\omega_{\mathbf{k}}} |B_{10}(t)|^2 |V_{10}(t)|^2 \coth(\beta\omega_{\mathbf{k}}/2)}{1 - \frac{\tanh(\frac{\beta\eta(t)}{2})}{\eta(t)} \left( \varepsilon(t) - 2(\varepsilon(t) - \varepsilon_i(t) - R_i(t)) - \frac{2|V_{10}(t)|^2 |B_{10}(t)|^2 \coth(\beta\omega_{\mathbf{k}}/2)}{\omega_{\mathbf{k}}} \right)}, \quad (21)$$

If  $i = 1$  then  $i' = 0$  and viceversa. Also we have the following definitions:

$$\eta(t) \equiv \sqrt{(\text{Tr}(\overline{H}_{\bar{S}}(t)))^2 - 4\text{Det}(\overline{H}_{\bar{S}}(t))} \quad (22)$$

$$\varepsilon(t) \equiv \text{Tr}(\overline{H}_{\bar{S}}(t)). \quad (23)$$

### IV. MASTER EQUATION

We transform any operator  $O(t)$  into the interaction picture in the following way:

$$\tilde{O}(t) \equiv U^{\dagger}(t) O(t) U(t) \quad (24)$$

$$U(t) \equiv \mathcal{T} \exp \left( -i \int_0^t dt' \overline{H}_T(t') \right). \quad (25)$$

Therefore:

$$\widetilde{\rho_S}(t) = U^\dagger(t) \overline{\rho_S}(t) U(t) \quad (26)$$

We will initialize the density operator as:  $\rho_{\text{Total}}(0) = \rho_S(0) \otimes \rho_B(0)$ , where  $\rho_B(0) \equiv \rho_B^{\text{Thermal}} \equiv \rho_B$ . Taking as reference state  $\rho_B$  and truncating at second order in  $\overline{H_I}(t)$ , we obtain our master equation in the interaction picture:

$$\frac{d\widetilde{\rho_S}(t)}{dt} = - \int_0^t \text{Tr}_B \left[ \widetilde{H_I}(t), \left[ \widetilde{H_I}(s), \widetilde{\rho_S}(t) \rho_B \right] \right] ds \quad (27)$$

To simplify this we define the following matrix:

$$\begin{pmatrix} A \\ B(t) \\ C(t) \end{pmatrix} = \begin{pmatrix} \sigma_x & \sigma_y & \frac{I-\sigma_z}{2} & \sigma_x & \sigma_y & \frac{I+\sigma_z}{2} \\ B_x(t) & B_y(t) & B_{1z}(t) & B_y(t) & B_x(t) & B_{0z}(t) \\ V_{10}^{\Re}(t) & V_{10}^{\Im}(t) & 1 & V_{10}^{\Im}(t) & -V_{10}^{\Re}(t) & 1 \end{pmatrix}. \quad (28)$$

$$\overline{H_I}(t) = \sum_i C_i(t) (A_i \otimes B_i(t)) \quad (29)$$

$$\widetilde{H_I}(t) = \sum_i C_i(t) (\widetilde{A}_i(t) \otimes \widetilde{B}_i(t)), \quad (30)$$

and expanding the commutators yields:

$$\frac{d\widetilde{\rho_S}(t)}{dt} = - \int_0^t \text{Tr}_B \left( \sum_j C_j(t) (\widetilde{A}_j(t) \otimes \widetilde{B}_j(t)) \sum_i C_i(s) (\widetilde{A}_i(s) \otimes \widetilde{B}_i(s)) \widetilde{\rho_S}(t) \rho_B - \sum_j C_j(t) (\widetilde{A}_j(t) \otimes \widetilde{B}_j(t)) \widetilde{\rho_S}(t) \rho_B \sum_i C_i(s) (\widetilde{A}_i(s) \otimes \widetilde{B}_i(s)) \right. \quad (31)$$

$$\left. - \sum_i C_i(s) (\widetilde{A}_i(s) \otimes \widetilde{B}_i(s)) \widetilde{\rho_S}(t) \rho_B \sum_j C_j(t) (\widetilde{A}_j(t) \otimes \widetilde{B}_j(t)) + \widetilde{\rho_S}(t) \rho_B \sum_i C_i(s) (\widetilde{A}_i(s) \otimes \widetilde{B}_i(s)) \sum_j C_j(t) (\widetilde{A}_j(t) \otimes \widetilde{B}_j(t)) \right) ds. \quad (32)$$

We can keep the  $A(t)$  and  $C(t)$  as they are when tracing over the bath degrees of freedom, but we will replace the expected value of the  $B(t)$  operators by  $\mathcal{B}(t)$  such that:

$$\mathcal{B}_{ij}(t, s) \equiv \text{Tr}_B (\widetilde{B}_i(t) \widetilde{B}_j(s) \rho_B) \quad (33)$$

An useful property of the expected values  $\mathcal{B}_{ij}(t, s)$  is that they verify  $\mathcal{B}_{ji}^*(t, s) = \mathcal{B}_{ij}(s, t)$ . In order to calculate the correlation functions we rearranged the expression (33) such that:

$$B_i(t, \tau) \equiv e^{iH_B \tau} B_i(t) e^{-iH_B \tau} \quad (34)$$

$$\mathcal{B}_{ij}(t, s) = \text{Tr}_B (B_i(t, \tau) B_j(s, 0) \rho_B) \quad (35)$$

This allows us to remove the trace over the bath and write down a more tangible master equation:

$$\frac{d\widetilde{\rho_S}(t)}{dt} = - \int_0^t \left( \sum_{ij} C_i(t) C_j(s) \left( \mathcal{B}_{ij}(t, s) \left[ \widetilde{A}_i(t), \widetilde{A}_j(s) \widetilde{\rho_S}(t) \right] - \mathcal{B}_{ij}^*(t, s) \left[ \widetilde{A}_i(t), \widetilde{\rho_S}(t) \widetilde{A}_j(s) \right] \right) \right) ds \quad (36)$$

For returning the Schrödinger we define the following notation:

$$\widetilde{A}_j(s, t) = U(t) U^\dagger(s) A_j(t) U(s) U^\dagger(t) \quad (37)$$

Given that  $s = t - \tau$  then we can perform the change of variables in the integral of the equation (36), doing the reverse of the transformation to interaction picture we get:

$$\frac{d\overline{\rho_S}(t)}{dt} = -i[\overline{H_S}(t), \overline{\rho_S}(t)] - \sum_{ij} \int_0^t d\tau C_i(t) C_j(t-\tau) (\mathcal{B}_{ij}(t, t-\tau) [\widetilde{A_i}(t), \widetilde{A_j}(t-\tau, t) \overline{\rho_S}(t)] + \mathcal{B}_{ij}^*(t, t-\tau) [\overline{\rho_S}(t) \widetilde{A_j}(t-\tau, t), \widetilde{A_i}(t)]) \quad (38)$$

Let's consider the unitary operator  $U(t)$ :

$$U(t) \equiv \mathcal{T} \exp \left( -i \int_0^t dt' \overline{H_S}(t') \right) \quad (39)$$

$$= \mathbb{I} + \sum_{n=1}^{\infty} (-i)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \dots \int_0^{t_{n-1}} dt_n H(t_1) H(t_2) \dots H(t_n). \quad (40)$$

Here  $0 < t_1 < t_2 < \dots < t_{n-1} < t_n = t$  is a partition of the set  $[0, t]$ . We will use a perturbative solution to the exponential of a time-varying operator, this can be done if we write an effective hamiltonian  $H_E(t)$  such that  $\mathcal{T} \exp \left( -i \int_0^t dt' \overline{H_S}(t') \right) \equiv \exp(-it H_E(t))$ . The effective Hamiltonian is expanded in a series of terms of increasing order in time  $H_E(t) = H_E^{(0)}(t) + H_E^{(1)}(t) + H_E^{(2)}(t) + \dots$  so we can write:

$$U(t) = \exp \left( -it \left( H_E^{(0)}(t) + H_E^{(1)}(t) + H_E^{(2)}(t) + \dots \right) \right). \quad (41)$$

The terms can be found expanding  $\mathcal{T} \exp \left( -i \int_0^t dt' \overline{H_S}(t') \right)$  and  $U(t)$  then equating the terms of the same power. The lowest terms are:

$$H_E^{(0)}(t) = \frac{1}{t} \int_0^t \overline{H_S}(t') dt', \quad (42)$$

$$H_E^{(1)}(t) = -\frac{i}{2t} \int_0^t dt' \int_0^{t'} dt'' [\overline{H_S}(t'), \overline{H_S}(t'')], \quad (43)$$

$$H_E^{(2)}(t) = \frac{1}{6t} \int_0^t dt' \int_0^{t'} dt'' \int_0^{t''} dt''' ([\overline{H_S}(t'), \overline{H_S}(t'')], \overline{H_S}(t''')) + [\overline{H_S}(t'''), \overline{H_S}(t'')], \overline{H_S}(t')]. \quad (44)$$

The Fourier decomposition of the operator  $\widetilde{A_i}(t)$  using the expansion  $H_E(t)$  is:

$$\widetilde{A_i}(t) = U^\dagger(t) A_i(t) U(t) \quad (45)$$

$$= e^{iH_E(t)t} A_i(t) e^{-iH_E(t)t} \quad (46)$$

$$= \sum_{w(t)} e^{-itw(t)} \mathcal{A}_i(t, w(t)). \quad (47)$$

$w(t)$  belongs to the set of differences of eigenvalues of  $H_E(t)$  that depends of the time. As we can see the decomposition matrices are time-dependent as well.

Extending the Fourier decomposition to the matrix  $\widetilde{A_j}(t - \tau, t)$  we obtain :

$$\widetilde{A_j}(t - \tau, t) = \sum_{w(t-\tau), w'(t)} e^{i\tau w(t-\tau)} e^{-it(w(t-\tau) - w'(t))} \mathcal{A}_j(t; w(t-\tau), w'(t)) \quad (48)$$

Let's define:

$$\mathcal{A}_j(t; w(t-\tau), w'(t)) = \mathcal{A}_{jww'}(t; t-\tau, t). \quad (49)$$

So we can show that:

$$\widetilde{A}_j(t-\tau, t) = \sum_{w(t-\tau), w'(t)} e^{i\tau w(t-\tau)} e^{-it(w(t-\tau)-w'(t))} \mathcal{A}_{jww'}(t; t-\tau, t).$$

where  $w(t)$  and  $w'(t-\tau)$  belongs to the set of the differences of the eigenvalues of the Hamiltonian  $H_E(t)$  and  $H_E(t-\tau)$  respectively.

In order to show the explicit form of the matrices present in the RHS of the equation (46) for a general  $2 \times 2$  matrix in a given time let's write the matrix  $A_i(t)$  in the base  $W(t) = \{|+_t\rangle, |-_t\rangle\}$ , where the index  $t$  represents the time, formed by the time-dependent eigenvectors of  $H_E(t)$  in the following way:

$$A_i(t) = \sum_{\alpha_t, \beta_t \in W(t)} \langle \alpha_t | A_i(t) | \beta_t \rangle | \alpha_t \rangle \langle \beta_t |. \quad (50)$$

Given that  $[|+_t\rangle \langle +_t|, |-_t\rangle \langle -_t|] = 0$  because the normalized eigenvectors of a hermitic matrix form an orthonormal system, where  $H_E(t) |+_t\rangle = \lambda_+(t) |+_t\rangle$  and  $H_E(t) |-_t\rangle = \lambda_-(t) |-_t\rangle$ . The subscript  $t$  introduce the fact that the eigenvalues and eigenvectors are time-dependent. Using the Zassenhaus formula we obtain:

$$e^{i\tau H_E(\tau)} = e^{i\tau \lambda_+(\tau)} |+_t\rangle \langle +_t| + e^{i\tau \lambda_-(\tau)} |-_t\rangle \langle -_t|. \quad (51)$$

Calculating the transformation (46) directly using the previous relationship we find that:

$$U^\dagger(t-\tau) A_i(t) U(t-\tau) = \mathcal{A}_i(t; 0) + \mathcal{A}_i(t; -w(t-\tau)) e^{i(t-\tau)w(t-\tau)} + \mathcal{A}_i(t; w(t-\tau)) e^{-i(t-\tau)w(t-\tau)}. \quad (52)$$

Here  $w(t-\tau) = \lambda_+(t-\tau) - \lambda_-(t-\tau)$ . The expansion matrices of the Fourier decomposition for a general  $2 \times 2$  matrix are:

$$\mathcal{A}_i(t; 0) = \langle +_{t-\tau} | A_i(t) | +_{t-\tau} \rangle | +_{t-\tau} \rangle \langle +_{t-\tau} | + \langle -_{t-\tau} | A_i(t) | -_{t-\tau} \rangle | -_{t-\tau} \rangle \langle -_{t-\tau} |, \quad (53)$$

$$\mathcal{A}_i(t; -w(t-\tau)) = \langle +_{t-\tau} | A_i(t) | -_{t-\tau} \rangle | +_{t-\tau} \rangle \langle -_{t-\tau} |, \quad (54)$$

$$\mathcal{A}_i(t; w(t-\tau)) = \langle -_{t-\tau} | A_i(t) | +_{t-\tau} \rangle | -_{t-\tau} \rangle \langle +_{t-\tau} | \quad (55)$$

Given that  $\mathcal{A}_j(t; w(t-\tau), w'(t)) = \mathcal{A}_j^\dagger(t; -w(t-\tau), -w'(t))$  it's enough to describe the decomposition matrix of the double Fourier decomposition (48) as:

$$\mathcal{A}_i(t; 0, 0) = \langle +_t | \mathcal{A}_i(t; 0) | +_t \rangle | +_t \rangle \langle +_t | + \langle -_t | \mathcal{A}_i(t; 0) | -_t \rangle | -_t \rangle \langle -_t |, \quad (56)$$

$$\mathcal{A}_i(t; 0, w'(t)) = \langle -_t | \mathcal{A}_i(t; 0) | +_t \rangle | -_t \rangle \langle +_t | \quad (57)$$

$$\mathcal{A}_i(t; w(t-\tau), 0) = \langle +_t | \mathcal{A}_i(t; -w(t-\tau)) | +_t \rangle | +_t \rangle \langle +_t | + \langle -_t | \mathcal{A}_i(t; -w(t-\tau)) | -_t \rangle | -_t \rangle \langle -_t |, \quad (58)$$

$$\mathcal{A}_i(t; w(t-\tau), w'(t)) = \langle -_t | \mathcal{A}_i(t; -w(t-\tau)) | +_t \rangle | -_t \rangle \langle +_t | \quad (59)$$

$$\mathcal{A}_i(t; w(t-\tau), -w'(t)) = \langle +_t | \mathcal{A}_i(t; -w(t-\tau)) | -_t \rangle | +_t \rangle \langle -_t | \quad (60)$$

Replacing (48) in (38) we deduce that:

$$\frac{d\overline{\rho_S}(t)}{dt} = -i[\overline{H_S}(t), \overline{\rho_S}(t)] - \sum_{ijww'} \int_0^t d\tau C_i(t) C_j(t-\tau) \left( \mathcal{B}_{ij}(t, t-\tau) \left[ A_i(t), e^{i\tau w(t-\tau)} e^{-it(w(t-\tau)-w'(t))} \mathcal{A}_{jww'}(t-\tau, t) \overline{\rho_S}(t) \right] \right. \quad (61)$$

$$\left. + \mathcal{B}_{ij}^*(t, t-\tau) \left[ \overline{\rho_S}(t) e^{-i\tau w(t-\tau)} e^{it(w(t-\tau)-w'(t))} \mathcal{A}_{jww'}^\dagger(t-\tau, t), A_i(t) \right] \right) \quad (62)$$

Let's define the operator:

$$D_{ijww'}(t-\tau, t) \equiv C_i(t) C_j(t-\tau) \mathcal{B}_{ij}(t, t-\tau) e^{i\tau w(t-\tau)} e^{-it(w(t-\tau)-w'(t))} \mathcal{A}_{jww'}(t-\tau, t) \quad (63)$$

as we can see the adjoint of  $D_{ijww'}(t-\tau, t)$  is:

$$D_{ijww'}^\dagger(t-\tau, t) = C_i(t) C_j(t-\tau) \mathcal{B}_{ij}^*(t, t-\tau) e^{-i\tau w(t-\tau)} e^{it(w(t-\tau)-w'(t))} \mathcal{A}_{jww'}^\dagger(t-\tau, t) \quad (64)$$

we used the fact that  $C_i(t) \in \mathbb{R}$  for all  $i$ . With this notation applied to (62) we arrive to the following master equation:

$$\frac{d\overline{\rho_S}(t)}{dt} = -i [\overline{H_S}(t), \overline{\rho_S}(t)] - \sum_{ijww'} \int_0^t d\tau \left( [A_i(t), D_{ijww'}(t-\tau, t) \overline{\rho_S}(t)] - [\overline{\rho_S}(t) D_{ijww'}^\dagger(t-\tau, t), A_i(t)] \right) \quad (65)$$

We define a response matrix  $\mathcal{D}_{ijww'}(t)$  as:

$$\mathcal{D}_{ijww'}(t) = \int_0^t D_{ijww'}(t-\tau, t) d\tau \quad (66)$$

In particular, the  $\mathcal{B}(t, s)$  operators matrix it's defined in terms of  $\mathcal{B}(t, s) \equiv \mathcal{B}_{ij}(t, s)$  following the notation of the matrix (28) is:

$$\mathcal{B}(t, s) \equiv \begin{pmatrix} \mathcal{B}_{11}(t, s) & \mathcal{B}_{12}(t, s) & \mathcal{B}_{13}(t, s) & \mathcal{B}_{12}(t, s) & \mathcal{B}_{11}(t, s) & \mathcal{B}_{16}(t, s) \\ \mathcal{B}_{21}(t, s) & \mathcal{B}_{22}(t, s) & \mathcal{B}_{23}(t, s) & \mathcal{B}_{22}(t, s) & \mathcal{B}_{21}(t, s) & \mathcal{B}_{26}(t, s) \\ \mathcal{B}_{31}(t, s) & \mathcal{B}_{32}(t, s) & \mathcal{B}_{33}(t, s) & \mathcal{B}_{32}(t, s) & \mathcal{B}_{31}(t, s) & \mathcal{B}_{36}(t, s) \\ \mathcal{B}_{21}(t, s) & \mathcal{B}_{22}(t, s) & \mathcal{B}_{23}(t, s) & \mathcal{B}_{22}(t, s) & \mathcal{B}_{21}(t, s) & \mathcal{B}_{26}(t, s) \\ \mathcal{B}_{11}(t, s) & \mathcal{B}_{12}(t, s) & \mathcal{B}_{13}(t, s) & \mathcal{B}_{12}(t, s) & \mathcal{B}_{11}(t, s) & \mathcal{B}_{16}(t, s) \\ \mathcal{B}_{61}(t, s) & \mathcal{B}_{62}(t, s) & \mathcal{B}_{63}(t, s) & \mathcal{B}_{62}(t, s) & \mathcal{B}_{61}(t, s) & \mathcal{B}_{66}(t, s) \end{pmatrix}, \quad (67)$$

We can define:

$$N(\omega) \equiv (e^{\beta\omega} - 1)^{-1} \quad (68)$$

and the spectral density is defined in the usual way:

$$J_i(\omega) \equiv \sum_{\mathbf{k}} |g_{i\mathbf{k}}|^2 \delta(\omega - \omega_{\mathbf{k}}), \quad (69)$$

$$v_{i\mathbf{k}}(\omega_{\mathbf{k}}, t) = g_{i\mathbf{k}} F_i(\omega_{\mathbf{k}}, t). \quad (70)$$

In this case  $g_i(\omega)$  and  $v_i(\omega, t)$  are the continuous version of  $g_i(\omega_{\mathbf{k}})$  and  $v_{i\mathbf{k}}(\omega_{\mathbf{k}}, t)$  respectively.

The integral version of the correlation functions  $\text{Tr}_B(\widetilde{B}_i(t) \widetilde{B}_j(s) \rho_B)$  are equal to:

$$\chi_{10}(t) = \int_0^\infty \frac{\sqrt{J_1^*(\omega)} J_0(\omega) F_1^*(\omega, t) F_0(\omega, t) - \sqrt{J_1(\omega)} J_0^*(\omega) F_1(\omega, t) F_0^*(\omega, t)}{2\omega^2} d\omega \quad (71)$$

$$U_{10}(t, s) = \exp \left( i \left( \int_0^\infty \frac{(\sqrt{J_1(\omega)} F_1(\omega, t) - \sqrt{J_0(\omega)} F_0(\omega, t)) (\sqrt{J_1(\omega)} F_1(\omega, s) - \sqrt{J_0(\omega)} F_0(\omega, s))^* \exp(i\omega\tau)}{\omega^2} d\omega \right)^3 \right) \quad (72)$$

$$B_{10}(t) = \exp(\chi_{10}(t)) \exp \left( -\frac{1}{2} \int_0^\infty \left| \frac{\sqrt{J_1(\omega)} F_1(\omega, t) - \sqrt{J_0(\omega)} F_0(\omega, t)}{\omega} \right|^2 \coth \left( \frac{\beta\omega}{2} \right) d\omega \right), \quad (73)$$

$$\xi^+(t, s) = \exp \left( -\int_0^\infty \frac{|\left( \sqrt{J_1(\omega)} F_1(\omega, t) - \sqrt{J_0(\omega)} F_0(\omega, t) \right) \exp(i\omega\tau) + \sqrt{J_1(\omega)} F_1(\omega, s) - \sqrt{J_0(\omega)} F_0(\omega, s)|^2}{2\omega^2} \coth \left( \frac{\beta\omega}{2} \right) d\omega \right) \quad (74)$$

$$\xi^-(t, s) = \exp \left( -\int_0^\infty \frac{|\left( \sqrt{J_1(\omega)} F_1(\omega, t) - \sqrt{J_0(\omega)} F_0(\omega, t) \right) \exp(i\omega\tau) - \left( \sqrt{J_1(\omega)} F_1(\omega, s) - \sqrt{J_0(\omega)} F_0(\omega, s) \right)|^2}{2\omega^2} \coth \left( \frac{\beta\omega}{2} \right) d\omega \right) \quad (75)$$

$$Q(\omega, t) = \frac{\sqrt{J_1(\omega)} F_1(\omega, t) - \sqrt{J_0(\omega)} F_0(\omega, t)}{\omega} \quad (76)$$

$$\langle \widetilde{B}_x(t) \widetilde{B}_x(s) \rangle_B = \mathcal{B}_{11}(t, s) \quad (77)$$

$$= \frac{1}{2} \left( (\exp(\chi_{10}(t) + \chi_{10}(s)))^{\Re} U_{10}(t, s) \xi^+(t, s) + (\exp(\chi_{10}(t) + \chi_{01}(s)))^{\Re} U_{10}^*(t, s) \xi^-(t, s) \right) \quad (78)$$

$$- (B_{10}(t))^{\Re} (B_{01}(s))^{\Re} \quad (79)$$

$$\langle \widetilde{B}_y(t) \widetilde{B}_y(s) \rangle_B = \mathcal{B}_{22}(t, s) \quad (80)$$

$$= -\frac{1}{2} \left( (\exp(\chi_{01}(t) + \chi_{01}(s)))^{\Re} U_{10}(t, s) \xi^+(t, s) - (\exp(\chi_{10}(t) + \chi_{01}(s)))^{\Re} U_{10}^*(t, s) \xi^-(t, s) \right) \quad (81)$$

$$+ (B_{01}(t))^{\Im} (B_{10}(s))^{\Im} \quad (82)$$

$$\langle \widetilde{B}_x(t) \widetilde{B}_y(s) \rangle_B = \mathcal{B}_{12}(t, s) \quad (83)$$

$$= \frac{1}{2} \left( (\exp(\chi_{10}(t) + \chi_{01}(s)))^{\Im} U_{10}^*(t, s) \xi^-(t, s) + (\exp(\chi_{01}(t) + \chi_{01}(s)))^{\Im} U_{10}(t, s) \xi^+(t, s) \right) \quad (84)$$

$$+ (B_{10}(t))^{\Re} (B_{10}(s))^{\Im} \quad (85)$$

$$\langle \widetilde{B}_y(t) \widetilde{B}_x(s) \rangle_B = \mathcal{B}_{21}(t, s) \quad (86)$$

$$= \frac{1}{2} \left( (\exp(\chi_{01}(t) + \chi_{10}(s)))^{\Im} U_{10}^*(t, s) \xi^-(t, s) + (\exp(\chi_{01}(t) + \chi_{01}(s)))^{\Im} U_{10}(t, s) \xi^+(t, s) \right) \quad (87)$$

$$+ (B_{10}(t))^{\Im} (B_{10}(s))^{\Re} \quad (88)$$

$$\langle \widetilde{B}_{iz}(t) \widetilde{B}_{jz}(s) \rangle_B = \mathcal{B}_{nm}(t, s), (n, m \in \{3, 6\}) \quad (89)$$

$$= \int_0^\infty \left( \sqrt{J_i(\omega) J_j^*(\omega)} (1 - F_i(\omega, t)) (1 - F_j^*(\omega, s)) e^{i\omega\tau} N(\omega) + \sqrt{J_i^*(\omega) J_j(\omega)} (1 - F_i^*(\omega, t)) (1 - F_j(\omega, s)) e^{-i\omega\tau} (N(\omega) + 1) \right) d\omega, \quad (90)$$

$$\langle \widetilde{B}_{iz}(t) \widetilde{B}_x(s) \rangle_B = \mathcal{B}_{n1}(t, s), (n \in \{3, 6\}) \quad (91)$$

$$= i B_{01}^{\Im}(s) \int_0^\infty \left( \sqrt{J_i(\omega)} (1 - F_i(\omega, t)) Q^*(\omega, s) N(\omega) e^{i\omega\tau} - \sqrt{J_i^*(\omega)} (1 - F_i^*(\omega, t)) Q(\omega, s) e^{-i\omega\tau} (N(\omega) + 1) \right) d\omega, \quad (92)$$

$$\langle \widetilde{B}_x(t) \widetilde{B}_{iz}(s) \rangle_B = \mathcal{B}_{1n}(t, s), (n \in \{3, 6\}) \quad (93)$$

$$= i B_{01}^{\Im}(t) \int_0^\infty \left( \sqrt{J_i^*(\omega)} (1 - F_i^*(\omega, s)) Q(\omega, t) N(\omega) e^{i\omega\tau} - \sqrt{J_i(\omega)} (1 - F_i(\omega, s)) Q^*(\omega, t) e^{-i\omega\tau} (N(\omega) + 1) \right) d\omega, \quad (94)$$

$$\langle \widetilde{B}_{iz}(t) \widetilde{B}_y(s) \rangle_B = \mathcal{B}_{n2}(t, s), (n \in \{3, 6\}) \quad (95)$$

$$= i B_{10}^{\Re}(s) \int_0^\infty \left( \sqrt{J_i^*(\omega)} (1 - F_i^*(\omega, s)) Q(\omega, s) (N(\omega) + 1) e^{-i\omega\tau} - \sqrt{J_i(\omega)} (1 - F_i(\omega, s)) Q^*(\omega, s) e^{i\omega\tau} N(\omega) \right) d\omega, \quad (96)$$

$$\langle \widetilde{B}_y(t) \widetilde{B}_{iz}(s) \rangle_B = \mathcal{B}_{2n}(t, s), (n \in \{3, 6\}) \quad (97)$$

$$= i B_{10}^{\Re}(t) \int_0^\infty \left( \sqrt{J_i(\omega)} (1 - F_i(\omega, s)) Q(\omega, t) N(\omega) e^{i\omega\tau} - \sqrt{J_i^*(\omega)} (1 - F_i^*(\omega, s)) Q^*(\omega, t) e^{-i\omega\tau} (N(\omega) + 1) \right) d\omega. \quad (98)$$

Finally we end up with our final master equation in the variationally optimized frame in the Schrödinger picture:

$$\frac{d\overline{\rho_S}(t)}{dt} = -i [\overline{H_S}(t), \overline{\rho_S}(t)] - \sum_{ijww'} \left( [A_i(t), \mathcal{D}_{ijww'}(t) \overline{\rho_S}(t)] - [\overline{\rho_S}(t) \mathcal{D}_{ijww'}^\dagger(t), A_i(t)] \right) \quad (99)$$

If we extend the upper limit of integration to  $\infty$  in the equation (66) then the system will be independent of any preparation at  $t = 0$ , so the evolution of the system will depend only on its present state as expected in the Markovian approximation.

Applying the inverse transformation we will obtain that:

$$e^{-V(t)} \frac{d\overline{\rho_S}(t)}{dt} e^{V(t)} = e^{-V(t)} V'(t) e^{V(t)} \rho_S(t) + \dot{\rho_S}(t) - \rho_S(t) V'(t) \quad (100)$$

$$= -i e^{-V(t)} [\overline{H_S}(t), \overline{\rho_S}(t)] e^{V(t)} - \sum_{ijww'} \int_0^t d\tau \left( e^{-V(t)} [A_i, \mathcal{D}_{ijww'}(t - \tau, t) \overline{\rho_S}(t)] e^{V(t)} - e^{-V(t)} [A_i, \overline{\rho_S}(t) \mathcal{D}_{ijww'}^\dagger(t - \tau, t)] e^{V(t)} \right). \quad (101)$$

For a product and a commutator we have the inverse transformation:

$$e^{-V(t)} \overline{A(t) B(t)} e^{V(t)} = A(t) B(t) \quad (102)$$

$$e^{-V(t)} [A(t), B(t)] e^{V(t)} = [A(t), B(t)]. \quad (103)$$

So we will obtain that

$$e^{-V(t)} \frac{d\overline{\rho_S(t)}}{dt} e^{V(t)} = -i[H_S(t), \rho_S(t)] - \sum_{ijww'} \left( [e^{-V(t)} A_i(t) e^{V(t)}, e^{-V(t)} \mathcal{D}_{ijww'}(t) e^{V(t)} \rho_S(t)] - [e^{-V(t)} A_i(t) e^{V(t)}, \rho_S(t) e^{-V(t)} \mathcal{D}_{ijww'}^\dagger(t) e^{V(t)}] \right) \quad (104)$$

Re-defining  $\rho_{\bar{S}}(t) \equiv \rho(t)$  and  $H_{\bar{S}}(t) \equiv H(t)$ , we get:

$$e^{-V(t)} V'(t) e^{V(t)} \rho(t) + \dot{\rho}(t) - \rho(t) V'(t) = -i[H(t), \rho(t)] - \sum_{ijww'} \left( [e^{-V(t)} A_i(t) e^{V(t)}, e^{-V(t)} \mathcal{D}_{ijww'}(t) e^{V(t)} \rho(t)] \right) \quad (105)$$

$$- [e^{-V(t)} A_i(t) e^{V(t)}, \rho(t) e^{-V(t)} \mathcal{D}_{ijww'}^\dagger(t) e^{V(t)}] \quad (106)$$

We will now show that many useful master equations can be derived as special cases of the above “mother” of all master equations.

## V. LIMITING CASES

Many limiting cases can be derived from the “mother” of all master equations. We can set  $g_{ik}^{\Im} = 0$ , or  $V_{10}^{\Im} = 0$ ,  $g_{1k} = g_{0k}$ , for example. Let us look at some particular cases.

### A. Time-independent VPQME of 2011

The hamiltonian associated to this system is given by:

$$H = \left( \delta + \sum_{\mathbf{k}} g_{\mathbf{k}} (b_{\mathbf{k}}^\dagger + b_{\mathbf{k}}) \right) |1\rangle\langle 1| + \frac{\Omega}{2} \sigma_x + \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}}. \quad (107)$$

It's possible to summarize this hamiltonian in terms of the hamiltonian (1) using the following matrix:

$$\begin{pmatrix} V_{10}^{\Im}(t) & g_{0\mathbf{k}}^{\Re} & v_{0\mathbf{k}}(t) & B_{10}(t) \\ V_{10}^{\Re}(t) & g_{0\mathbf{k}}^{\Im} & v_{1\mathbf{k}}(t) & \Omega_r \\ \varepsilon_0(t) & g_{1\mathbf{k}}^{\Re} & B_{0z}(t) & R_0(t) \\ \varepsilon_1(t) & g_{1\mathbf{k}}^{\Im} & B_{1z}(t) & R_1(t) \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & B \\ \frac{\Omega}{2} & 0 & v_{\mathbf{k}} & B\Omega \\ 0 & g_{\mathbf{k}} & 0 & 0 \\ \delta & 0 & B_z & R \end{pmatrix} \quad (108)$$

We now have the corresponding set of hamiltonian that satisfy the separation shown in (14)-(18):

$$\overline{H_S} = (\delta + R) |1\rangle\langle 1| + \frac{\Omega_r}{2} \sigma_x, \quad (109)$$

$$\overline{H_I} = B_z |1\rangle\langle 1| + \frac{\Omega}{2} (B_x \sigma_x + B_y \sigma_y), \quad (110)$$

$$H_B = \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}}. \quad (111)$$

Let's look now at  $v_{\mathbf{k}}$ :



$$v_{\mathbf{k}} = \frac{g_i(\omega_{\mathbf{k}}) \left( 1 - \frac{\tanh(\frac{\beta\eta(t)}{2})}{\eta(t)} (2\varepsilon_i(t) + 2R_i - \varepsilon(t)) \right) + 2 \frac{\tanh(\frac{\beta\eta(t)}{2})}{\eta(t)} \frac{v_{i'\mathbf{k}}}{\omega_{\mathbf{k}}} |B_{10}|^2 |V_{10}(t)|^2 \coth(\beta\omega_{\mathbf{k}}/2)}{1 - \frac{\tanh(\frac{\beta\eta(t)}{2})}{\eta(t)} \left( \varepsilon(t) - 2(\varepsilon(t) - \varepsilon_i(t) - R_i) - \frac{2|V_{10}(t)|^2 |B_{10}|^2 \coth(\beta\omega_{\mathbf{k}}/2)}{\omega_{\mathbf{k}}} \right)} \quad (112)$$

$$= \frac{g_{\mathbf{k}} \left( 1 - \frac{\varepsilon(t)}{\eta} \tanh\left(\frac{\beta\eta}{2}\right) \right)}{1 - \frac{\varepsilon(t)}{\eta} \tanh\left(\frac{\beta\eta}{2}\right) \left( 1 - \frac{\Omega_r^2}{2\varepsilon(t)\omega_{\mathbf{k}}} \coth(\beta\omega_{\mathbf{k}}/2) \right)} \quad (113)$$

The bath and system-bath interaction operators become:

$$\begin{pmatrix} B_z(t) & B^\pm(t) \\ B_x(t) & B(t) \\ B_y(t) & R(t) \end{pmatrix} \equiv \begin{pmatrix} \sum_{\mathbf{k}} (g_{\mathbf{k}} - v_{\mathbf{k}}(t)) (b_{\mathbf{k}}^\dagger + b_{\mathbf{k}}) & e^{\pm \sum_{\mathbf{k}} \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} (b_{\mathbf{k}}^\dagger - b_{\mathbf{k}})} \\ \frac{B^+ + B^- - 2B}{2} & e^{-(1/2) \sum_{\mathbf{k}} \left( \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} \right)^2 \coth(\beta\omega_{\mathbf{k}}/2)} \\ \frac{B^- - B^+}{2i} & \sum_{\mathbf{k}} \left( \frac{v_{\mathbf{k}}^2}{\omega_{\mathbf{k}}} - 2g_{\mathbf{k}} \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} \right) \end{pmatrix}, \quad (114)$$

$$\begin{pmatrix} A \\ B(t) \\ C(t) \end{pmatrix} = \begin{pmatrix} \sigma_x & \sigma_y & \frac{I - \sigma_z}{2} & \sigma_x & \sigma_y & \frac{I + \sigma_z}{2} \\ B_x & B_y & B_z & B_y & B_x & 0 \\ \frac{\Omega}{2} & \frac{\Omega}{2} & 1 & 0 & 0 & 1 \end{pmatrix}. \quad (115)$$

Therefore  $C(t)$  is no longer time-dependent. Defining:

$$\Lambda_{ij}(\tau) \equiv C_i C_j \mathcal{B}_{ij}(\tau), \quad (116)$$

We get:

$$K_{ijww'}(t) = \int_0^t \Lambda_{ij}(\tau) e^{i\omega\tau} e^{-it(w-w')} d\tau. \quad (117)$$

Now for a time-independent hamiltonian is possible to show that for the decomposition matrix  $\mathcal{A}_j(w(t)) = \mathcal{A}_j(w)$ :

$$U^\dagger(t) \mathcal{A}_j(t) U(t) = \sum_w e^{-i\omega t} \mathcal{A}_j(w) \quad (118)$$

It means that a decomposition matrix of  $\widetilde{\mathcal{A}}_j(t)$  associated to the eigenvector under evolution for the same time-independent hamiltonian  $U(t) \mathcal{A}_j(w) U^\dagger(t)$  generates the same decomposition matrix multiplied by a phase  $e^{i\omega t}$ . It means that the decomposition matrix  $A_{jww'}$  for a time-independent hamiltonian fulfill  $A_{jww'} = A_j(w) \delta_{ww'}$  so only if  $w = w'$  then the response function is relevant for taking account and it's equal to:

$$\begin{aligned} K_{ijww}(t) &= \int_0^t C_i(t) C_j(t - \tau) \mathcal{B}_{ij}(\tau) e^{i\omega\tau} e^{-it(w-w)} d\tau \\ &= \int_0^t C_i(t) C_j(t - \tau) \mathcal{B}_{ij}(\tau) e^{i\omega\tau} d\tau \\ &\equiv K_{ijw}(t) \end{aligned}$$

The master equation can be written as:

$$\frac{d\bar{\rho}_S(t)}{dt} = -i[\overline{H}_S(t), \bar{\rho}_S(t)] - \sum_{ijw} \left( K_{ijw}^{\mathcal{R}}(t) [A_i, A_{jw} \bar{\rho}_S(t) - \bar{\rho}_S(t) A_{jw}^\dagger] + i K_{ijw}^{\mathcal{I}}(t) [A_i, A_{jw} \bar{\rho}_S(t) + \bar{\rho}_S(t) A_{jw}^\dagger] \right) \quad (119)$$

The spectral density in this case is:

$$J(\omega) = \sum_{\mathbf{k}} |g_{\mathbf{k}}|^2 \delta(\omega - \omega_{\mathbf{k}}), \quad (120)$$

$$v_{\mathbf{k}}(t) = g_{\mathbf{k}} F(\omega_{\mathbf{k}}, t). \quad (121)$$

The relevant correlation functions are given by the matrix  $\Lambda(\tau)$ :

$$\Lambda(\tau) = \begin{pmatrix} \frac{\Omega_r^2}{4} (\cosh(\phi(\tau)) - 1) & 0 & 0 \\ 0 & \frac{\Omega_r^2}{4} \sinh(\phi(\tau)) & -\frac{\Omega_r}{2} \int_0^\infty d\omega \frac{J(\omega)}{\omega} F(\omega) (1 - F(\omega)) iG_-(\tau) \\ 0 & \frac{\Omega_r}{2} \int_0^\infty d\omega \frac{J(\omega)}{\omega} F(\omega) (1 - F(\omega)) iG_-(\tau) & \int_0^\infty d\omega J(\omega) (1 - F(\omega))^2 G_+(\tau) \end{pmatrix}. \quad (122)$$

Here  $G_{\pm}(\omega, \tau) = e^{i\omega\tau} N(\omega) + e^{-i\omega\tau} (N(\omega) + 1)$  and  $\phi(\tau) = \int_0^\infty \frac{J_1(\omega) F_1^2(\omega)}{\omega^2} G_+(\omega, \tau) d\omega$  defines the phonon propagator. Applying the inverse transformation to the equation (119) and using the fact that for the time-independent model we have  $V(t) = V$  then:

$$\dot{\rho}(t) = -i[H, \rho(t)] - \sum_{ijw} (K_{ijw}^{\Re}(t) [e^{-V} A_i e^V, e^{-V} A_{jw} e^V \rho(t) - \rho(t) e^{-V} A_{jw}^\dagger e^V] + i K_{ijw}^{\Im}(t) [e^{-V} A_i e^V, e^{-V} A_{jw} e^V \rho(t) + \rho(t) e^{-V} A_{jw}^\dagger e^V]) \quad (123)$$

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