

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:

$$A(t) \leq A_B(t) \equiv -\frac{1}{\beta} \ln \left(\text{Tr} \left(e^{-\beta \overline{H}_{\bar{S}}(t) + \overline{H}_{\bar{B}}} \right) \right) + \langle \overline{H}_{\bar{I}}(t) \rangle_{\overline{H}_{\bar{S}}(t) + \overline{H}_{\bar{B}}} + O \left(\langle \overline{H}_{\bar{I}}^2(t) \rangle_{\overline{H}_{\bar{S}}(t) + \overline{H}_{\bar{B}}} \right). \quad (19)$$

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 ρ_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 related to describe $\overline{H_I}(t)$:

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

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

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

Taking the master equation (27) 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 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, known as correlation functions, 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), also 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 degree 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:

$$\widetilde{A}_j(t-\tau, t) = \sum_{w(t-\tau), w'(t)} e^{i\tau w(t-\tau)} e^{-it(w(t-\tau)-w'(t))} \mathcal{A}_{jww'}(t; t-\tau, t). \quad (50)$$

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 2×2 matrix in a given time let's write the matrix $A_i(t)$ in the base $W(t) = \{|+\rangle, |-\rangle\}$, where the index t represents the time, formed by the time-dependent eigenvectors of $H_E(t)$ in the following way:

$$A_i(t) = \sum_{\alpha_t, \beta_t \in W(t)} \langle \alpha_t | A_i(t) | \beta_t \rangle | \alpha_t \rangle \langle \beta_t |. \quad (51)$$

Given that $\langle +_t | +_t \rangle = 1$ and $\langle -_t | -_t \rangle = 1$ 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:

$$e^{i\tau H_E(t)} = e^{i\tau \lambda_+(t)} | +_t \rangle \langle +_t | + e^{i\tau \lambda_-(t)} | -_t \rangle \langle -_t |. \quad (52)$$

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

$$U^\dagger(t-\tau) A_i(t) U(t-\tau) = A_i(t; 0) + A_i(t; -w(t-\tau)) e^{i(t-\tau)w(t-\tau)} + A_i(t; w(t-\tau)) e^{-i(t-\tau)w(t-\tau)}. \quad (53)$$

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

$$\mathcal{A}_i(t; 0) = \langle +_{t-\tau} | A_i(t) | +_{t-\tau} \rangle | +_{t-\tau} \rangle \langle +_{t-\tau} | + \langle -_{t-\tau} | A_i(t) | -_{t-\tau} \rangle | -_{t-\tau} \rangle \langle -_{t-\tau} |, \quad (54)$$

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

$$\mathcal{A}_i(t; w(t-\tau)) = \langle -_{t-\tau} | A_i(t) | +_{t-\tau} \rangle | -_{t-\tau} \rangle \langle +_{t-\tau} |. \quad (56)$$

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:

$$\mathcal{A}_i(t; 0, 0) = \langle +_t | \mathcal{A}_i(t; 0) | +_t \rangle | +_t \rangle \langle +_t | + \langle -_t | \mathcal{A}_i(t; 0) | -_t \rangle | -_t \rangle \langle -_t |, \quad (57)$$

$$\mathcal{A}_i(t; 0, w'(t)) = \langle -_t | \mathcal{A}_i(t; 0) | +_t \rangle | -_t \rangle \langle +_t |, \quad (58)$$

$$\mathcal{A}_i(t; w(t-\tau), 0) = \langle +_t | \mathcal{A}_i(t; -w(t-\tau)) | +_t \rangle | +_t \rangle \langle +_t | + \langle -_t | \mathcal{A}_i(t; -w(t-\tau)) | -_t \rangle | -_t \rangle \langle -_t |, \quad (59)$$

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

$$\mathcal{A}_i(t; w(t-\tau), -w'(t)) = \langle +_t | \mathcal{A}_i(t; -w(t-\tau)) | -_t \rangle | +_t \rangle \langle -_t |. \quad (61)$$

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

$$\frac{d\overline{\rho_S}(t)}{dt} = -i[\overline{H_S}(t), \overline{\rho_S}(t)] - \sum_{ijww'} \int_0^t d\tau C_i(t) C_j(t-\tau) \left(\mathcal{B}_{ij}(t, t-\tau) \left[A_i(t), e^{i\tau w(t-\tau)} e^{-it(w(t-\tau)-w'(t))} \mathcal{A}_{jww'}(t-\tau, t) \overline{\rho_S}(t) \right] \right. \quad (62)$$

$$\left. + \mathcal{B}_{ij}^*(t, t-\tau) \left[\overline{\rho_S}(t) e^{-i\tau w(t-\tau)} e^{it(w(t-\tau)-w'(t))} \mathcal{A}_{jww'}^\dagger(t-\tau, t), A_i(t) \right] \right). \quad (63)$$

Let's define the operator:

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

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

$$D_{ijww'}^\dagger(t-\tau, t) = C_i(t) C_j(t-\tau) \mathcal{B}_{ij}^*(t, t-\tau) e^{-i\tau w(t-\tau)} e^{it(w(t-\tau)-w'(t))} \mathcal{A}_{jww'}^\dagger(t-\tau, t). \quad (65)$$

we used the fact that $C_i(t) \in \mathbb{R}$ for all i . With this notation applied to (63) we arrive to the following master equation:

$$\frac{d\overline{\rho_S}(t)}{dt} = -i [\overline{H_S}(t), \overline{\rho_S}(t)] - \sum_{ijww'} \int_0^t d\tau \left([A_i(t), D_{ijww'}(t-\tau, t) \overline{\rho_S}(t)] - [\overline{\rho_S}(t) D_{ijww'}^\dagger(t-\tau, t), A_i(t)] \right). \quad (66)$$

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

$$\mathcal{D}_{ijww'}(t) = \int_0^t D_{ijww'}(t-\tau, t) d\tau. \quad (67)$$

In particular, the $\mathcal{B}(t, s)$ operators matrix is defined in terms of $\mathcal{B}(t, s) \equiv \mathcal{B}_{ij}(t, s)$, following the notation of the matrix (28) we have:

$$\mathcal{B}(t, s) \equiv \begin{pmatrix} \mathcal{B}_{11}(t, s) & \mathcal{B}_{12}(t, s) & \mathcal{B}_{13}(t, s) & \mathcal{B}_{12}(t, s) & \mathcal{B}_{11}(t, s) & \mathcal{B}_{16}(t, s) \\ \mathcal{B}_{21}(t, s) & \mathcal{B}_{22}(t, s) & \mathcal{B}_{23}(t, s) & \mathcal{B}_{22}(t, s) & \mathcal{B}_{21}(t, s) & \mathcal{B}_{26}(t, s) \\ \mathcal{B}_{31}(t, s) & \mathcal{B}_{32}(t, s) & \mathcal{B}_{33}(t, s) & \mathcal{B}_{32}(t, s) & \mathcal{B}_{31}(t, s) & \mathcal{B}_{36}(t, s) \\ \mathcal{B}_{21}(t, s) & \mathcal{B}_{22}(t, s) & \mathcal{B}_{23}(t, s) & \mathcal{B}_{22}(t, s) & \mathcal{B}_{21}(t, s) & \mathcal{B}_{26}(t, s) \\ \mathcal{B}_{11}(t, s) & \mathcal{B}_{12}(t, s) & \mathcal{B}_{13}(t, s) & \mathcal{B}_{12}(t, s) & \mathcal{B}_{11}(t, s) & \mathcal{B}_{16}(t, s) \\ \mathcal{B}_{61}(t, s) & \mathcal{B}_{62}(t, s) & \mathcal{B}_{63}(t, s) & \mathcal{B}_{62}(t, s) & \mathcal{B}_{61}(t, s) & \mathcal{B}_{66}(t, s) \end{pmatrix}. \quad (68)$$

We can define:

$$N(\omega) \equiv (e^{\beta\omega} - 1)^{-1}. \quad (69)$$

and the spectral density is defined in the usual way:

$$J_i(\omega) \equiv \sum_{\mathbf{k}} |g_{i\mathbf{k}}|^2 \delta(\omega - \omega_{\mathbf{k}}), \quad (70)$$

$$v_{i\mathbf{k}}(\omega_{\mathbf{k}}, t) = g_{i\mathbf{k}} F_i(\omega_{\mathbf{k}}, t). \quad (71)$$

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 $\mathcal{B}_{ij}(t, s)$ is equal to:

$$\chi_{10}(t) = \int_0^\infty \frac{\sqrt{J_1^*(\omega)} J_0(\omega) F_1^*(\omega, t) F_0(\omega, t) - \sqrt{J_1(\omega)} J_0^*(\omega) F_1(\omega, t) F_0^*(\omega, t)}{2\omega^2} d\omega, \quad (72)$$

$$U_{10}(t, s) = \exp \left(i \left(\int_0^\infty \frac{(\sqrt{J_1(\omega)} F_1(\omega, t) - \sqrt{J_0(\omega)} F_0(\omega, t)) (\sqrt{J_1(\omega)} F_1(\omega, s) - \sqrt{J_0(\omega)} F_0(\omega, s))^* \exp(i\omega\tau)}{\omega^2} d\omega \right)^3 \right), \quad (73)$$

$$B_{10}(t) = \exp(\chi_{10}(t)) \exp \left(-\frac{1}{2} \int_0^\infty \left| \frac{\sqrt{J_1(\omega)} F_1(\omega, t) - \sqrt{J_0(\omega)} F_0(\omega, t)}{\omega} \right|^2 \coth \left(\frac{\beta\omega}{2} \right) d\omega \right), \quad (74)$$

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

$$\xi^-(t, s) = \exp \left(-\int_0^\infty \frac{|\sqrt{J_1(\omega)} F_1(\omega, t) - \sqrt{J_0(\omega)} F_0(\omega, t)| \exp(i\omega\tau) - (\sqrt{J_1(\omega)} F_1(\omega, s) - \sqrt{J_0(\omega)} F_0(\omega, s))|^2}{2\omega^2} \coth \left(\frac{\beta\omega}{2} \right) d\omega \right), \quad (76)$$

$$Q(\omega, t) = \frac{\sqrt{J_1(\omega)} F_1(\omega, t) - \sqrt{J_0(\omega)} F_0(\omega, t)}{\omega}, \quad (77)$$

$$\langle \widetilde{B}_x(t) \widetilde{B}_x(s) \rangle_B = \mathcal{B}_{11}(t, s) \quad (78)$$

$$= \frac{1}{2} \left((\exp(\chi_{10}(t) + \chi_{10}(s)))^{\Re} U_{10}(t, s) \xi^+(t, s) + (\exp(\chi_{10}(t) + \chi_{01}(s)))^{\Re} U_{10}^*(t, s) \xi^-(t, s) \right) \quad (79)$$

$$- (B_{10}(t))^{\Re} (B_{01}(s))^{\Re}, \quad (80)$$

$$\langle \widetilde{B}_y(t) \widetilde{B}_y(s) \rangle_B = \mathcal{B}_{22}(t, s) \quad (81)$$

$$= -\frac{1}{2} \left((\exp(\chi_{01}(t) + \chi_{01}(s)))^{\Re} U_{10}(t, s) \xi^+(t, s) - (\exp(\chi_{10}(t) + \chi_{01}(s)))^{\Re} U_{10}^*(t, s) \xi^-(t, s) \right) \quad (82)$$

$$+ (B_{01}(t))^{\Im} (B_{10}(s))^{\Im}, \quad (83)$$

$$\langle \widetilde{B}_x(t) \widetilde{B}_y(s) \rangle_B = \mathcal{B}_{12}(t, s) \quad (84)$$

$$= \frac{1}{2} \left((\exp(\chi_{10}(t) + \chi_{01}(s)))^{\Im} U_{10}^*(t, s) \xi^-(t, s) + (\exp(\chi_{01}(t) + \chi_{01}(s)))^{\Im} U_{10}(t, s) \xi^+(t, s) \right) \quad (85)$$

$$+ (B_{10}(t))^{\Re} (B_{10}(s))^{\Im}. \quad (86)$$

$$\langle \widetilde{B}_y(t) \widetilde{B}_x(s) \rangle_B = \mathcal{B}_{21}(t, s) \quad (87)$$

$$= \frac{1}{2} \left((\exp(\chi_{01}(t) + \chi_{10}(s)))^{\Im} U_{10}^*(t, s) \xi^-(t, s) + (\exp(\chi_{01}(t) + \chi_{01}(s)))^{\Im} U_{10}(t, s) \xi^+(t, s) \right) \quad (88)$$

$$+ (B_{10}(t))^{\Im} (B_{10}(s))^{\Re}, \quad (89)$$

$$\langle \widetilde{B}_{iz}(t) \widetilde{B}_{jz}(s) \rangle_B = \mathcal{B}_{nm}(t, s), \quad (n, m \in \{3, 6\}) \quad (90)$$

$$= \int_0^\infty \left(\sqrt{J_i(\omega) J_j^*(\omega)} (1 - F_i(\omega, t)) (1 - F_j^*(\omega, s)) e^{i\omega\tau} N(\omega) + \sqrt{J_i^*(\omega) J_j(\omega)} (1 - F_i^*(\omega, t)) (1 - F_j(\omega, s)) e^{-i\omega\tau} (N(\omega) + 1) \right) d\omega, \quad (91)$$

$$\langle \widetilde{B}_{iz}(t) \widetilde{B}_x(s) \rangle_B = \mathcal{B}_{n1}(t, s), \quad (n \in \{3, 6\}) \quad (92)$$

$$= i B_{01}^{\Im}(s) \int_0^\infty \left(\sqrt{J_i(\omega)} (1 - F_i(\omega, t)) Q^*(\omega, s) N(\omega) e^{i\omega\tau} - \sqrt{J_i^*(\omega)} (1 - F_i^*(\omega, t)) Q(\omega, s) e^{-i\omega\tau} (N(\omega) + 1) \right) d\omega, \quad (93)$$

$$\langle \widetilde{B}_x(t) \widetilde{B}_{iz}(s) \rangle_B = \mathcal{B}_{1n}(t, s), \quad (n \in \{3, 6\}) \quad (94)$$

$$= i B_{01}^{\Im}(t) \int_0^\infty \left(\sqrt{J_i^*(\omega)} (1 - F_i^*(\omega, s)) Q(\omega, t) N(\omega) e^{i\omega\tau} - \sqrt{J_i(\omega)} (1 - F_i(\omega, s)) Q^*(\omega, t) e^{-i\omega\tau} (N(\omega) + 1) \right) d\omega, \quad (95)$$

$$\langle \widetilde{B}_{iz}(t) \widetilde{B}_y(s) \rangle_B = \mathcal{B}_{n2}(t, s), \quad (n \in \{3, 6\}) \quad (96)$$

$$= i B_{10}^{\Re}(s) \int_0^\infty \left(\sqrt{J_i^*(\omega)} (1 - F_i^*(\omega, s)) Q(\omega, s) (N(\omega) + 1) e^{-i\omega\tau} - \sqrt{J_i(\omega)} (1 - F_i(\omega, s)) Q^*(\omega, s) e^{i\omega\tau} N(\omega) \right) d\omega, \quad (97)$$

$$\langle \widetilde{B}_y(t) \widetilde{B}_{iz}(s) \rangle_B = \mathcal{B}_{2n}(t, s), \quad (n \in \{3, 6\}) \quad (98)$$

$$= i B_{10}^{\Re}(t) \int_0^\infty \left(\sqrt{J_i(\omega)} (1 - F_i(\omega, s)) Q(\omega, t) N(\omega) e^{i\omega\tau} - \sqrt{J_i^*(\omega)} (1 - F_i^*(\omega, s)) Q^*(\omega, t) e^{-i\omega\tau} (N(\omega) + 1) \right) d\omega. \quad (99)$$

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

$$\frac{d\overline{\rho_S}(t)}{dt} = -i [\overline{H_S}(t), \overline{\rho_S}(t)] - \sum_{ijww'} \left([A_i(t), \mathcal{D}_{ijww'}(t) \overline{\rho_S}(t)] - [\overline{\rho_S}(t) \mathcal{D}_{ijww'}^\dagger(t), A_i(t)] \right). \quad (100)$$

If we extend the upper limit of integration to ∞ in the equation (67) 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:

$$e^{-V(t)} \frac{d\overline{\rho_S}(t)}{dt} e^{V(t)} = e^{-V(t)} V'(t) e^{V(t)} \rho_S(t) + \dot{\rho}_S(t) - \rho_S(t) V'(t) \quad (101)$$

$$= -ie^{-V(t)} [\overline{H_S}(t), \overline{\rho_S}(t)] e^{V(t)} - \sum_{ijww'} \int_0^t d\tau \left(e^{-V(t)} [A_i, \mathcal{D}_{ijww'}(t-\tau, t) \overline{\rho_S}(t)] e^{V(t)} - e^{-V(t)} [A_i, \overline{\rho_S}(t) \mathcal{D}_{ijww'}^\dagger(t-\tau, t)] e^{V(t)} \right). \quad (102)$$

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

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

$$e^{-V(t)} [A(t), B(t)] e^{V(t)} = [A(t), B(t)]. \quad (104)$$

So we will obtain that

$$e^{-V(t)} \frac{d\overline{\rho_S(t)}}{dt} e^{V(t)} = -i[H_S(t), \rho_S(t)] - \sum_{ijww'} \left([e^{-V(t)} A_i(t) e^{V(t)}, e^{-V(t)} \mathcal{D}_{ijww'}(t) e^{V(t)} \rho_S(t)] - [e^{-V(t)} A_i(t) e^{V(t)}, \rho_S(t) e^{-V(t)} \mathcal{D}_{ijww'}^\dagger(t) e^{V(t)}] \right). \quad (105)$$

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

$$e^{-V(t)} V'(t) e^{V(t)} \rho(t) + \dot{\rho}(t) - \rho(t) V'(t) = -i[H(t), \rho(t)] - \sum_{ijww'} \left([e^{-V(t)} A_i(t) e^{V(t)}, e^{-V(t)} \mathcal{D}_{ijww'}(t) e^{V(t)} \rho(t)] \right. \quad (106)$$

$$\left. - [e^{-V(t)} A_i(t) e^{V(t)}, \rho(t) e^{-V(t)} \mathcal{D}_{ijww'}^\dagger(t) e^{V(t)}] \right). \quad (107)$$

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 $g_{ik}^{\mathfrak{S}} = 0$, or $V_{10}^{\mathfrak{S}} = 0$, $g_{1k} = g_{0k}$, for example. Let us look at some particular cases.

A. Time-independent VPQME of 2011

The hamiltonian associated to this system is given by:

$$H = \left(\delta + \sum_{\mathbf{k}} g_{\mathbf{k}} (b_{\mathbf{k}}^\dagger + b_{\mathbf{k}}) \right) |1\rangle\langle 1| + \frac{\Omega}{2} \sigma_x + \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}}. \quad (108)$$

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

$$\begin{pmatrix} V_{10}^{\mathfrak{S}}(t) & g_{0\mathbf{k}}^{\mathfrak{R}} & v_{0\mathbf{k}}(t) & B_{10}(t) \\ V_{10}^{\mathfrak{R}}(t) & g_{0\mathbf{k}}^{\mathfrak{S}} & v_{1\mathbf{k}}(t) & \Omega_r \\ \varepsilon_0(t) & g_{1\mathbf{k}}^{\mathfrak{R}} & B_{0z}(t) & R_0(t) \\ \varepsilon_1(t) & g_{1\mathbf{k}}^{\mathfrak{S}} & B_{1z}(t) & R_1(t) \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & B \\ \frac{\Omega}{2} & 0 & v_{\mathbf{k}} & B\Omega \\ 0 & g_{\mathbf{k}} & 0 & 0 \\ \delta & 0 & B_z & R \end{pmatrix}. \quad (109)$$

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

$$\overline{H_S} = (\delta + R) |1\rangle\langle 1| + \frac{\Omega_r}{2} \sigma_x, \quad (110)$$

$$\overline{H_I} = B_z |1\rangle\langle 1| + \frac{\Omega}{2} (B_x \sigma_x + B_y \sigma_y), \quad (111)$$

$$H_B = \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}}. \quad (112)$$

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

$$v_{\mathbf{k}} = \frac{g_i(\omega_{\mathbf{k}}) \left(1 - \frac{\tanh(\frac{\beta\eta(t)}{2})}{\eta(t)} (2\varepsilon_i(t) + 2R_i - \varepsilon(t)) \right) + 2 \frac{\tanh(\frac{\beta\eta(t)}{2})}{\eta(t)} \frac{v_{i'\mathbf{k}}}{\omega_{\mathbf{k}}} |B_{10}|^2 |V_{10}(t)|^2 \coth(\beta\omega_{\mathbf{k}}/2)}{1 - \frac{\tanh(\frac{\beta\eta(t)}{2})}{\eta(t)} \left(\varepsilon(t) - 2(\varepsilon(t) - \varepsilon_i(t) - R_i) - \frac{2|V_{10}(t)|^2 |B_{10}|^2 \coth(\beta\omega_{\mathbf{k}}/2)}{\omega_{\mathbf{k}}} \right)}$$
(113)

$$= \frac{g_{\mathbf{k}} \left(1 - \frac{\varepsilon(t)}{\eta} \tanh\left(\frac{\beta\eta}{2}\right) \right)}{1 - \frac{\varepsilon(t)}{\eta} \tanh\left(\frac{\beta\eta}{2}\right) \left(1 - \frac{\Omega_r^2}{2\varepsilon(t)\omega_{\mathbf{k}}} \coth(\beta\omega_{\mathbf{k}}/2) \right)}.$$
(114)

The bath and system-bath interaction operators become:

$$\begin{pmatrix} B_z(t) & B^\pm(t) \\ B_x(t) & B(t) \\ B_y(t) & R(t) \end{pmatrix} \equiv \begin{pmatrix} \sum_{\mathbf{k}} (g_{\mathbf{k}} - v_{\mathbf{k}}(t)) (b_{\mathbf{k}}^\dagger + b_{\mathbf{k}}) & e^{\pm \sum_{\mathbf{k}} \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} (b_{\mathbf{k}}^\dagger - b_{\mathbf{k}})} \\ \frac{B^+ + B^- - 2B}{2} & e^{-(1/2) \sum_{\mathbf{k}} \left(\frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} \right)^2 \coth(\beta\omega_{\mathbf{k}}/2)} \\ \frac{B^- - B^+}{2i} & \sum_{\mathbf{k}} \left(\frac{v_{\mathbf{k}}^2}{\omega_{\mathbf{k}}} - 2g_{\mathbf{k}} \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} \right) \end{pmatrix},$$
(115)

$$\begin{pmatrix} A \\ B(t) \\ C(t) \end{pmatrix} = \begin{pmatrix} \sigma_x & \sigma_y & \frac{I - \sigma_z}{2} & \sigma_x & \sigma_y & \frac{I + \sigma_z}{2} \\ B_x & B_y & B_z & B_y & B_x & 0 \\ \frac{\Omega}{2} & \frac{\Omega}{2} & 1 & 0 & 0 & 1 \end{pmatrix}.$$
(116)

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

$$\Lambda_{ij}(\tau) \equiv C_i C_j \mathcal{B}_{ij}(\tau).$$
(117)

We get:

$$K_{ijww'}(t) = \int_0^t \Lambda_{ij}(\tau) e^{i\omega\tau} e^{-it(w-w')} d\tau.$$
(118)

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

$$U^\dagger(t) \mathcal{A}_j(t) U(t) = \sum_w e^{-i\omega t} \mathcal{A}_j(w).$$
(119)

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 $A_{jww'} = \mathcal{A}_j(w) \delta_{ww'}$ so only if $w = w'$ then the response function is relevant for taking account and it's equal to:

$$K_{ijww}(t) = \int_0^t C_i(t) C_j(t - \tau) \mathcal{B}_{ij}(\tau) e^{i\omega\tau} e^{-it(w-w)} d\tau$$
(120)

$$= \int_0^t C_i(t) C_j(t - \tau) \mathcal{B}_{ij}(\tau) e^{i\omega\tau} d\tau$$
(121)

$$\equiv K_{ijw}(t).$$
(122)

The master equation can be written as:

$$\frac{d\bar{\rho}_S(t)}{dt} = -i[\overline{H}_S(t), \bar{\rho}_S(t)] - \sum_{ijw} \left(K_{ijw}^{\mathcal{R}}(t) [A_i, A_{jw} \bar{\rho}_S(t) - \bar{\rho}_S(t) A_{jw}^\dagger] + i K_{ijw}^{\mathcal{S}}(t) [A_i, A_{jw} \bar{\rho}_S(t) + \bar{\rho}_S(t) A_{jw}^\dagger] \right). \quad (123)$$

The spectral density in this case is:

$$J(\omega) = \sum_{\mathbf{k}} |g_{\mathbf{k}}|^2 \delta(\omega - \omega_{\mathbf{k}}), \quad (124)$$

$$v_{\mathbf{k}}(t) = g_{\mathbf{k}} F(\omega_{\mathbf{k}}, t). \quad (125)$$

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

$$\Lambda(\tau) = \begin{pmatrix} \frac{\Omega_r^2}{4} (\cosh(\phi(\tau)) - 1) & 0 & 0 \\ 0 & \frac{\Omega_r^2}{4} \sinh(\phi(\tau)) & -\frac{\Omega_r}{2} \int_0^\infty d\omega \frac{J(\omega)}{\omega} F(\omega) (1 - F(\omega)) iG_-(\tau) \\ 0 & \frac{\Omega_r}{2} \int_0^\infty d\omega \frac{J(\omega)}{\omega} F(\omega) (1 - F(\omega)) iG_-(\tau) & \int_0^\infty d\omega J(\omega) (1 - F(\omega))^2 G_+(\tau) \end{pmatrix}. \quad (126)$$

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 (123) and using the fact that for the time-independent model we have $V(t) = V$ then:

$$\dot{\rho}(t) = -i[H, \rho(t)] - \sum_{ijw} (K_{ijw}^{\Re}(t) [e^{-V} A_i e^V, e^{-V} A_{jw} e^V \rho(t) - \rho(t) e^{-V} A_{jw}^\dagger e^V] + iK_{ijw}^{\Im}(t) [e^{-V} A_i e^V, e^{-V} A_{jw} e^V \rho(t) + \rho(t) e^{-V} A_{jw}^\dagger e^V]). \quad (127)$$

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