

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 $\beta = 1/k_B T$:

$$\rho_B \equiv \rho_B(0) = \frac{e^{-\beta H_B}}{\text{Tr}(e^{-\beta H_B})}. \quad (7)$$

With the following definitions:

$$\begin{pmatrix} B_{iz}(t) & B_i^\pm(t) \\ B_x(t) & B_i(t) \\ B_y(t) & B_{ij}(t) \end{pmatrix} \equiv \begin{pmatrix} \sum_{\mathbf{k}} \left((g_{i\mathbf{k}} - v_{i\mathbf{k}}(t)) b_{\mathbf{k}}^\dagger + (g_{i\mathbf{k}} - v_{i\mathbf{k}}(t))^* b_{\mathbf{k}} \right) & e^{\pm \sum_{\mathbf{k}} \left(\frac{v_{i\mathbf{k}}(t)}{\omega_{\mathbf{k}}} b_{\mathbf{k}}^\dagger - \frac{v_{i\mathbf{k}}^*(t)}{\omega_{\mathbf{k}}} b_{\mathbf{k}} \right)} \\ \frac{B_1^+(t)B_0^-(t) + B_0^+(t)B_1^-(t) - B_{10}(t) - B_{01}(t)}{2} & e^{-\frac{1}{2} \sum_{\mathbf{k}} \left| \frac{v_{i\mathbf{k}}(t)}{\omega_{\mathbf{k}}} \right|^2 \coth(\beta\omega_{\mathbf{k}}/2)} \\ \frac{B_0^+(t)B_1^-(t) - B_1^+(t)B_0^-(t) + B_{10}(t) - B_{01}(t)}{2i} & e^{-\frac{1}{2} \sum_{\mathbf{k}} \left| \frac{v_{i\mathbf{k}}(t) - v_{j\mathbf{k}}(t)}{\omega_{\mathbf{k}}} \right|^2 \coth\left(\frac{\beta\omega_{\mathbf{k}}}{2}\right)} e^{\chi_{ij}(t)} \end{pmatrix}, \quad (8)$$

$$R_i(t) \equiv \sum_{\mathbf{k}} \left(\frac{|v_{i\mathbf{k}}(t)|^2}{\omega_{\mathbf{k}}} - \left(g_{i\mathbf{k}} \frac{v_{i\mathbf{k}}^*(t)}{\omega_{\mathbf{k}}} + g_{i\mathbf{k}}^* \frac{v_{i\mathbf{k}}(t)}{\omega_{\mathbf{k}}} \right) \right), \quad (9)$$

$$\chi_{ij}(t) \equiv \sum_{\mathbf{k}} \left(\frac{v_{i\mathbf{k}}^*(t) v_{j\mathbf{k}}(t) - v_{i\mathbf{k}}(t) v_{j\mathbf{k}}^*(t)}{2\omega_{\mathbf{k}}^2} \right), \quad (10)$$

$$(\cdot)^{\Re} \equiv \Re(\cdot), \quad (11)$$

$$(\cdot)^{\Im} \equiv \Im(\cdot). \quad (12)$$

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

$$\overline{H}_T(t) \equiv \overline{H}_{\bar{S}}(t) + \overline{H}_{\bar{I}}(t) + \overline{H}_{\bar{B}}, \quad (13)$$

$$\overline{H}_{\bar{S}}(t) \equiv \sum_i (\varepsilon_i(t) + R_i(t)) |i\rangle\langle i| + \sigma_x (B_{10}^{\Re}(t) V_{10}^{\Re}(t) - B_{10}^{\Im}(t) V_{10}^{\Im}(t)) - \sigma_y (B_{10}^{\Re}(t) V_{10}^{\Im}(t) + B_{10}^{\Im}(t) V_{10}^{\Re}(t)), \quad (14)$$

$$\overline{H}_{\bar{I}}(t) \equiv \sum_i B_{iz}(t) |i\rangle\langle i| + V_{10}^{\Re}(t) (B_x(t) \sigma_x + B_y(t) \sigma_y) - V_{10}^{\Im}(t) (B_x(t) \sigma_y - B_y(t) \sigma_x), \quad (15)$$

$$\overline{H}_{\bar{B}} \equiv \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} = H_B. \quad (16)$$

III. FREE-ENERGY MINIMIZATION

The true free energy $E_{\text{Free}}(t)$ is bounded by the Bogoliubov inequality:

$$E_{\text{Free}}(t) \leq E_{\text{Free,B}}(t) \equiv -\frac{1}{\beta} \ln \left(\text{Tr} \left(e^{-\beta \overline{H}_{\bar{S}}(t) + \overline{H}_{\bar{B}}} \right) \right) + \langle \overline{H}_{\bar{I}}(t) \rangle_{\overline{H}_{\bar{S}}(t) + \overline{H}_{\bar{B}}} + O \left(\langle \overline{H}_{\bar{I}}^2(t) \rangle_{\overline{H}_{\bar{S}}(t) + \overline{H}_{\bar{B}}} \right). \quad (17)$$

We will optimize the set of variational parameters $\{v_{\mathbf{k}}(t)\}$ in order to minimize $E_{\text{Free,B}}(t)$ (i.e. to make it as close to the true free energy $E_{\text{Free}}(t)$ 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 $\{v_{\mathbf{k}}(t)\}$:

$$\frac{\partial A_B(\{v_{\mathbf{k}}(t)\}; t)}{\partial v_{i\mathbf{k}}(t)} = 0. \quad (18)$$

This leads us to:

$$v_{i\mathbf{k}}(\omega_{\mathbf{k}}, t) = \frac{g_i(\omega_{\mathbf{k}}) \left(1 - \frac{\tanh\left(\frac{\beta\eta(t)}{2}\right)}{\eta(t)} (2\varepsilon_i(t) + 2R_i(t) - \varepsilon(t)) \right) + 2 \frac{\tanh\left(\frac{\beta\eta(t)}{2}\right)}{\eta(t)} \frac{v_{i'\mathbf{k}}(\omega_{\mathbf{k}}, t)}{\omega_{\mathbf{k}}} |B_{10}(t)|^2 |V_{10}(t)|^2 \coth(\beta\omega_{\mathbf{k}}/2)}{1 - \frac{\tanh\left(\frac{\beta\eta(t)}{2}\right)}{\eta(t)} \left(\varepsilon(t) - 2(\varepsilon(t) - \varepsilon_i(t) - R_i(t)) - \frac{2|B_{10}(t)|^2 |V_{10}(t)|^2 \coth(\beta\omega_{\mathbf{k}}/2)}{\omega_{\mathbf{k}}} \right)}, \quad (19)$$

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

$$\eta(t) \equiv \sqrt{(\text{Tr}(\overline{H}_{\bar{S}}(t)))^2 - 4\text{Det}(\overline{H}_{\bar{S}}(t))}, \quad (20)$$

$$\varepsilon(t) \equiv \text{Tr}(\overline{H}_{\bar{S}}(t)). \quad (21)$$

IV. MASTER EQUATION

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

$$\tilde{O}(t) \equiv U^\dagger(t) O(t) U(t), \quad (22)$$

$$U(t) \equiv \mathcal{T} \exp \left(-i \int_0^t dt' \overline{H_T}(t') \right) \quad (23)$$

$$= \exp \left(-i \overline{H_{T,\text{eff}}}(t) \right), \text{ where} \quad (24)$$

$$H_X^{\text{eff}}(t) \equiv \frac{1}{t} \int_0^t H_X(t') dt' - \frac{i}{2t} \int_0^t \int_0^{t'} [H_X(t'), H_X(t'')] dt' dt'' + \frac{1}{6t} \int_0^t \int_0^{t'} \int_0^{t''} \left([[\overline{H_S}(t'), \overline{H_S}(t'')], \overline{H_S}(t''')] + [[\overline{H_S}(t'''), \overline{H_S}(t'')], \overline{H_S}(t')] \right) dt' dt'' dt''' + \dots \quad (25)$$

Therefore:

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

We will initialize the total density operator as: $\rho_T(0) = \rho_S(0) \otimes \rho_B$. 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:

$$\frac{d\widetilde{\overline{\rho_S}}(t)}{dt} = - \int_0^t \text{Tr}_B \left[\widetilde{\overline{H_I}}(t), \left[\widetilde{\overline{H_I}}(t'), \widetilde{\overline{\rho_S}}(t) \rho_B \right] \right] dt'. \quad (27)$$

Since $\overline{H_I}(t)$ contains a lot of terms, we will write it as:

$$\overline{H_I}(t) = \sum_i C_i(t) (A_i \otimes B_i(t)), \text{ where}, \quad (28)$$

$$\begin{pmatrix} A \\ B(t) \\ C(t) \end{pmatrix} = \begin{pmatrix} \sigma_x & \sigma_y & \frac{I-\sigma_z}{2} & \sigma_x & \sigma_y & \frac{I+\sigma_z}{2} \\ B_x(t) & B_y(t) & B_{1z}(t) & B_y(t) & B_x(t) & B_{0z}(t) \\ V_{10}^{\Re}(t) & V_{10}^{\Im}(t) & 1 & V_{10}^{\Im}(t) & -V_{10}^{\Re}(t) & 1 \end{pmatrix}, \quad (29)$$

We plug this expression for $\overline{H_I}(t)$ into the master equation and expand the commutators:

$$\frac{d\widetilde{\overline{\rho_S}}(t)}{dt} = - \int_0^t \text{Tr}_B \left(\sum_j C_j(t) (\widetilde{A_j}(t) \otimes \widetilde{B_j}(t)) \sum_i C_i(t') (\widetilde{A_i}(t') \otimes \widetilde{B_i}(t')) \widetilde{\overline{\rho_S}}(t) \rho_B - \sum_j C_j(t) (\widetilde{A_j}(t) \otimes \widetilde{B_j}(t)) \widetilde{\overline{\rho_S}}(t) \rho_B \sum_i C_i(t') (\widetilde{A_i}(t') \otimes \widetilde{B_i}(t')) \right) \quad (30)$$

$$- \sum_i C_i(t') (\widetilde{A_i}(t') \otimes \widetilde{B_i}(t')) \widetilde{\overline{\rho_S}}(t) \rho_B \sum_j C_j(t) (\widetilde{A_j}(t) \otimes \widetilde{B_j}(t)) + \widetilde{\overline{\rho_S}}(t) \rho_B \sum_i C_i(t') (\widetilde{A_i}(t') \otimes \widetilde{B_i}(t')) \sum_j C_j(t) (\widetilde{A_j}(t) \otimes \widetilde{B_j}(t)) \right) dt'. \quad (31)$$

A. Trace over the bath

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 $\mathcal{B}(t, t')$ such that:

$$\mathcal{B}_{ij}(t, t') \equiv \text{Tr}_B \left(\widetilde{B_i}(t) \widetilde{B_j}(t') \rho_B \right). \quad (32)$$

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

$$\frac{d\widetilde{\overline{\rho_S}}(t)}{dt} = - \int_0^t \left(\sum_{ij} C_i(t) C_j(t') \left(\mathcal{B}_{ij}(t, t') \left[\widetilde{A_i}(t), \widetilde{A_j}(t') \widetilde{\overline{\rho_S}}(t) \right] - \mathcal{B}_{ij}^*(t, t') \left[\widetilde{A_i}(t), \widetilde{\overline{\rho_S}}(t) \widetilde{A_j}(t') \right] \right) \right) dt'. \quad (33)$$

here we considered the following notation:

$$\widetilde{A}_j(t', t) = U(t) U^\dagger(t') A_j U(t') U^\dagger(t). \quad (34)$$

Given that $t' = t - \tau$ then we can perform the change of variables in the integral of the equation (33), also doing the reverse of the transformation to interaction picture we get:

$$\frac{d\overline{\rho_S}(t)}{dt} = -i [\overline{H_S}(t), \overline{\rho_S}(t)] - \sum_{ij} \int_0^t d\tau C_i(t) C_j(t - \tau) \left(\mathcal{B}_{ij}(t, t - \tau) [\widetilde{A}_i(t - \tau, t) \overline{\rho_S}(t)] + \mathcal{B}_{ij}^*(t, t - \tau) [\overline{\rho_S}(t) \widetilde{A}_j(t - \tau, t), A_i] \right). \quad (35)$$

The Fourier decomposition of the operators $\widetilde{A}_i(t)$ and $\widetilde{A}_j(t - \tau, t)$ using the expansion $\overline{H_{S, \text{eff}}}(t)$ is:

$$\widetilde{A}_i(t) = \sum_{w(t)} e^{-itw(t)} A_i(w(t)). \quad (36)$$

$$\widetilde{A}_j(t - \tau, t) = \sum_{w(t-\tau), w'(t)} e^{i\tau w(t-\tau)} e^{-it(w(t-\tau) - w'(t))} A_j(w(t - \tau), w'(t)), \quad (37)$$

where $w(t)$ belongs to the set of differences of eigenvalues of $\overline{H_{S, \text{eff}}}(t)$.

Replacing (37) in (35) we deduce that:

$$\frac{d\overline{\rho_S}(t)}{dt} = -i [\overline{H_S}(t), \overline{\rho_S}(t)] - \sum_{ijww'} \int_0^t d\tau C_i(t) C_j(t - \tau) \left(\mathcal{B}_{ij}(t, t - \tau) [A_i, e^{i\tau w(t-\tau)} e^{-it(w(t-\tau) - w'(t))} A_{jww'}(t - \tau, t) \overline{\rho_S}(t)] \right) \quad (38)$$

$$+ \mathcal{B}_{ij}^*(t, t - \tau) [\overline{\rho_S}(t) e^{-i\tau w(t-\tau)} e^{it(w(t-\tau) - w'(t))} A_{jww'}^\dagger(t - \tau, t), A_i] \right). \quad (39)$$

Let's define the operator:

$$D_{ijww'}(t - \tau, t) \equiv C_i(t) C_j(t - \tau) \mathcal{B}_{ij}(t, t - \tau) e^{i\tau w(t-\tau)} e^{-it(w(t-\tau) - w'(t))} A_{jww'}(t - \tau, t). \quad (40)$$

With this notation applied to (39) we arrive to the following master equation:

$$\frac{d\overline{\rho_S}(t)}{dt} = -i [\overline{H_S}(t), \overline{\rho_S}(t)] - \sum_{ijww'} \int_0^t d\tau \left([A_i, D_{ijww'}(t - \tau, t) \overline{\rho_S}(t)] - [\overline{\rho_S}(t) D_{ijww'}^\dagger(t - \tau, t), A_i] \right). \quad (41)$$

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

$$\mathcal{D}_{ijww'}(t) = \int_0^t D_{ijww'}(t - \tau, t) d\tau. \quad (42)$$

Finally we end up with our final master equation in the variationally optimized

$$\frac{d\overline{\rho_S}(t)}{dt} = -i [\overline{H_S}(t), \overline{\rho_S}(t)] - \sum_{ijww'} \left([A_i, \mathcal{D}_{ijww'}(t) \overline{\rho_S}(t)] - [\overline{\rho_S}(t) \mathcal{D}_{ijww'}^\dagger(t), A_i] \right) \quad (43)$$

$$\dot{\rho} = -i [(t), \rho] - \sum_{ijww'} \left([A_i, \mathcal{D}_{ijww'}(t) \rho] - [\rho \mathcal{D}_{ijww'}^\dagger(t), A_i] \right) \quad (44)$$

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

A. Time-independent VPQME of 2011

The hamiltonian associated to this system is given by:

$$H = \left(\delta + \sum_{\mathbf{k}} g_{\mathbf{k}} (b_{\mathbf{k}}^{\dagger} + b_{\mathbf{k}}) \right) |1\rangle\langle 1| + \frac{\Omega}{2} \sigma_x + \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}. \quad (45)$$

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

$$\begin{pmatrix} V_{10}^{\Im}(t) & g_{0\mathbf{k}}^{\Re} & v_{0\mathbf{k}}(t) & B_{10}(t) \\ V_{10}^{\Re}(t) & g_{0\mathbf{k}}^{\Im} & v_{1\mathbf{k}}(t) & \Omega_r \\ \varepsilon_0(t) & g_{1\mathbf{k}}^{\Re} & B_{0z}(t) & R_0(t) \\ \varepsilon_1(t) & g_{1\mathbf{k}}^{\Im} & B_{1z}(t) & R_1(t) \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & B \\ \frac{\Omega}{2} & 0 & v_{\mathbf{k}} & B\Omega \\ 0 & g_{\mathbf{k}} & 0 & 0 \\ \delta & 0 & B_z & R \end{pmatrix}. \quad (46)$$

We now have the corresponding set of hamiltonians that satisfy the separation shown in (13)-(??):

$$\overline{H}_S = (\delta + R) |1\rangle\langle 1| + \frac{\Omega_r}{2} \sigma_x, \quad (47)$$

$$\overline{H}_I = B_z |1\rangle\langle 1| + \frac{\Omega}{2} (B_x \sigma_x + B_y \sigma_y), \quad (48)$$

$$H_B = \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}. \quad (49)$$

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

$$v_{\mathbf{k}} = \frac{g_i(\omega_{\mathbf{k}}) \left(1 - \frac{\tanh(\frac{\beta\eta(t)}{2})}{\eta(t)} (2\varepsilon_i(t) + 2R_i - \varepsilon(t)) \right) + 2 \frac{\tanh(\frac{\beta\eta(t)}{2})}{\eta(t)} \frac{v_{i'\mathbf{k}}}{\omega_{\mathbf{k}}} |B_{10}|^2 |V_{10}(t)|^2 \coth(\beta\omega_{\mathbf{k}}/2)}{1 - \frac{\tanh(\frac{\beta\eta(t)}{2})}{\eta(t)} \left(\varepsilon(t) - 2(\varepsilon(t) - \varepsilon_i(t) - R_i) - \frac{2|V_{10}(t)|^2 |B_{10}|^2 \coth(\beta\omega_{\mathbf{k}}/2)}{\omega_{\mathbf{k}}} \right)} \quad (50)$$

$$= \frac{g_{\mathbf{k}} \left(1 - \frac{\varepsilon(t)}{\eta} \tanh\left(\frac{\beta\eta}{2}\right) \right)}{1 - \frac{\varepsilon(t)}{\eta} \tanh\left(\frac{\beta\eta}{2}\right) \left(1 - \frac{\Omega_r^2}{2\varepsilon(t)\omega_{\mathbf{k}}} \coth(\beta\omega_{\mathbf{k}}/2) \right)}. \quad (51)$$

The bath and system-bath interaction operators become:

$$\begin{pmatrix} B_z(t) & B^{\pm}(t) \\ B_x(t) & B(t) \\ B_y(t) & R(t) \end{pmatrix} \equiv \begin{pmatrix} \sum_{\mathbf{k}} (g_{\mathbf{k}} - v_{\mathbf{k}}(t)) (b_{\mathbf{k}}^{\dagger} + b_{\mathbf{k}}) & e^{\pm \sum_{\mathbf{k}} \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} (b_{\mathbf{k}}^{\dagger} - b_{\mathbf{k}})} \\ \frac{B^+ + B^- - 2B}{2} & e^{-(1/2) \sum_{\mathbf{k}} \left(\frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} \right)^2 \coth(\beta\omega_{\mathbf{k}}/2)} \\ \frac{B^- - B^+}{2i} & \sum_{\mathbf{k}} \left(\frac{v_{\mathbf{k}}^2}{\omega_{\mathbf{k}}} - 2g_{\mathbf{k}} \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} \right) \end{pmatrix}, \quad (52)$$

$$\begin{pmatrix} A \\ B(t) \\ C(t) \end{pmatrix} = \begin{pmatrix} \sigma_x & \sigma_y & \frac{I - \sigma_z}{2} & \sigma_x & \sigma_y & \frac{I + \sigma_z}{2} \\ B_x & B_y & B_z & B_y & B_x & 0 \\ \frac{\Omega}{2} & \frac{\Omega}{2} & 1 & 0 & 0 & 1 \end{pmatrix}. \quad (53)$$

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

$$\Lambda_{ij}(\tau) \equiv C_i C_j \mathcal{B}_{ij}(\tau). \quad (54)$$

We get:

$$K_{ijww'}(t) = \int_0^t \Lambda_{ij}(\tau) e^{i\omega\tau} e^{-it(w-w')} d\tau. \quad (55)$$

Now for a time-independent hamiltonian is possible to show that for the decomposition matrix $A_j(w(t)) = A_j(w)$:

$$U^\dagger(t) A_j(t) U(t) = \sum_w e^{-i\omega t} A_j(w). \quad (56)$$

It means that a decomposition matrix of $\widetilde{A}_j(t)$ associated to the eigenvector under evolution for the same time-independent hamiltonian $U(t) A_j(w) U^\dagger(t)$ 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:

$$K_{ijww}(t) = \int_0^t C_i C_j \mathcal{B}_{ij}(\tau) e^{i\omega\tau} d\tau \quad (57)$$

$$\equiv K_{ijw}(t). \quad (58)$$

The Fourier decomposition matrices for this case are:

$$A_1(0) = \sin(2\theta) (|\overline{H_{S,1}}\rangle\langle\overline{H_{S,1}}| - |\overline{H_{S,0}}\rangle\langle\overline{H_{S,0}}|), \quad (59)$$

$$A_1(\eta) = \cos(2\theta) |\overline{H_{S,0}}\rangle\langle\overline{H_{S,1}}|, \quad (60)$$

$$A_2(0) = 0, \quad (61)$$

$$A_2(\eta) = i |\overline{H_{S,0}}\rangle\langle\overline{H_{S,1}}|, \quad (62)$$

$$A_3(0) = \cos^2(\theta) |\overline{H_{S,1}}\rangle\langle\overline{H_{S,1}}| + \sin^2(\theta) |\overline{H_{S,0}}\rangle\langle\overline{H_{S,0}}|, \quad (63)$$

$$A_3(\eta) = -\sin(\theta) \cos(\theta) |\overline{H_{S,0}}\rangle\langle\overline{H_{S,1}}|. \quad (64)$$

where $\theta = \frac{1}{2} \tan^{-1}(\frac{\Omega_r}{\epsilon})$ characterises the tilt of the system eigenstates away from the x-axis in the variational frame, $|\overline{H_{S,1}}\rangle, |\overline{H_{S,0}}\rangle$ are the eigenstates of $\overline{H_S}$ with eigenvalues λ_1 and λ_0 respectively and $\eta = \lambda_1 - \lambda_0$ is the difference of eigenvalues. Also we can verify that $A_j(w) = A_j^\dagger(-w)$. Defining $A_j(w) \equiv A_{jw}$ then we can write the master equation as:

$$\frac{d\bar{\rho}_S(t)}{dt} = -i[\overline{H_S}(t), \bar{\rho}_S(t)] - \sum_{ijw} \left(K_{ijw}^{\mathcal{R}}(t) [A_i, A_{jw} \bar{\rho}_S(t) - \bar{\rho}_S(t) A_{jw}^\dagger] + i K_{ijw}^{\mathcal{I}}(t) [A_i, A_{jw} \bar{\rho}_S(t) + \bar{\rho}_S(t) A_{jw}^\dagger] \right). \quad (65)$$

The spectral density in this case is:

$$J(\omega) = \sum_{\mathbf{k}} |g_{\mathbf{k}}|^2 \delta(\omega - \omega_{\mathbf{k}}), \quad (66)$$

$$v_{\mathbf{k}}(t) = g_{\mathbf{k}} F(\omega_{\mathbf{k}}, t). \quad (67)$$

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

$$\Lambda(\tau) = \begin{pmatrix} \frac{\Omega_r^2}{4} (\cosh(\phi(\tau)) - 1) & 0 & 0 \\ 0 & \frac{\Omega_r^2}{4} \sinh(\phi(\tau)) & -\frac{\Omega_r}{2} \int_0^\infty d\omega \frac{J(\omega)}{\omega} F(\omega) (1 - F(\omega)) iG_-(\tau) \\ 0 & \frac{\Omega_r}{2} \int_0^\infty d\omega \frac{J(\omega)}{\omega} F(\omega) (1 - F(\omega)) iG_-(\tau) & \int_0^\infty d\omega J(\omega) (1 - F(\omega))^2 G_+(\tau) \end{pmatrix}. \quad (68)$$

Here $G_\pm(\omega, \tau) = e^{i\omega\tau} N(\omega) + e^{-i\omega\tau} (N(\omega) + 1)$ and $\phi(\tau) = \int_0^\infty \frac{J(\omega) F^2(\omega)}{\omega^2} G_+(\omega, \tau) d\omega$ defines the phonon propagator. Applying the inverse transformation to the equation (65) and using the fact that for the time-independent model we have $V(t) = V$ then:

$$\dot{\rho}(t) = -i[H, \rho(t)] - \sum_{ijw} \left(K_{ijw}^{\mathcal{R}}(t) [e^{-V} A_i e^V, e^{-V} A_{jw} e^V \rho(t) - \rho(t) e^{-V} A_{jw}^\dagger e^V] + i K_{ijw}^{\mathcal{I}}(t) [e^{-V} A_i e^V, e^{-V} A_{jw} e^V \rho(t) + \rho(t) e^{-V} A_{jw}^\dagger e^V] \right). \quad (69)$$

B. Time-dependent polaron master equation

Following the reference [1], if $v_{\mathbf{k}} \rightarrow g_{\mathbf{k}}$ then we recover the full polaron transformation. It means from the equation (8) that $B_z = 0$. The Hamiltonian studied in this case is given by:

$$H = \left(\delta + \sum_{\mathbf{k}} \left(g_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} + g_{\mathbf{k}}^* b_{\mathbf{k}} \right) \right) |1\rangle\langle 1| + \frac{\Omega(t)}{2} \sigma_x + \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}. \quad (70)$$

If $v_{\mathbf{k}} \rightarrow g_{\mathbf{k}}$ then $B(\tau) = B$ from the equation (8), so B is independent of the time. It's possible to summarize (70) in terms of the hamiltonian (1) using the following matrix:

$$\begin{pmatrix} V_{10}^{\Im}(t) & g_{0\mathbf{k}}^{\Re} & v_{0\mathbf{k}}(t) & B_{10}(t) \\ V_{10}^{\Re}(t) & g_{0\mathbf{k}}^{\Im} & v_{1\mathbf{k}}(t) & \Omega_r(t) \\ \varepsilon_0(t) & g_{1\mathbf{k}}^{\Re} & B_{0z}(t) & R_0(t) \\ \varepsilon_1(t) & g_{1\mathbf{k}}^{\Im} & B_{1z}(t) & R_1(t) \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & B \\ \frac{\Omega(t)}{2} & 0 & g_{\mathbf{k}} & B\Omega(t) \\ 0 & g_{\mathbf{k}}^{\Re} & 0 & 0 \\ \delta & g_{\mathbf{k}}^{\Im} & 0 & -\sum_{\mathbf{k}} \omega_{\mathbf{k}}^{-1} |g_{\mathbf{k}}|^2 \end{pmatrix}. \quad (71)$$

Using the equation (14) and (15) we obtain the following transformed Hamiltonians:

$$\overline{H_{\bar{S}}}(t) = (\delta + R_1) |1\rangle\langle 1| + \frac{B\sigma_x}{2} \Omega(t), \quad (72)$$

$$\overline{H_{\bar{I}}}(t) = \frac{\Omega(t)}{2} (B_x \sigma_x + B_y \sigma_y). \quad (73)$$

Let $\delta + R_1 = \delta'$, now taking the equation (72) with $\delta' |1\rangle\langle 1| = \frac{\delta'}{2} \sigma_z + \frac{\delta'}{2} \mathbb{I}$ help us to reproduce the hamiltonian of the reference [2] because for the time evolution the term proportional to the identity is negligible, so $\overline{H_{\bar{S}}}(t)$ is equal to:

$$\overline{H_{\bar{S}}}(t) = \frac{\delta'}{2} \sigma_z + \frac{B\sigma_x}{2} \Omega(t). \quad (74)$$

As we can see the function B is a time-independent function because we consider that $g_{\mathbf{k}}$ doesn't depend of the time. Writing the interaction Hamiltonian (73) in the similar way to the equation (28) allow us to write

$$\begin{pmatrix} A \\ B(t) \\ C(t) \end{pmatrix} = \begin{pmatrix} \sigma_x & \sigma_y & \frac{I-\sigma_z}{2} & \sigma_x & \sigma_y & \frac{I+\sigma_z}{2} \\ B_x & B_y & B_z & B_y & B_x & 0 \\ \frac{\Omega(t)}{2} & \frac{\Omega(t)}{2} & 0 & 0 & 0 & 1 \end{pmatrix}. \quad (75)$$

For the time-dependent polaron master equation we have $F(\omega_{\mathbf{k}}) = 1$ so it's continuous form is $F(\omega) = 1$ and using the matrix (68) we can deduce that the only terms that survive are $\Lambda_{11}(\tau)$ and $\Lambda_{22}(\tau)$:

$$\Lambda_{11}(\tau) = \frac{B^2}{2} \left(e^{\phi(\tau)} + e^{-\phi(\tau)} - 2 \right), \quad (76)$$

$$\Lambda_{22}(\tau) = \frac{B^2}{2} \left(e^{\phi(\tau)} + e^{-\phi(\tau)} \right). \quad (77)$$

The phonon propagator for this case is:

$$\phi(\tau) = \int_0^\infty \frac{J(\omega)}{\omega^2} G_+(\tau) d\omega. \quad (78)$$

Writing $G_+(\tau) = \coth\left(\frac{\beta\omega}{2}\right) \cos(\omega\tau) - i \sin(\omega\tau)$ then (78) can be written as:

$$\phi(\tau) = \int_0^\infty \frac{J(\omega)}{\omega^2} \left(\coth\left(\frac{\beta\omega}{2}\right) \cos(\omega\tau) - i \sin(\omega\tau) \right) d\omega. \quad (79)$$

These functions match with the equations $\Lambda_x(\tau)$ and $\Lambda_y(\tau)$ of the reference [2], also $\Lambda_i(\tau) = \Lambda_i(-\tau)$ for $i \in \{x, y\}$. The master equation for this section based on the equation (35) is:

$$\frac{d\rho_S(t)}{dt} = -i \left[\frac{\delta'}{2} \sigma_z + \frac{\Omega_r(t) \sigma_x}{2}, \rho_S(t) \right] - \sum_i \int_0^t d\tau \left(C_i(t) C_i(t-\tau) \Lambda_{ii}(\tau) \left[A_i, \widetilde{A}_i(t-\tau, t) \rho_S(t) \right] \right. \quad (80)$$

$$\left. + C_i(t) C_i(t-\tau) \Lambda_{ii}(-\tau) \left[\rho_S(t) \widetilde{A}_i(t-\tau, t), A_i \right] \right). \quad (81)$$

Replacing $C_i(t) = \frac{\Omega(t)}{2}$ and $\widetilde{A}_i(t-\tau, t) = \widetilde{\sigma}_i(t-\tau, t)$, also using the equations (76) and (77) on the equation (81) with $\Lambda_{11}(\tau) \equiv \Lambda_x(\tau)$ and $\Lambda_{22}(\tau) \equiv \Lambda_y(\tau)$ we obtain that:

$$\frac{d\rho_S(t)}{dt} = -\frac{i}{2} [\delta' \sigma_z + \Omega_r(t) \sigma_x, \rho_S(t)] - \frac{\Omega(t)}{4} \int_0^t d\tau \Omega(t-\tau) ([\sigma_x, \widetilde{\sigma}_x(t-\tau, t) \rho_S(t)] \Lambda_x(\tau) \quad (82)$$

$$+ [\sigma_y, \widetilde{\sigma}_y(t-\tau, t) \rho_S(t)] \Lambda_y(\tau) + [\rho_S(t) \widetilde{\sigma}_x(t-\tau, t), \sigma_x] \Lambda_x(\tau) + [\rho_S(t) \widetilde{\sigma}_y(t-\tau, t), \sigma_y] \Lambda_y(\tau)). \quad (83)$$

As we can see $[A_j, \widetilde{A}_i(t-\tau, t) \rho_S(t)]^\dagger = [\rho_S(t) \widetilde{A}_i(t-\tau, t), A_j]$, $\Lambda_x(\tau) = \Lambda_x(-\tau)$ and $\Lambda_y(\tau) = \Lambda_y(-\tau)$, so the result obtained is the same master equation (21) of the reference [2] extending the hermitian conjugate.

C. Time-Dependent Weak-Coupling Limit

In order to prove that the master equation deduced reproduces the equation (S17) of the reference [3] we will impose that $F(\omega) = 0$, so there is no transformation in this case. As we can see from the matrix (68) the only term that survives is $\Lambda_{33}(\tau)$. Taking $\hbar = 1$ the Hamiltonian of the reference can be written as:

$$H = \Delta |1\rangle\langle 1| + \frac{\Omega(t)}{2} (|1\rangle\langle 0| + |0\rangle\langle 1|) + \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + |1\rangle\langle 1| \sum_{\mathbf{k}} \left(g_{\mathbf{k}} b_{\mathbf{k}}^\dagger + g_{\mathbf{k}}^* b_{\mathbf{k}} \right). \quad (84)$$

The correlation functions are relevant if $F(\omega) = 0$, for the weak-coupling approximation we have:

$$\Lambda_{33}(\tau) = \int_0^\infty d\omega J(\omega) G_+(\tau). \quad (85)$$

In our case $A_3 = \frac{\mathbb{I} + \sigma_z}{2}$, the equation (81) can be transformed in:

$$\frac{d\rho_S}{dt} = -i [H_S(t), \rho_S(t)] - \sum_w \left(K_{33}(w, t) [A_3, A_3(w) \rho_S(t)] + K_{33}^*(w, t) \left[\rho_S(t) A_3^\dagger(w), A_3 \right] \right). \quad (86)$$

As the paper of refrence suggests we will consider that the quantum system is in resonance, so $\Delta = 0$. Furthermore the relaxation time of the bath is less than the evolution time to be considered, so the frequency of the Rabi frequency of the laser can be taken as constant and equal to $\tilde{\Omega}$. To find the matrices $A_3(w)$, we have to remember that $H_S = \frac{\Omega(t)}{2} (|1\rangle\langle 0| + |0\rangle\langle 1|)$, this Hamiltonian with $\Omega(t) \simeq \tilde{\Omega}$ have the following eigenstates

$$|H_{S,1}\rangle = \frac{1}{\sqrt{2}} (|1\rangle + |0\rangle), \quad (87)$$

$$|H_{S,0}\rangle = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle). \quad (88)$$

where $\lambda_1 = \frac{\tilde{\Omega}}{2}$ and $\lambda_0 = -\frac{\tilde{\Omega}}{2}$ are the eigenvalues of $|H_{S,1}\rangle$ and $|H_{S,0}\rangle$ respectively.

The decomposition matrices are:

$$A_3(0) = \frac{\mathbb{I}}{2}, \quad (89)$$

$$A_3(\eta) = \frac{1}{4}(\sigma_z + i\sigma_y), \quad (90)$$

$$A_3(-\eta) = \frac{1}{4}(\sigma_z - i\sigma_y), \quad (91)$$

Neglecting the term proportional to the identity in the Hamiltonian we obtain that:

$$\frac{d\rho_S(t)}{dt} = -i\frac{\tilde{\Omega}}{2}[\sigma_x, \rho_S(t)] - K_{33}(\tilde{\Omega}, t) \left[\frac{\sigma_z}{2}, \frac{1}{4}(\sigma_z + i\sigma_y)\rho_S(t) \right] - K_{33}(-\tilde{\Omega}, t) \left[\frac{\sigma_z}{2}, \frac{1}{4}(\sigma_z - i\sigma_y)\rho_S(t) \right] \quad (92)$$

$$- K_{33}^*(\tilde{\Omega}, t) \left[\rho_S(t) \frac{1}{4}(\sigma_z + i\sigma_y), \frac{\sigma_z}{2} \right] - K_{33}^*(-\tilde{\Omega}, t) \left[\rho_S(t) \frac{1}{4}(\sigma_z - i\sigma_y), \frac{\sigma_z}{2} \right]. \quad (93)$$

Calculating the response functions extending the upper limit of τ to ∞ , we obtain:

$$K_{33}(\tilde{\Omega}) = \pi J(\tilde{\Omega}) (n(\tilde{\Omega}) + 1), \quad (94)$$

$$K_{33}(-\tilde{\Omega}) = \pi J(\tilde{\Omega}) n(\tilde{\Omega}). \quad (95)$$

Replacing in the equation (92) lead us to obtain:

$$\frac{d\rho_S(t)}{dt} = -i\frac{\tilde{\Omega}}{2}[\sigma_x, \rho_S(t)] - \frac{\pi}{8}J(\tilde{\Omega}) \left((n(\tilde{\Omega}) + 1) [\sigma_z, (\sigma_z + i\sigma_y)\rho_S(t)] + n(\tilde{\Omega}) [\sigma_z, (\sigma_z - i\sigma_y)\rho_S(t)] \right) \quad (96)$$

$$- \frac{\pi}{8}J(\tilde{\Omega}) \left((n(\tilde{\Omega}) + 1) [\rho_S(t)(\sigma_z + i\sigma_y), \sigma_z] + n(\tilde{\Omega}) [\rho_S(t)(\sigma_z - i\sigma_y), \sigma_z] \right). \quad (97)$$

This is the same result than the equation (S17), so we have proved that our general master equation allows to reproduce the results of the weak-coupling time-dependent. Now the master equation in the evolution time is given by

$$\frac{d\rho_S(t)}{dt} = -i\frac{\Omega(t)}{2}[\sigma_x, \rho_S(t)] - \frac{\pi}{8}J(\Omega(t)) ((n(\Omega(t)) + 1)[\sigma_z, (\sigma_z + i\sigma_y)\rho_S(t)] + n(\Omega(t))[\sigma_z, (\sigma_z - i\sigma_y)\rho_S(t)]) \quad (98)$$

$$- \frac{\pi}{8}J(\Omega(t)) ((n(\Omega(t)) + 1)[\rho_S(t)(\sigma_z + i\sigma_y), \sigma_z] + n(\Omega(t))[\rho_S(t)(\sigma_z - i\sigma_y), \sigma_z]). \quad (99)$$

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