The Mother of all Master Equations

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I. THE HAMILTONIAN

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

$$H_T(t) = H_S(t) + H_I + H_B, \tag{1}$$

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

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

$$H_B = \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}}. \tag{4}$$

II. UNITARY TRANSFORMATION INTO THE VARIATIONALLY OPTIMIZABLE FRAME

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

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

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 in the variational frame will be written as:

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

We assume that the bath starts equilibrium with inverse temperature $\beta = 1/k_{\mathrm{B}}T$:

$$\rho_B \equiv \rho_B(0) \tag{7}$$

$$= \frac{e^{-\beta H_B}}{\mathrm{Tr}\left(e^{-\beta H_B}\right)} \tag{8}$$

With the following definitions:

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

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

$$(\cdot)^{\Re} \equiv \Re(\cdot) \tag{11}$$
$$(\cdot)^{\Im} \equiv \Im(\cdot) \tag{12}$$

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

$$\overline{H_T}(t) \equiv \overline{H_{\bar{S}}}(t) + \overline{H_{\bar{I}}}(t) + \overline{H_{\bar{B}}} \tag{13}$$
$$\overline{H_{\bar{S}}}(t) \equiv \sum_i (\varepsilon_i(t)+R_i(t))|i\rangle\langle i| + \sigma_x\big(B_{10}^{\Re}(t)V_{10}^{\Re}(t) - B_{10}^{\Im}(t)V_{10}^{\Im}(t)\big) - \sigma_y\big(B_{10}^{\Re}(t)V_{10}^{\Im}(t) + B_{10}^{\Im}(t)V_{10}^{\Re}(t)\big) \tag{14}$$
$$\overline{H_{\bar{I}}}(t) \equiv \sum_i B_{iz}(t)|i\rangle\langle i| + V_{10}^{\Re}(t)(B_x(t)\sigma_x + B_y(t)\sigma_y) - V_{10}^{\Im}(t)(B_x(t)\sigma_y - B_y(t)\sigma_x) \tag{15}$$
$$\overline{H_{\bar{B}}} \equiv \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} \tag{16}$$
$$= H_B \tag{17}$$

III. FREE-ENERGY MINIMIZATION

The true free energy A is bounded by the Bogoliubov inequality:

$$A \leq A_{\mathrm{B}}(t) \equiv -\frac{1}{\beta}\ln\left(\mathrm{Tr}\left(e^{-\beta\overline{H_{\bar{S}}(t)+H_{\bar{B}}}}\right)\right) + \langle\overline{H_{\bar{I}}}(t)\rangle_{\overline{H_{\bar{S}}(t)+H_{\bar{B}}}} + O\left(\langle\overline{H_{\bar{I}}}(t)\rangle_{\overline{H_{\bar{S}}(t)+H_{\bar{B}}}}\right) \tag{18}$$

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

$$\frac{\partial A_{\mathrm{B}}(\{v_{\mathbf{k}}(t)\};t)}{\partial v_{i\mathbf{k}}(t)} = 0. \tag{19}$$

This leads us to:

$$v_{i\mathbf{k}}(\omega_{\mathbf{k}},t) = \frac{g_i(\omega_{\mathbf{k}})\left(1 - \frac{\tanh\left(\frac{\beta\eta(t)}{2}\right)}{\eta(t)}(2\varepsilon_i(t) + 2R_i(t) - \varepsilon(t))\right) + 2\frac{\tanh\left(\frac{\beta\eta(t)}{2}\right)}{\eta(t)}\frac{v_{i'\mathbf{k}}(\omega_{\mathbf{k}},t)}{\omega_{\mathbf{k}}}|B_{10}(t)|^2|V_{10}(t)|^2\coth(\beta\omega_{\mathbf{k}}/2)}{1 - \frac{\tanh\left(\frac{\beta\eta(t)}{2}\right)}{\eta(t)}\left(\varepsilon(t) - 2(\varepsilon(t) - \varepsilon_i(t) - R_i(t)) - \frac{2|V_{10}(t)|^2|B_{10}(t)|^2\coth(\beta\omega_{\mathbf{k}}/2)}{\omega_{\mathbf{k}}}\right)}, \tag{20}$$

with the following definitions:

$$\eta(t) \equiv \sqrt{\left(\mathrm{Tr}\left(\overline{H_{\bar{S}}}(t)\right)\right)^2 - 4\mathrm{Det}\left(\overline{H_{\bar{S}}}(t)\right)} \tag{21}$$
$$\varepsilon(t) \equiv \mathrm{Tr}\left(\overline{H_{\bar{S}}}(t)\right). \tag{22}$$

IV. MASTER EQUATION

We transform any operator O into the interaction picture in the following way:

$$\widetilde{O} \equiv U^{\dagger}(t)\,O\,U(t) \tag{23}$$
$$U(t) \equiv \mathcal{T}\exp\left(-\mathrm{i}\int_0^t \mathrm{d}t'\,\overline{H_T}(t')\right). \tag{24}$$

Therefore:

$$\widetilde{\overline{\rho_S}}\left(t\right) = U^{\dagger}\left(t\right)\overline{\rho_S}\left(t\right)U\left(t\right) \tag{25}$$

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

$$\frac{\mathrm{d}\widetilde{\overline{\rho_S}}\left(t\right)}{\mathrm{d}t} = -\int_0^t \mathrm{Tr}_B\left[\widetilde{\overline{H_{\bar{I}}}}\left(t\right), \left[\widetilde{\overline{H_{\bar{I}}}}\left(s\right), \widetilde{\overline{\rho_S}}\left(t\right)\rho_B\right]\right]\mathrm{d}s \tag{26}$$

To simplify this we define the following matrix:

$$\begin{pmatrix} A \\ B\left(t\right) \\ C\left(t\right) \end{pmatrix} = \begin{pmatrix} \sigma_x & \sigma_y & \frac{I-\sigma_z}{2} & \sigma_x & \sigma_y & \frac{I+\sigma_z}{2} \\ B_x\left(t\right) & B_y\left(t\right) & B_{1z}\left(t\right) & B_y\left(t\right) & B_x\left(t\right) & B_{0z}\left(t\right) \\ V_{10}^{\Re}\left(t\right) & V_{10}^{\Re}\left(t\right) & 1 & V_{10}^{\Im}\left(t\right) & -V_{10}^{\Im}\left(t\right) & 1 \end{pmatrix}. \tag{27}$$

$$\overline{H_{\bar{I}}}\left(t\right) = \sum_i C_i\left(t\right)\left(A_i \otimes B_i\left(t\right)\right) \tag{28}$$

$$\widetilde{\overline{H_{\bar{I}}}}\left(t\right) = \sum_i C_i\left(t\right)\left(\widetilde{A_i}\left(t\right) \otimes \widetilde{B_i}\left(t\right)\right), \tag{29}$$

and expanding the commutators yields:

$$\frac{\mathrm{d}\widetilde{\overline{\rho_S}}\left(t\right)}{\mathrm{d}t} = -\int_0^t \mathrm{Tr}_B\left(\sum_j C_j(t)\left(\widetilde{A_j}(t)\otimes\widetilde{B_j}(t)\right)\sum_i C_i\left(s\right)\left(\widetilde{A_i}(s)\otimes\widetilde{B_i}(s)\right)\widetilde{\overline{\rho_S}}\left(t\right)\rho_B - \sum_j C_j(t)\left(\widetilde{A_j}(t)\otimes\widetilde{B_j}(t)\right)\widetilde{\overline{\rho_S}}\left(t\right)\rho_B\sum_i C_i\left(s\right)\left(\widetilde{A_i}(s)\otimes\widetilde{B_i}(s)\right)\right. \tag{30}$$

$$\left. - \sum_i C_i\left(s\right)\left(\widetilde{A_i}(s)\otimes\widetilde{B_i}(s)\right)\widetilde{\overline{\rho_S}}\left(t\right)\rho_B\sum_j C_j\left(t\right)\left(\widetilde{A_j}(t)\otimes\widetilde{B_j}(t)\right) + \widetilde{\overline{\rho_S}}\left(t\right)\rho_B\sum_i C_i\left(s\right)\left(\widetilde{A_i}(s)\otimes\widetilde{B_i}(s)\right)\sum_j C_j\left(t\right)\left(\widetilde{A_j}(t)\otimes\widetilde{B_j}(t)\right)\right)\mathrm{d}s. \tag{31}$$

The correlation functions are equal to:

$$\left\langle\widetilde{B_{iz}}\left(\tau\right)\widetilde{B_{jz}}\left(0\right)\right\rangle_B = \sum_{\mathbf{k}}\left(\left(g_{i\mathbf{k}} - v_{i\mathbf{k}}\right)\left(g_{j\mathbf{k}} - v_{j\mathbf{k}}\right)^* e^{\mathrm{i}\omega_{\mathbf{k}}\tau}N_{\mathbf{k}} + \left(g_{i\mathbf{k}} - v_{i\mathbf{k}}\right)^*\left(g_{j\mathbf{k}} - v_{j\mathbf{k}}\right)e^{-\mathrm{i}\omega_{\mathbf{k}}\tau}\left(N_{\mathbf{k}} + 1\right)\right), \tag{32}$$

$$U = \prod_{\mathbf{k}}\left(\exp\left(\frac{v_{0\mathbf{k}}^* v_{1\mathbf{k}} - v_{0\mathbf{k}}v_{1\mathbf{k}}^*}{\omega_{\mathbf{k}}^2}\right)\right), \tag{33}$$

$$\phi\left(\tau\right) = \sum_{\mathbf{k}}\left|\frac{v_{1\mathbf{k}} - v_{0\mathbf{k}}}{\omega_{\mathbf{k}}}\right|^2\left(-\mathrm{i}\sin\left(\omega_{\mathbf{k}}\tau\right) + \cos\left(\omega_{\mathbf{k}}\tau\right)\coth\left(\frac{\beta\omega_{\mathbf{k}}}{2}\right)\right), \tag{34}$$

$$\left\langle\widetilde{B_x}\left(\tau\right)\widetilde{B_x}\left(0\right)\right\rangle_B = \frac{\left|B_{10}\right|^2}{2}\left(U^{\Re}\exp\left(-\phi\left(\tau\right)\right) + \exp\left(\phi\left(\tau\right)\right) - U^{\Re} - 1\right), \tag{35}$$

$$\left\langle\widetilde{B_y}\left(\tau\right)\widetilde{B_y}\left(0\right)\right\rangle_B = \frac{\left|B_{10}\right|^2}{2}\left(\exp\left(\phi\left(\tau\right)\right) - U^{\Re}\exp\left(-\phi\left(\tau\right)\right) - 1 + U^{\Re}\right), \tag{36}$$

$$\left\langle\widetilde{B_x}\left(\tau\right)\widetilde{B_y}\left(0\right)\right\rangle_B = \frac{U^{\Im}\left|B_{10}\right|^2}{2}\left(\exp\left(-\phi\left(\tau\right)\right) - 1\right), \tag{37}$$

$$\left\langle\widetilde{B_y}\left(\tau\right)\widetilde{B_x}\left(0\right)\right\rangle_B = \frac{U^{\Im}\left|B_{10}\right|^2}{2}\left(\exp\left(-\phi\left(\tau\right)\right) - 1\right), \tag{38}$$

$$\left\langle\widetilde{B_{iz}}\left(\tau\right)\widetilde{B_x}\left(0\right)\right\rangle_B = \mathrm{i}B_{10}^{\Im}\sum_{\mathbf{k}}\left(\left(g_{i\mathbf{k}} - v_{i\mathbf{k}}\right)N_{\mathbf{k}}e^{\mathrm{i}\omega_{\mathbf{k}}\tau}\left(\frac{v_{1\mathbf{k}} - v_{0\mathbf{k}}}{\omega_{\mathbf{k}}}\right)^* - \left(g_{i\mathbf{k}} - v_{i\mathbf{k}}\right)^*\frac{v_{1\mathbf{k}} - v_{0\mathbf{k}}}{\omega_{\mathbf{k}}}e^{-\mathrm{i}\omega_{\mathbf{k}}\tau}\left(N_{\mathbf{k}} + 1\right)\right), \tag{39}$$

$$\left\langle \widetilde{B_x}\left(\tau\right)\widetilde{B_{iz}}\left(0\right)\right\rangle_B = \mathrm{i}B_{10}^{\Im}\sum_{\mathbf{k}}\left(\left(g_{i\mathbf{k}}-v_{i\mathbf{k}}\right)^{*}N_{\mathbf{k}}e^{\mathrm{i}\omega_{\mathbf{k}}\tau}\left(\frac{v_{1\mathbf{k}}-v_{0\mathbf{k}}}{\omega_{\mathbf{k}}}\right)-\left(g_{i\mathbf{k}}-v_{i\mathbf{k}}\right)\left(\frac{v_{1\mathbf{k}}-v_{0\mathbf{k}}}{\omega_{\mathbf{k}}}\right)^{*}e^{-\mathrm{i}\omega_{\mathbf{k}}\tau}\left(N_{\mathbf{k}}+1\right)\right), \tag{40}$$

$$\left\langle \widetilde{B_{iz}}\left(\tau\right)\widetilde{B_y}\left(0\right)\right\rangle_B = \mathrm{i}B_{10}^{\Re}\sum_{\mathbf{k}}\left(e^{-\mathrm{i}\omega_{\mathbf{k}}\tau}\left(g_{i\mathbf{k}}-v_{i\mathbf{k}}\right)^{*}\left(\frac{v_{1\mathbf{k}}-v_{0\mathbf{k}}}{\omega_{\mathbf{k}}}\right)\left(N_{\mathbf{k}}+1\right)-e^{\mathrm{i}\omega_{\mathbf{k}}\tau}\left(g_{i\mathbf{k}}-v_{i\mathbf{k}}\right)\left(\frac{v_{1\mathbf{k}}-v_{0\mathbf{k}}}{\omega_{\mathbf{k}}}\right)^{*}N_{\mathbf{k}}\right), \tag{41}$$

$$\left\langle \widetilde{B_y}\left(\tau\right)\widetilde{B_{iz}}\left(0\right)\right\rangle_B = \mathrm{i}B_{10}^{\Re}\sum_{\mathbf{k}}\left(\left(g_{i\mathbf{k}}-v_{i\mathbf{k}}\right)^{*}N_{\mathbf{k}}e^{\mathrm{i}\omega_{\mathbf{k}}\tau}\left(\frac{v_{1\mathbf{k}}-v_{0\mathbf{k}}}{\omega_{\mathbf{k}}}\right)-\left(g_{i\mathbf{k}}-v_{i\mathbf{k}}\right)\left(N_{\mathbf{k}}+1\right)e^{-\mathrm{i}\omega_{\mathbf{k}}\tau}\left(\frac{v_{1\mathbf{k}}-v_{0\mathbf{k}}}{\omega_{\mathbf{k}}}\right)^{*}\right). \tag{42}$$

The integral version of the correlation functions are given by:

$$\left\langle \widetilde{B_{iz}}(\tau)\widetilde{B_{jz}}(0)\right\rangle_B = \int_0^{\infty}\left(\sqrt{J_i(\omega)J_j^{*}(\omega)}(1-F_i(\omega))\left(1-F_j^{*}(\omega)\right)e^{\mathrm{i}\omega\tau}N(\omega)+\sqrt{J_i^{*}(\omega)J_j(\omega)}(1-F_i^{*}(\omega))(1-F_j(\omega))e^{-\mathrm{i}\omega\tau}(N(\omega)+1)\right)\mathrm{d}\omega, \tag{43}$$

$$U = \exp\left(\int_0^{\infty}\frac{\sqrt{J_0^{*}\left(\omega\right)J_1\left(\omega\right)}F_0^{*}\left(\omega\right)F_1\left(\omega\right)-\sqrt{J_0\left(\omega\right)J_1^{*}\left(\omega\right)}F_0\left(\omega\right)F_1^{*}\left(\omega\right)}{\omega^2}\mathrm{d}\omega\right), \tag{44}$$

$$\phi\left(\tau\right) = \int_0^{\infty}\left|\frac{\sqrt{J_1\left(\omega\right)}F_1\left(\omega\right)-\sqrt{J_0\left(\omega\right)}F_0\left(\omega\right)}{\omega}\right|^2\left(-\mathrm{i}\sin\left(\omega\tau\right)+\cos\left(\omega\tau\right)\coth\left(\frac{\beta\omega}{2}\right)\right)\mathrm{d}\omega, \tag{45}$$

$$B_{10} = \exp\left(-\frac{1}{2}\int_0^{\infty}\left|\frac{\sqrt{J_1(\omega)}F_1(\omega)-\sqrt{J_0(\omega)}F_0(\omega)}{\omega}\right|^2\coth\left(\frac{\beta\omega}{2}\right)\mathrm{d}\omega\right)\exp\left(\int_0^{\infty}\frac{1}{2}\left(\frac{\sqrt{J_0(\omega)J_1^{*}(\omega)}F_0(\omega)F_1^{*}(\omega)-\sqrt{J_0^{*}(\omega)J_1(\omega)}F_0^{*}(\omega)F_1(\omega)}{\omega^2}\right)\mathrm{d}\omega\right), \tag{46}$$

$$\left\langle \widetilde{B_x}(\tau)\widetilde{B_x}(0)\right\rangle_B = \frac{\left|B_{10}\right|^2}{2}\left(U^{\Re}\exp\left(-\phi\left(\tau\right)\right)+\exp\left(\phi\left(\tau\right)\right)-U^{\Re}-1\right), \tag{47}$$

$$\left\langle \widetilde{B_y}(\tau)\widetilde{B_y}(0)\right\rangle_B = \frac{\left|B_{10}\right|^2}{2}\left(\exp\left(\phi\left(\tau\right)\right)-U^{\Re}\exp\left(-\phi\left(\tau\right)\right)-1+U^{\Re}\right), \tag{48}$$

$$\left\langle \widetilde{B_x}(\tau)\widetilde{B_y}(0)\right\rangle_B = \frac{U^{\Im}\left|B_{10}\right|^2}{2}\left(\exp\left(-\phi\left(\tau\right)\right)-1\right), \tag{49}$$

$$\left\langle \widetilde{B_y}(\tau)\widetilde{B_x}(0)\right\rangle_B = \frac{U^{\Im}\left|B_{10}\right|^2}{2}\left(\exp\left(-\phi\left(\tau\right)\right)-1\right), \tag{50}$$

$$\left\langle \widetilde{B_{iz}}(\tau)\widetilde{B_x}(0)\right\rangle_B = \mathrm{i}B_{10}^{\Im}\sum_{\mathbf{k}}\left(g_{i\mathbf{k}}(1-F_i(\omega_{\mathbf{k}}))N_{\mathbf{k}}e^{\mathrm{i}\omega_{\mathbf{k}}\tau}\left(\frac{g_{1\mathbf{k}}F_1(\omega_{\mathbf{k}})-g_{0\mathbf{k}}F_0(\omega_{\mathbf{k}})}{\omega_{\mathbf{k}}}\right)^{*}-g_{i\mathbf{k}}^{*}(1-F_i(\omega_{\mathbf{k}}))^{*}\frac{g_{1\mathbf{k}}F_1(\omega_{\mathbf{k}})-g_{0\mathbf{k}}F_0(\omega_{\mathbf{k}})}{\omega_{\mathbf{k}}}e^{-\mathrm{i}\omega_{\mathbf{k}}\tau}(N_{\mathbf{k}}+1)\right), \tag{51}$$

$$Q_i\left(\omega\right) = \sqrt{J_i\left(\omega\right)}\left(1-F_i\left(\omega\right)\right)\left(\frac{\sqrt{J_1\left(\omega\right)}F_1\left(\omega\right)-\sqrt{J_0\left(\omega\right)}F_0\left(\omega\right)}{\omega}\right)^{*}, \tag{52}$$

$$\left\langle \widetilde{B_{iz}}(\tau)\widetilde{B_x}(0)\right\rangle_B = \mathrm{i}B_{10}^{\Im}\int_0^{\infty}\left(Q_i\left(\omega\right)N\left(\omega\right)e^{\mathrm{i}\omega\tau}-Q_i^{*}\left(\omega\right)\left(N\left(\omega\right)+1\right)e^{-\mathrm{i}\omega\tau}\right)\mathrm{d}\omega, \tag{53}$$

$$\left\langle \widetilde{B_x}(\tau)\widetilde{B_{iz}}(0)\right\rangle_B = \mathrm{i}B_{10}^{\Im}\int_0^{\infty}\left(Q_i^{*}\left(\omega\right)N\left(\omega\right)e^{\mathrm{i}\omega\tau}-Q_i\left(\omega\right)\left(N\left(\omega\right)+1\right)e^{-\mathrm{i}\omega\tau}\right)\mathrm{d}\omega, \tag{54}$$

$$\left\langle \widetilde{B_{iz}}(\tau)\widetilde{B_y}(0)\right\rangle_B = \mathrm{i}B_{10}^{\Re}\int_0^{\infty}\left(e^{-\mathrm{i}\omega\tau}Q_i^{*}\left(\omega\right)\left(N\left(\omega\right)+1\right)-e^{\mathrm{i}\omega\tau}Q_i\left(\omega\right)N\left(\omega\right)\right)\mathrm{d}\omega, \tag{55}$$

$$\left\langle \widetilde{B_y}(\tau)\widetilde{B_{iz}}(0)\right\rangle_B = \mathrm{i}B_{10}^{\Re}\int_0^{\infty}\left(e^{\mathrm{i}\omega\tau}Q_i^{*}\left(\omega\right)N\left(\omega\right)-e^{-\mathrm{i}\omega\tau}Q_i\left(\omega\right)\left(N\left(\omega\right)+1\right)\right)\mathrm{d}\omega. \tag{56}$$

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

$$\mathcal{B}_{ij}\left(\tau\right) = \mathrm{Tr}_B\left(\widetilde{B_i}\left(t\right)\widetilde{B_j}\left(s\right)\rho_B\right) \tag{57}$$

$$= \mathrm{Tr}_B\left(\widetilde{B_i}\left(\tau\right)\widetilde{B_j}\left(0\right)\rho_B\right). \tag{58}$$

The $\mathcal{B}$ operators matrix it's defined in terms of (43)-(56) following the notation of the matrix (27) as:

$$\mathcal{B}\left(t\right) \equiv \begin{pmatrix} \mathcal{B}_{11}\left(t\right) & \mathcal{B}_{12}\left(t\right) & \mathcal{B}_{13}\left(t\right) & \mathcal{B}_{12}\left(t\right) & \mathcal{B}_{11}\left(t\right) & \mathcal{B}_{16}\left(t\right) \\ \mathcal{B}_{12}\left(t\right) & \mathcal{B}_{22}\left(t\right) & \mathcal{B}_{23}\left(t\right) & \mathcal{B}_{22}\left(t\right) & \mathcal{B}_{12}\left(t\right) & \mathcal{B}_{26}\left(t\right) \\ \mathcal{B}_{11}\left(t\right) & \mathcal{B}_{32}\left(t\right) & \mathcal{B}_{33}\left(t\right) & \mathcal{B}_{32}\left(t\right) & \mathcal{B}_{31}\left(t\right) & \mathcal{B}_{36}\left(t\right) \\ \mathcal{B}_{12}\left(t\right) & \mathcal{B}_{22}\left(t\right) & \mathcal{B}_{23}\left(t\right) & \mathcal{B}_{22}\left(t\right) & \mathcal{B}_{12}\left(t\right) & \mathcal{B}_{26}\left(t\right) \\ \mathcal{B}_{11}\left(t\right) & \mathcal{B}_{12}\left(t\right) & \mathcal{B}_{13}\left(t\right) & \mathcal{B}_{12}\left(t\right) & \mathcal{B}_{11}\left(t\right) & \mathcal{B}_{16}\left(t\right) \\ \mathcal{B}_{61}\left(t\right) & \mathcal{B}_{62}\left(t\right) & \mathcal{B}_{63}\left(t\right) & \mathcal{B}_{62}\left(t\right) & \mathcal{B}_{61}\left(t\right) & \mathcal{B}_{66}\left(t\right) \end{pmatrix}, \tag{59}$$

$$\begin{pmatrix} \mathcal{B}_{11}\left(t\right) & \cdot & \cdots \\ \cdot & \mathcal{B}_{22}\left(t\right) & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \equiv \begin{pmatrix} \frac{\left|B_{10}\right|^2}{2}\left(U^{\Re}\exp\left(-\phi\left(\tau\right)\right)+\exp\left(\phi\left(\tau\right)\right)-U^{\Re}-1\right) & & \cdots \\ & \frac{\left|B_{10}\right|^2}{2}\left(\exp\left(\phi\left(\tau\right)\right)-U^{\Re}\exp\left(-\phi\left(\tau\right)\right)-1+U^{\Re}\right) & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \tag{60}$$

where we have defined:

$$G_{\pm}\left(t\right) \equiv \left(N\left(\omega\right)+1\right)\mathrm{e}^{-\mathrm{i}t\omega} \pm N\left(\omega\right)e^{\mathrm{i}t\omega} \tag{61}$$

$$N\left(\omega\right) \equiv \left(\mathrm{e}^{\beta\omega}-1\right)^{-1}, \tag{62}$$

and the spectral density is defined in the usual way:

$$J_i\left(\omega\right) \equiv \sum_{\mathbf{k}}\left|g_{i\mathbf{k}}\right|^2\delta\left(\omega-\omega_{\mathbf{k}}\right), \tag{63}$$

$$v_{i\mathbf{k}} = g_{i\mathbf{k}}F_i\left(\omega_{\mathbf{k}}\right). \tag{64}$$

In this case $g_i\left(\omega\right)$ and $v_i\left(\omega\right)$ are the continuous version of $g_i\left(\omega_{\mathbf{k}}\right)$ and $v_{i\mathbf{k}}\left(\omega_{\mathbf{k}},t\right)$ respectively.
This allows us to remove the trace over the bath and write down a more tangible master equation:

$$\frac{\mathrm{d}\widetilde{\overline{\rho_S}}\left(t\right)}{\mathrm{d}t} = -\int_0^t\sum_{ij}\left(C_i\left(t\right)C_j\left(s\right)\left(\mathcal{B}_{ij}\left(\tau\right)\left[\widetilde{A_i}\left(t\right),\widetilde{A_j}\left(s\right)\widetilde{\overline{\rho_S}}\left(t\right)\right]+\mathcal{B}_{ji}\left(-\tau\right)\left[\widetilde{\overline{\rho_S}}\left(t\right)\widetilde{A_j}\left(s\right),\widetilde{A_i}\left(t\right)\right]\right)\right)\mathrm{d}s \tag{65}$$

Doing the reverse of the transformation to interaction picture we get:

$$\frac{\mathrm{d}\overline{\rho_S}\left(t\right)}{\mathrm{d}t} = -\mathrm{i}\left[H_S\left(t\right),\overline{\rho_S}\left(t\right)\right]-\sum_{ij}\int_0^t C_i\left(t\right)C_j\left(t-\tau\right)\mathcal{B}_{ij}\left(\tau\right)\left[A_i,\widetilde{A_j}\left(t-\tau,t\right)\overline{\rho_S}\left(t\right)\right]+C_j\left(t\right)C_i\left(t-\tau\right)\mathcal{B}_{ji}\left(-\tau\right)\left[\overline{\rho_S}\left(t\right)\widetilde{A_j}\left(t-\tau,t\right),A_i\right]\mathrm{d}\tau. \tag{66}$$

We still have interaction picture versions of A_j, so we will decompose $\widetilde{A_j}\left(t\right)$ in terms of the Schroedinger picture version A_i:

$$\widetilde{A_j}\left(t\right) = \sum_{w(t)}e^{-\mathrm{i}w(t)\tau}A_j\left(w\left(t\right)\right) \tag{67}$$

$$\widetilde{A_j}\left(t-\tau,t\right) = \sum_{w'(t),w(t-\tau)}e^{-\mathrm{i}(t-\tau)w(t-\tau)}e^{\mathrm{i}tw'(t)}A_{jww'}\left(t,t-\tau\right) \tag{68}$$

Where the sum is defined on the set of all the differences between the eigenvalues of the system and we furthermore define $A_j\left(w\left(t-\tau\right),w'\left(t\right)\right) \equiv A_{jww'}\left(t,t-\tau\right)$, in our case $w\left(t\right) \in \{0,\pm\eta\left(t\right)\}$. We also have that $w\left(t\right)$ belongs to the set of differences of eigenvalues of $H_E\left(t\right)$ that depends of the time. As we can see the decomposition matrices are time-dependent as well. Also, $w\left(t-\tau\right)$ and $w'\left(t\right)$ belong to the set of the differences of the eigenvalues of the Hamiltonian $H_E\left(t-\tau\right)$ and $H_E\left(t\right)$ respectively. In matrix form for the 2×2 these are:

$$A_i\left(0\right) = \langle +|\widetilde{A_i}\left(t\right)|+\rangle\,|+\rangle\!\langle +| + \langle -|\widetilde{A_i}\left(t\right)|-\rangle\,|-\rangle\!\langle -| \tag{69}$$

$$A_i\left(w\right) = \langle +|\widetilde{A_i}\left(t\right)|-\rangle\,|+\rangle\!\langle -| \tag{70}$$

$$A_i\left(-w\right) = \langle -|\widetilde{A_i}\left(t\right)|+\rangle\,|-\rangle\!\langle +|. \tag{71}$$

The Fourier exponentials $e^{\mathrm{i}w\tau}$ and $e^{-\mathrm{i}t\left(w-w'\right)}$ can be combined with the C and Λ functions:

$$K_{ijww'}\left(t\right)=\int_0^t C_i\left(t\right)C_j\left(t-\tau\right)\mathcal{B}_{ij}\left(\tau\right)e^{\mathrm{i}w\tau}e^{-\mathrm{i}t\left(w-w'\right)}\mathrm{d}\tau \tag{72}$$

Finally we end up with our final master equation in the variationally optimized frame in the Schroedinger picture, in terms of only K and A:

$$\frac{\mathrm{d}\overline{\rho_{\bar{S}}}(t)}{\mathrm{d}t}=-\mathrm{i}\left[\overline{H}_{\bar{S}}\left(t\right),\overline{\rho_{\bar{S}}}\right]-\sum_{ijww'}\left(K_{ijww'}\left(t\right)\left[A_i,A_{jww'}\overline{\rho}_S\left(t\right)\right]-K^*_{ijww'}\left(t\right)\left[A_i,\overline{\rho}_S\left(t\right)A^\dagger_{jww'}\right]\right) \tag{73}$$

$$=-\mathrm{i}\left[\overline{H}_{\bar{S}}(t),\overline{\rho}_{\bar{S}}(t)\right]-\sum_{ijww'}\left(K^{\Re}_{ijww'}(t)\left[A_i,A_{jww'}\overline{\rho}_S(t)-\overline{\rho}_S(t)A^\dagger_{jww'}\right]+\mathrm{i}K^{\Im}_{ijww'}(t)\left[A_i,A_{jww'}\overline{\rho}_S(t)+\overline{\rho}_S(t)A^\dagger_{jww'}\right]\right) \tag{74}$$

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

$$\dot{\rho}=-\mathrm{i}\left[H\left(t\right),\rho\right]-\sum_{ijww'}\left(K_{ijww'}\left(t\right)\left[A_i,A_{jww'}\rho\right]-K^*_{ijww'}\left(t\right)\left[A_i,\rho A^\dagger_{jww'}\right]\right) \tag{75}$$

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

A. Time-independent VPQME of 2011

$$\begin{pmatrix} V^{\Im}_{10}\left(t\right) & g_{0\mathbf{k}} & v_{0\mathbf{k}}\left(t\right) & B\left(t\right) \\ V^{\Re}_{10}\left(t\right) & g^{\Im}_{1\mathbf{k}} & v_{1\mathbf{k}}\left(t\right) & \Omega_r \\ \varepsilon_0\left(t\right) & g^{\Re}_{1\mathbf{k}} & & R_0\left(t\right) \\ \varepsilon_1\left(t\right) & & & R_1\left(t\right) \end{pmatrix}=\begin{pmatrix} 0 & 0 & 0 & B_{10} \\ \frac{\Omega}{2} & 0 & v_{\mathbf{k}} & B\Omega \\ 0 & g_{\mathbf{k}} & & 0 \\ \delta & & & R \end{pmatrix} \tag{76}$$

We now have a simpler $\bar{H}_{\bar{S}}$:

$$\overline{H_{\bar{S}}}\left(t\right)\equiv R|0\rangle\langle 0|+\delta|1\rangle\langle 1|+\sigma_x\Omega_r. \tag{77}$$

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

$$v_{\mathbf{k}}=\frac{g_i\left(\omega_{\mathbf{k}}\right)\left(1-\frac{\tanh\left(\frac{\beta\eta(t)}{2}\right)}{\eta(t)}\left(2\varepsilon_i\left(t\right)+2R_i-\varepsilon\left(t\right)\right)\right)+2\frac{\tanh\left(\frac{\beta\eta(t)}{2}\right)}{\eta(t)}\frac{v_{i'\mathbf{k}}}{\omega_{\mathbf{k}}}\left|B_{10}\right|^2\left|V_{10}\left(t\right)\right|^2\coth\left(\beta\omega_{\mathbf{k}}/2\right)}{1-\frac{\tanh\left(\frac{\beta\eta(t)}{2}\right)}{\eta(t)}\left(\varepsilon\left(t\right)-2\left(\varepsilon\left(t\right)-\varepsilon_i\left(t\right)-R_i\right)-\frac{2|V_{10}(t)|^2|B_{10}|^2\coth(\beta\omega_{\mathbf{k}}/2)}{\omega_{\mathbf{k}}}\right)} \tag{78}$$

$$=\frac{g_{\mathbf{k}}\left(1-\frac{\varepsilon(t)}{\eta}\tanh\left(\frac{\beta\eta}{2}\right)\right)}{1-\frac{\varepsilon(t)}{\eta}\tanh\left(\frac{\beta\eta}{2}\right)\left(1-\frac{\Omega_r^2}{2\varepsilon(t)\omega_{\mathbf{k}}}\coth\left(\beta\omega_{\mathbf{k}}/2\right)\right)} \tag{79}$$

The bath and system-bath interaction operators become:

$$\begin{pmatrix} B_z(t) & B^{\pm}(t) \\ B_x(t) & B_{10}(t) \\ B_y(t) & R(t) \end{pmatrix} \equiv \begin{pmatrix} 2\sum_{\mathbf{k}}\left(g_{\mathbf{k}}-v_{\mathbf{k}}\right)b_{\mathbf{k}}^{\dagger} & e^{\pm\sum_{\mathbf{k}}\frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}}\left(b_{\mathbf{k}}^{\dagger}-b_{\mathbf{k}}\right)} \\ \frac{B^{+}+B^{-}-2B}{2} & e^{-(1/2)\sum_{\mathbf{k}}\left(\frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}}\right)^{2}\coth(\beta\omega_{\mathbf{k}}/2)} \\ \frac{B^{-}-B^{+}}{2\mathrm{i}} & \sum_{\mathbf{k}}\left(\frac{|v_{\mathbf{k}}|^{2}}{\omega_{\mathbf{k}}}-2g_{\mathbf{k}}\frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}}\right) \end{pmatrix}, \tag{80}$$

$$\begin{pmatrix} A \\ B(t) \\ C(t) \end{pmatrix} = \begin{pmatrix} \sigma_x & \sigma_y & \frac{I-\sigma_z}{2} & \sigma_x & \sigma_y & \frac{I+\sigma_z}{2} \\ B_x & B_y & B_z & B_y & B_x & 0 \\ \frac{\Omega}{2} & \frac{\Omega}{2} & 1 & 0 & 0 & 1 \end{pmatrix}. \tag{81}$$

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

$$\Lambda_{ij}(t) \equiv C_i C_j \mathcal{B}_{ij}(t), \tag{82}$$

We get:

$$K_{ijww'}(t) = \int_0^t \Lambda_{ij}(\tau)\, e^{\mathrm{i}w\tau} e^{-\mathrm{i}t\left(w-w'\right)} \mathrm{d}\tau. \tag{83}$$

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

$$U(t)\, A_j(w)\, U^{\dagger}(t) = e^{\mathrm{i}wt} A_j(w) \tag{84}$$

It means that a decomposition matrix of $\widetilde{A_j}(t)$ 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 $e^{\mathrm{i}wt}$. 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:

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

Replacing in the equation (73) we obtain that:

$$\frac{\mathrm{d}\overline{\rho}_{\bar{S}}(t)}{\mathrm{d}t} = -\mathrm{i}\left[\overline{H}_{\bar{S}}(t), \overline{\rho}_S(t)\right] - \sum_{ijw}\left(K_{ijw}^{\Re}(t)\left[A_i, A_{jw}\overline{\rho}_S(t) - \overline{\rho}_S(t)\, A_{jw}^{\dagger}\right] + \mathrm{i}K_{ijw}^{\Im}(t)\left[A_i, A_{jw}\overline{\rho}_S(t) + \overline{\rho}_S(t)\, A_{jw}^{\dagger}\right]\right) \tag{85}$$

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