

# 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  $e^{\pm V}$  where  $V$  is the variationally optimizable anti-Hermitian operator:

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

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  $O$  in the variational frame will be written as:

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

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:

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

$$(\cdot)^{\Re} \equiv \Re(\cdot) \quad (9)$$

$$(\cdot)^{\Im} \equiv \Im(\cdot) \quad (10)$$

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

$$\overline{H}_T(t) \equiv \overline{H}_{\overline{S}}(t) + \overline{H}_{\overline{I}} + \overline{H}_{\overline{B}} \quad (11)$$

$$\overline{H}_{\overline{S}}(t) \equiv \sum_i (\varepsilon_i(t) + R_i) |i\rangle \langle i| + \sigma_x (B_{10}^{\Re}(t) V_{10}^{\Re}(t) - B_{10}^{\Im}(t) V_{10}^{\Im}(t)) - \sigma_y (B_{10}^{\Re}(t) V_{10}^{\Im}(t) + B_{10}^{\Im}(t) V_{10}^{\Re}(t)) \quad (12)$$

$$\overline{H}_{\overline{I}} \equiv \sum_i B_{iz} |i\rangle \langle i| + V_{10}^{\Re}(t) (B_x \sigma_x + B_y \sigma_y) - V_{10}^{\Im}(t) (B_x \sigma_y - B_y \sigma_x) \quad (13)$$

$$\overline{H}_{\overline{B}} \equiv \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} \quad (14)$$

$$= H_B \quad (15)$$

### III. FREE-ENERGY MINIMIZATION

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

$$A \leq A_B \equiv -\frac{1}{\beta} \ln \left( \text{Tr} \left( e^{-\beta \overline{H}_{\overline{S}}(t) + H_B} \right) \right) + \langle \overline{H}_{\overline{I}} \rangle_{\overline{H}_{\overline{S}}(t) + H_B} + O \left( \langle \overline{H}_{\overline{I}}^2 \rangle_{\overline{H}_{\overline{S}}(t) + H_B} \right) \quad (16)$$

We will optimize the set of variational parameters  $\{v_{\mathbf{k}}\}$  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  $\langle \overline{H}_{\overline{I}} \rangle_{\overline{H}_{\overline{S}}(t) + H_B} = 0$  we can obtain the following condition to obtain the set  $\{v_{\mathbf{k}}\}$ :

$$\frac{\partial A_B}{\partial v_{i\mathbf{k}}} = 0. \quad (17)$$

This leads us to:

$$v_i(\omega_{\mathbf{k}}) = \frac{g_i(\omega_{\mathbf{k}}) \left( 1 - \frac{\tanh(\frac{\beta \eta(t)}{2})}{\eta(t)} (2\varepsilon_i(t) + 2R_i - \varepsilon(t)) \right) + 2 \frac{\tanh(\frac{\beta \eta(t)}{2})}{\eta(t)} \frac{v_{i'\mathbf{k}}}{\omega_{\mathbf{k}}} |B_{10}|^2 |V_{10}(t)|^2 \coth(\beta \omega_{\mathbf{k}}/2)}{1 - \frac{\tanh(\frac{\beta \eta(t)}{2})}{\eta(t)} \left( \varepsilon(t) - 2(\varepsilon(t) - \varepsilon_i(t) - R_i) - \frac{2|V_{10}(t)|^2 |B_{10}|^2 \coth(\beta \omega_{\mathbf{k}}/2)}{\omega_{\mathbf{k}}} \right)}, \quad (18)$$

with the following definitions:

$$\eta \equiv \sqrt{(\text{Tr}(\overline{H}_{\overline{S}}(t)))^2 - 4 \text{Det}(\overline{H}_{\overline{S}}(t))} \quad (19)$$

$$\varepsilon(t) \equiv \text{Tr}(\overline{H}_{\overline{S}}(t)). \quad (20)$$

### IV. MASTER EQUATION

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

$$\tilde{O} \equiv U^{\dagger}(t) O U(t) \quad (21)$$

$$U(t) \equiv \mathcal{T} \exp \left( -i \int_0^t dt' \overline{H}_T(t') \right). \quad (22)$$

Therefore:

$$\widetilde{\rho_S}(t) = U^\dagger(t) \overline{\rho_S}(t) U(t) \quad (23)$$

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  $H_I(t)$ , we obtain our master equation in the interaction picture:

$$\frac{d\widetilde{\rho_S}(t)}{dt} = - \int_0^t \text{Tr}_B \left[ \widetilde{H_I}(t), \left[ \widetilde{H_I}(s), \widetilde{\rho_S}(t) \rho_B \right] \right] ds \quad (24)$$

To simplify this we define the following matrix:

$$\begin{pmatrix} A \\ B \\ C(t) \end{pmatrix} = \begin{pmatrix} \sigma_x & \sigma_y & \frac{I-\sigma_z}{2} & \sigma_x & \sigma_y & \frac{I+\sigma_z}{2} \\ B_x & B_y & B_{1z} & B_y & B_x & B_{0z} \\ V_{10}^{\Re}(t) & V_{10}^{\Re}(t) & 1 & V_{10}^{\Im}(t) & -V_{10}^{\Im}(t) & 1 \end{pmatrix}. \quad (25)$$

Then we have:

$$\overline{H_I}(t) = \sum_i C_i(t) (A_i \otimes B_i(t)) \quad (26)$$

$$\widetilde{H_I}(t) = \sum_i C_i(t) (\widetilde{A}_i(t) \otimes \widetilde{B}_i(t)), \quad (27)$$

and expanding the commutators yields:

$$\frac{d\widetilde{\rho_S}(t)}{dt} = - \int_0^t \text{Tr}_B \left( \sum_j C_j(t) (\widetilde{A}_j(t) \otimes \widetilde{B}_j(t)) \sum_i C_i(s) (\widetilde{A}_i(s) \otimes \widetilde{B}_i(s)) \widetilde{\rho_S}(t) \rho_B - \sum_j C_j(t) (\widetilde{A}_j(t) \otimes \widetilde{B}_j(t)) \widetilde{\rho_S}(t) \rho_B \sum_i C_i(s) (\widetilde{A}_i(s) \otimes \widetilde{B}_i(s)) \right. \quad (28)$$

$$\left. - \sum_i C_i(s) (\widetilde{A}_i(s) \otimes \widetilde{B}_i(s)) \widetilde{\rho_S}(t) \rho_B \sum_j C_j(t) (\widetilde{A}_j(t) \otimes \widetilde{B}_j(t)) + \widetilde{\rho_S}(t) \rho_B \sum_i C_i(s) (\widetilde{A}_i(s) \otimes \widetilde{B}_i(s)) \sum_j C_j(t) (\widetilde{A}_j(t) \otimes \widetilde{B}_j(t)) \right) ds. \quad (29)$$

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  $\Lambda$  operators:

$$\Lambda(\tau) \equiv \begin{pmatrix} \Lambda_{11}(\tau) & 0 & 0 & 0 & -\Lambda_{11}(\tau) \\ 0 & \Lambda_{22}(\tau) & \Lambda_{23}(\tau) & \Lambda_{22}(\tau) & 0 \\ 0 & \Lambda_{32}(\tau) & \Lambda_{33}(\tau) & \Lambda_{32}(\tau) & 0 \\ 0 & \Lambda_{22}(\tau) & \Lambda_{23}(\tau) & \Lambda_{22}(\tau) & 0 \\ -\Lambda_{11}(\tau) & 0 & 0 & 0 & \Lambda_{11}(\tau) \end{pmatrix}, \quad (30)$$

$$\begin{pmatrix} \Lambda_{11} & \cdot & \cdot \\ \cdot & \Lambda_{22} & \Lambda_{23} \\ \cdot & \Lambda_{32} & \Lambda_{33} \end{pmatrix} \equiv \begin{pmatrix} \frac{B(\tau)B(0)}{2} (e^{\phi(\tau)} + e^{-\phi(\tau)} - 2) & \frac{B(\tau)B(0)}{2} (e^{\phi(\tau)} + e^{-\phi(\tau)}) & -B(0) \int_0^\infty d\omega \frac{J(\omega)v(\omega)}{\omega g(\omega)} \left(1 - \frac{v(\omega)}{g(\omega)}\right) iG_-(\tau) \\ B(\tau) \int_0^\infty d\omega \frac{J(\omega)v(\omega)}{\omega g(\omega)} \left(1 - \frac{v(\omega)}{g(\omega)}\right) iG_-(\tau) & \int_0^\infty d\omega J(\omega) \left(1 - \frac{v(\omega)}{g(\omega)}\right)^2 G_+(\tau) \end{pmatrix} \quad (31)$$

with the phonon propagator given by:

$$\phi(\tau) \equiv \int_0^\infty d\omega \frac{J(\omega) v^2(\omega)}{\omega^2 g^2(\omega)} G_+(\tau), \quad (32)$$

$$G_\pm(\tau) \equiv (n(\omega) + 1) e^{-i\tau\omega} \pm n(\omega) e^{-i\tau\omega} \quad (33)$$

$$n(\omega) \equiv (e^{\beta\omega} - 1)^{-1}, \quad (34)$$

and the spectral density is defined in the usual way:

$$J(\omega) \equiv \sum_{\mathbf{k}} |g_{\mathbf{k}}|^2 \delta(\omega - \omega_{\mathbf{k}}). \quad (35)$$

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

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

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

$$\frac{d\overline{\rho_S}(t)}{dt} = -i[H_S(t), \overline{\rho_S}(t)] - \sum_{ij} \int_0^t C_i(t) C_j(t-\tau) \Lambda_{ij}(\tau) \left[ A_i, \widetilde{A}_j(t-\tau, t) \overline{\rho_S}(t) \right] + C_j(t) C_i(t-\tau) \Lambda_{ji}(-\tau) \left[ \overline{\rho_S}(t) \widetilde{A}_j(t-\tau, t), A_i \right] d\tau. \quad (37)$$

We still have interaction picture versions of  $A_j$ , so we will decompose  $\widetilde{A}_j(\tau)$  in terms of the Schroedinger picture version  $A_j$ :

$$\widetilde{A}_j(t) = \sum_{w(t)} e^{-i w(t) \tau} A_j(w(t)) \quad (38)$$

$$\widetilde{A}_j(t-\tau, t) = \sum_{w(t), w'(t-\tau)} e^{-i w(t) t} e^{i w'(t-\tau)} A'_j(w(t), w'(t-\tau)) \quad (39)$$

Where the sum is defined on the set of all the differences between the eigenvalues of the system, in our case  $w \in \{0, \pm\eta\}$ . We also have that  $w(t)$  belongs to the set of differences of eigenvalues that depends of the time. As we can see the eigenvectors are time dependent as well. Also,  $w'(t-\tau)$  and  $w(t)$  belong to the set of the differences of the eigenvalues of the Hamiltonian  $H_S(t-\tau)$  and  $H_S(t)$  respectively. In matrix form, these are:

$$A_i(0) = \langle + | A_i | + \rangle | + \rangle \langle + | + \langle - | A_i | - \rangle | - \rangle \langle - | \quad (40)$$

$$A_i(w) = \langle + | A_i | - \rangle | + \rangle \langle - | \quad (41)$$

$$A_i(-w) = \langle - | A_i | + \rangle | - \rangle \langle + |. \quad (42)$$

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

$$K_{ijww'}(t) = \int_0^t C_i(t) C_j(t-\tau) \Lambda_{ij}(\tau) e^{i w \tau} e^{-i t(w-w')} d\tau \quad (43)$$

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

$$\frac{d\overline{\rho_S}(t)}{dt} = -i[\overline{H_S}(t), \overline{\rho_S}] - \sum_{ijww'} K_{ijww'}(t) \left[ A_i, A_{jww'} \overline{\rho_S}(t) - \overline{\rho_S}(t) A_{jww'}^\dagger \right] \quad (44)$$

Re-defining  $\overline{\rho_S}(t) \equiv \rho$  and  $\overline{H_S} \equiv H$ , we get:

$$\dot{\rho} = -i[H(t), \rho] - \sum_{ijww'} K_{ijww'}(t) \left[ A_i, A_{jww'} \rho - \rho A_{jww'}^\dagger \right] \quad (45)$$

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

### A. Time-independent VPQME of 2011

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

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

$$\overline{H_{\bar{S}}}(t) \equiv R|0\rangle\langle 0| + \delta(t)|1\rangle\langle 1| + \sigma_x \Omega_r. \quad (47)$$

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

$$v_{\mathbf{k}} = \frac{g_i(\omega_{\mathbf{k}}) \left( 1 - \frac{\tanh(\frac{\beta\eta(t)}{2})}{\eta(t)} (2\varepsilon_i(t) + 2R_i - \varepsilon(t)) \right) + 2 \frac{\tanh(\frac{\beta\eta(t)}{2})}{\eta(t)} \frac{v_{i'\mathbf{k}}}{\omega_{\mathbf{k}}} |B_{10}|^2 |V_{10}(t)|^2 \coth(\beta\omega_{\mathbf{k}}/2)}{1 - \frac{\tanh(\frac{\beta\eta(t)}{2})}{\eta(t)} \left( \varepsilon(t) - 2(\varepsilon(t) - \varepsilon_i(t) - R_i) - \frac{2|V_{10}(t)|^2 |B_{10}|^2 \coth(\beta\omega_{\mathbf{k}}/2)}{\omega_{\mathbf{k}}} \right)} \quad (48)$$

$$= \frac{g_{\mathbf{k}} \left( 1 - \frac{\varepsilon(t)}{\eta} \tanh\left(\frac{\beta\eta}{2}\right) \right)}{1 - \frac{\varepsilon(t)}{\eta} \tanh\left(\frac{\beta\eta}{2}\right) \left( 1 - \frac{\Omega^2}{2\varepsilon(t)\omega_{\mathbf{k}}} \coth(\beta\omega_{\mathbf{k}}/2) \right)} \quad (49)$$

The bath and system-bath interaction operators become:

$$\begin{pmatrix} B_z & B^{\pm} \\ B_x & B_{10} \\ B_y & R \end{pmatrix} \equiv \begin{pmatrix} 2 \sum_{\mathbf{k}} (g_{\mathbf{k}} - v_{\mathbf{k}}) b_{\mathbf{k}}^{\dagger} & e^{\pm \sum_{\mathbf{k}} \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} (b_{\mathbf{k}}^{\dagger} - b_{\mathbf{k}})} \\ \frac{B^+ + B^- - 2B}{2} & e^{-(1/2) \sum_{\mathbf{k}} \left( \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} \right)^2 \coth(\beta\omega_{\mathbf{k}}/2)} \\ \frac{B^- - B^+}{2i} & \sum_{\mathbf{k}} \left( \frac{|v_{\mathbf{k}}|^2}{\omega_{\mathbf{k}}} - 2g_{\mathbf{k}} \frac{v_{\mathbf{k}}}{\omega_{\mathbf{k}}} \right) \end{pmatrix}, \quad (50)$$

$$\begin{pmatrix} A \\ B \\ C(t) \end{pmatrix} = \begin{pmatrix} \sigma_x & \sigma_y & \frac{I - \sigma_z}{2} & \sigma_x & \sigma_y & \frac{I + \sigma_z}{2} \\ B_x & B_y & B_z & B_y & B_x & 0 \\ \frac{\Omega}{2} & \frac{\Omega}{2} & 1 & 0 & 0 & 1 \end{pmatrix}. \quad (51)$$

Therefore  $C(t)$  is no longer time-dependent and we have:

$$K_{ijww'}(t) = \int_0^t C_i C_j \Lambda_{ij}(\tau) e^{i w \tau} e^{-i t(w - w')} d\tau \quad (52)$$

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