The Mother of all Master Equations

Nike Dattani[*]
Harvard-Smithsonian Center for Astrophysics

Camilo Chaparro Sogamoso[†]
National University of Colombia

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:

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

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:

$$\overline{O} \equiv e^{V} O e^{-V}. \tag{6}$$

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

$$\rho_B \equiv \rho_B(0) = \frac{e^{-\beta H_B}}{\mathrm{Tr}\left(e^{-\beta H_B}\right)} \tag{7}$$

With the following definitions:

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

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

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

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

$$\overline{H_T}(t) \equiv \overline{H_{\bar{S}}}(t) + \overline{H_{\bar{I}}} + \overline{H_{\bar{B}}} \tag{11}$$

$$\overline{H_{\bar{S}}}(t) \equiv \sum_i \left(\varepsilon_i(t) + R_i\right)|i\rangle\langle i| + \sigma_x\left(B_{10}^{\Re}(t)V_{10}^{\Re}(t) - B_{10}^{\Im}(t)V_{10}^{\Im}(t)\right) - \sigma_y\left(B_{10}^{\Re}(t)V_{10}^{\Im}(t) + B_{10}^{\Im}(t)V_{10}^{\Re}(t)\right) \tag{12}$$

$$\overline{H_{\bar{I}}} \equiv \sum_i B_{iz}|i\rangle\langle i| + V_{10}^{\Re}(t)\left(B_x\sigma_x + B_y\sigma_y\right) - V_{10}^{\Im}(t)\left(B_x\sigma_y - B_y\sigma_x\right) \tag{13}$$

$$\overline{H_{\bar{B}}} \equiv \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} \tag{14}$$

$$= H_B \tag{15}$$

III. FREE-ENERGY MINIMIZATION

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

$$A \leq A_{\mathrm{B}} \equiv -\frac{1}{\beta}\ln\left(\mathrm{Tr}\left(e^{-\beta\overline{H_{\bar{S}}}(t) + H_B}\right)\right) + \left\langle\overline{H_{\bar{I}}}\right\rangle_{\overline{H_{\bar{S}}}(t) + H_{\bar{B}}} + O\left(\left\langle\overline{H_{\bar{I}}}^2\right\rangle_{\overline{H_{\bar{S}}}(t) + H_{\bar{B}}}\right) \tag{16}$$

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 $\left\langle\overline{H_{\bar{I}}}\right\rangle_{\overline{H_{\bar{S}}}(t) + H_{\bar{B}}} = 0$ we can obtain the following condition to obtain the set $\{v_{\mathbf{k}}\}$:

$$\frac{\partial A_{\mathrm{B}}}{\partial v_{i\mathbf{k}}} = 0. \tag{17}$$

This leads us to:

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

with the following definitions:

$$\eta \equiv \sqrt{\left(\mathrm{Tr}\left(\overline{H_{\bar{S}}}(t)\right)\right)^2 - 4\mathrm{Det}\left(\overline{H_{\bar{S}}}(t)\right)} \tag{19}$$

$$\varepsilon(t) \equiv \mathrm{Tr}\left(\overline{H_{\bar{S}}}(t)\right). \tag{20}$$

IV. MASTER EQUATION

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

$$\widetilde{O} \equiv U^\dagger(t)OU(t) \tag{21}$$

$$U(t) \equiv \mathcal{T}\exp\left(-\mathrm{i}\int_0^t \mathrm{d}t'\overline{H_T}(t')\right). \tag{22}$$

Therefore:

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

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 ρ_B and truncating at second order in $H_I(t)$, we obtain our master equation in the interaction picture:

$$\frac{\mathrm{d}\widetilde{\rho_S}(t)}{\mathrm{d}t} = -\int_0^t \mathrm{Tr}_B\left[\widetilde{\overline{H_I}}(t), \left[\widetilde{\overline{H_I}}(s), \widetilde{\rho_S}(t)\rho_B\right]\right]\mathrm{d}s \tag{24}$$

To simplify this we define the following matrix:

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

Then we have:

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

$$\widetilde{H_I}(t) = \sum_i C_i(t)\left(\widetilde{A_i}(t) \otimes \widetilde{B_i}(t)\right), \tag{27}$$

and expanding the commutators yields:

$$\frac{\mathrm{d}\widetilde{\rho_S}(t)}{\mathrm{d}t} = -\int_0^t \mathrm{Tr}_B\left(\sum_j C_j(t)\left(\widetilde{A_j}(t)\otimes\widetilde{B_j}(t)\right)\sum_i C_i(s)\left(\widetilde{A_i}(s)\otimes\widetilde{B_i}(s)\right)\widetilde{\rho_S}(t)\rho_B - \sum_j C_j(t)\left(\widetilde{A_j}(t)\otimes\widetilde{B_j}(t)\right)\widetilde{\rho_S}(t)\rho_B\sum_i C_i(s)\left(\widetilde{A_i}(s)\otimes\widetilde{B_i}(s)\right) \tag{28}$$

$$-\sum_i C_i(s)\left(\widetilde{A_i}(s)\otimes\widetilde{B_i}(s)\right)\widetilde{\rho_S}(t)\rho_B\sum_j C_j(t)\left(\widetilde{A_j}(t)\otimes\widetilde{B_j}(t)\right) + \widetilde{\rho_S}(t)\rho_B\sum_i C_i(s)\left(\widetilde{A_i}(s)\otimes\widetilde{B_i}(s)\right)\sum_j C_j(t)\left(\widetilde{A_j}(t)\otimes\widetilde{B_j}(t)\right)\right)\mathrm{d}s. \tag{29}$$

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 Λ operators:

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

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

with the phonon propagator given by:

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

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

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

and the spectral density is defined in the usual way:

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

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

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

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

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

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_i:

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

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

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:

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

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

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

The Fourier exponentials $e^{iw\tau}$ and $e^{-it(w-w')}$ can be combined with the C and Λ functions:

$$K_{ijww'}(t) = \int_0^t C_i(t) C_j(t-\tau) \Lambda_{ij}(\tau) e^{iw\tau} e^{-it(w-w')} \mathrm{d}\tau \qquad (43)$$

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:

$$\frac{\mathrm{d}\overline{\rho_{\bar{S}}}(t)}{\mathrm{d}t} = -\mathrm{i}\left[\overline{H}_{\bar{S}}(t), \overline{\rho_{\bar{S}}} \right] - \sum_{ijww'} K_{ijww'}(t) \left[A_i, A_{jww'} \overline{\rho_{\bar{S}}}(t) - \overline{\rho_{\bar{S}}}(t) A^\dagger_{jww'} \right] \qquad (44)$$

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

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

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

A. Time-independent VPQME

B. Time-independent VPQME of McCutcheon *et al.*

$$g_{1\mathbf{k}} = 0 = v_{1\mathbf{k}} \tag{46}$$

$$g_{0\mathbf{k}}^{\Im} = 0 \tag{47}$$

$$g_{0\mathbf{k}}^{\Re} \equiv g_{\mathbf{k}} \tag{48}$$

$$V_{10}^{\Im} = 0 \tag{49}$$

$$V_{10}^{\Re} \equiv \frac{\Omega}{2} \tag{50}$$

$$\varepsilon_0 = 0 \tag{51}$$

$$\varepsilon_1 \equiv \delta \tag{52}$$

$$B \equiv B_{10} \tag{53}$$

$$\Omega_r \equiv B\Omega \tag{54}$$

$$R_0 \equiv R \tag{55}$$

$$v_{0\mathbf{k}} \equiv v_{\mathbf{k}} \tag{56}$$

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

$$\overline{H_{\bar{S}}}(t) \equiv R|0\rangle\langle 0| + \delta(t)|1\rangle\langle 1| + \sigma_x \Omega_r \tag{57}$$

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

$$v_{\mathbf{k}} = \frac{g_i(\omega_{\mathbf{k}})\left(1 - \frac{\tanh\left(\frac{\beta\eta(t)}{2}\right)}{\eta(t)}(2\varepsilon_i(t) + 2R_i - \varepsilon(t))\right) + 2\frac{\tanh\left(\frac{\beta\eta(t)}{2}\right)}{\eta(t)}\frac{v_{i'\mathbf{k}}}{\omega_{\mathbf{k}}}|B_{10}|^2|V_{10}(t)|^2\coth(\beta\omega_{\mathbf{k}}/2)}{1 - \frac{\tanh\left(\frac{\beta\eta(t)}{2}\right)}{\eta(t)}\left(\varepsilon(t) - 2(\varepsilon(t) - \varepsilon_i(t) - R_i) - \frac{2|V_{10}(t)|^2|B_{10}|^2\coth(\beta\omega_{\mathbf{k}}/2)}{\omega_{\mathbf{k}}}\right)} \tag{58}$$

$$= \frac{g_{\mathbf{k}}\left(1 - \frac{\tanh\left(\frac{\beta\eta}{2}\right)}{\eta}(2R - \varepsilon(t))\right)}{1 - \frac{\tanh\left(\frac{\beta\eta}{2}\right)}{\eta}\left(2R - \varepsilon(t) - \frac{\Omega_r^2\coth(\beta\omega_{\mathbf{k}}/2)}{1\omega_{\mathbf{k}}}\right)} \tag{59}$$

$$= \frac{g_{\mathbf{k}}\left(1 - \frac{(R-\delta)\tanh\left(\frac{\beta\eta}{2}\right)}{\eta}\right)}{1 - \frac{(R-\delta)\tanh\left(\frac{\beta\eta}{2}\right)}{\eta}\left(1 - \frac{\Omega_r^2\coth(\beta\omega_{\mathbf{k}}/2)}{2(R-\delta)\omega_{\mathbf{k}}}\right)} \tag{60}$$

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[*] n.dattani@cfa.harvard.edu

[†] edcchaparroso@unal.edu.co