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:

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

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

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

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

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

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

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

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

$$
= H_B \tag{15}
$$

III. FREE-ENERGY MINIMIZATION

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

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

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 $\langle \overline{H_{\bar{I}}} \rangle_{\overline{H_{\bar{S}}}(t) + H_{\bar{B}}} = 0$ 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:

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

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

In order to describe the dynamics of the QD under the influence of the phonon environment, we use the time-convolutionless projection operator technique. We consider the QD in its ground state. The initial density operator $\rho_{\text{Total}}(0) = \rho_S(0) \otimes \rho_B(0)$, where $\rho_B(0) \equiv \rho_B^{\text{Thermal}} \equiv \rho_B$ the transformed density operator is equal to:

$$\text{for } \rho_S(0) = |0\rangle\langle0|: = |0\rangle\langle0| \otimes B_0^+ \rho_B B_0^- \tag{21}$$

$$\text{for } \rho_S(0) = |1\rangle\langle1|: = |1\rangle\langle1| \otimes B_1^+ \rho_B B_1^- \tag{22}$$

$$\text{for } \rho_S(0) = |0\rangle\langle1|: = |0\rangle\langle1| \otimes B_0^+ \rho_B B_1^- \tag{23}$$

$$\text{for } \rho_S(0) = |1\rangle\langle0|: = |1\rangle\langle0| \otimes B_1^+ \rho_B B_0^- \tag{24}$$

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

$$\widetilde{O} \equiv U^\dagger(t) O U(t) \tag{25}$$

$$U(t) \equiv \mathcal{T} \exp\left(-\mathrm{i} \int_0^t \mathrm{d}t' \overline{H_T}(t')\right). \tag{26}$$

Therefore:

$$\widetilde{\overline{\rho_S}}(t) = U^\dagger(t) \overline{\rho_S}(t) U(t) \tag{27}$$

We define the following matrix:

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

Then we have:

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

$$\widetilde{H_I}(t) = \sum_i C_i(t) \left(\widetilde{A_i}(t) \otimes \widetilde{B_i}(t)\right) \tag{30}$$

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

$$\frac{\mathrm{d}\widetilde{\overline{\rho_S}}(t)}{\mathrm{d}t} = -\int_0^t \mathrm{Tr}_B\left[\widetilde{\overline{H_{\bar{I}}}}(t), \left[\widetilde{\overline{H_{\bar{I}}}}(s), \widetilde{\overline{\rho_S}}(t)\rho_B\right]\right] \mathrm{d}s \tag{31}$$

$$= -\int_0^t \sum_{ij} \left(C_i(t) C_j(s) \left(\Lambda_{ij}(\tau) \left[\widetilde{A_i}(t), \widetilde{A_j}(s)\widetilde{\overline{\rho_S}}(t)\right] + \Lambda_{ji}(-\tau) \left[\widetilde{\overline{\rho_S}}(t)\widetilde{A_j}(s), \widetilde{A_i}\right]\right)\right) \mathrm{d}s \tag{32}$$

where:

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

$$\Lambda_{11}\left(\tau\right) \equiv \frac{B\left(\tau\right)B\left(0\right)}{2}\left(e^{\phi\left(\tau\right)} + e^{-\phi\left(\tau\right)} - 2\right) \tag{34}$$

$$\Lambda_{22}\left(\tau\right) \equiv \frac{B\left(\tau\right)B\left(0\right)}{2}\left(e^{\phi\left(\tau\right)} + e^{-\phi\left(\tau\right)}\right) \tag{35}$$

$$\Lambda_{33}\left(\tau\right) \equiv \int_0^\infty \mathrm{d}\omega J\left(\omega\right)\left(1 - \frac{v(\omega)}{g(\omega)}\right)^2 G_+\left(\tau\right) \tag{36}$$

$$\Lambda_{32}\left(\tau\right) \equiv B\left(\tau\right)\int_0^\infty \mathrm{d}\omega \frac{J\left(\omega\right)v\left(\omega\right)}{\omega g(\omega)}\left(1 - \frac{v(\omega)}{g(\omega)}\right)iG_-\left(\tau\right) \tag{37}$$

$$\Lambda_{23}\left(\tau\right) \equiv -B\left(0\right)\int_0^\infty \mathrm{d}\omega \frac{J\left(\omega\right)v\left(\omega,\tau\right)}{\omega g(\omega,\tau)}\left(1 - \frac{v(\omega,\tau)}{g(\omega,\tau)}\right)iG_-\left(\tau\right) \tag{38}$$

with the phonon propagator given by:

$$\phi\left(\tau\right) = \int_0^\infty \mathrm{d}\omega \frac{J\left(\omega\right)}{\omega^2}F\left(\omega\right)^2 G_+\left(\tau\right), \tag{39}$$

$$G_\pm\left(\tau\right) = \left(n\left(\omega\right) + 1\right)e^{-\mathrm{i}\tau\omega} \pm n\left(\omega\right)e^{-\mathrm{i}\tau\omega} \tag{40}$$

$$n\left(\omega\right) = \left(e^{\beta\omega} - 1\right)^{-1}, \tag{41}$$

and the spectral density is defined in the usual way:

$$J(\omega) \equiv \sum_{\mathbf{k}} |g_{\mathbf{k}}|^2 \delta\left(\omega - \omega_{\mathbf{k}}\right). \tag{42}$$

and the

$$\frac{\mathrm{d}\overline{\rho_S}(t)}{\mathrm{d}t} = -\mathrm{i}\left[H_S\left(t\right), \overline{\rho_S}(t)\right] - \sum_{ij}\int_0^t C_i\left(t\right)C_j\left(t - \tau\right)\Lambda_{ij}\left(\tau\right)\left[A_i, \widetilde{A_j}\left(t - \tau, t\right)\overline{\rho_S}(t)\right] + C_j\left(t\right)C_i\left(t - \tau\right)\Lambda_{ji}\left(-\tau\right)\left[\overline{\rho_S}(t)\widetilde{A_j}\left(t - \tau, t\right), A_i\right]\mathrm{d}\tau. \tag{43}$$

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:

$$\widetilde{A_j}\left(\tau\right) = \sum_w e^{-\mathrm{i}w\tau}A_j\left(w\right) \tag{44}$$

$$\widetilde{A_j}\left(t\right) = \sum_{w(t)} e^{-\mathrm{i}w(t)\tau}A_j\left(w(t)\right) \tag{45}$$

$$\widetilde{A_j}\left(t - \tau, t\right) = \sum_{w(t), w'(t-\tau)} e^{-\mathrm{i}w(t)t}e^{\mathrm{i}w'(t-\tau)}A_j'\left(w\left(t\right), w'\left(t - \tau\right)\right) \tag{46}$$

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 $w\left(t\right)$ 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, $w'\left(t - \tau\right)$ and $w\left(t\right)$ belong to the set of the differences of the eigenvalues of the Hamiltonian $H_S\left(t - \tau\right)$ and $H_S\left(t\right)$ respectively. In matrix form, these are:

$$A_i\left(0\right) = \langle +|A_i|+\rangle |+\rangle \langle +| + \langle -|A_i|-\rangle |-\rangle \langle -| \tag{47}$$

$$A_i\left(w\right) = \langle +|A_i|-\rangle |+\rangle \langle -| \tag{48}$$

$$A_i\left(-w\right) = \langle -|A_i|+\rangle |-\rangle \langle +|. \tag{49}$$

We define the following response functions:

$$K_{ijww'}(t) = \int_0^t C_i\left(t\right)C_j\left(t - \tau\right)\Lambda_{ij}\left(\tau\right)e^{\mathrm{i}w\tau}e^{-\mathrm{i}t\left(w - w'\right)}\mathrm{d}\tau \tag{50}$$

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

$$\frac{\mathrm{d}\overline{\rho_S}(t)}{\mathrm{d}t} = -\mathrm{i}\left[H_S\left(t\right),\overline{\rho_S}\right] - \sum_{ijww'} K_{ijww'}(t)\left[A_i, A_{jww'}\overline{\rho_S(t)} - \overline{\rho_S}\left(t\right)A^\dagger_{jww'}\right] \tag{51}$$

$$\dot{\rho} = -\mathrm{i}\left[H_S\left(t\right),\rho\right] - \sum_{ijww'} K_{ijww'}(t)\left[A_i, A_{jww'}\rho - \rho A^\dagger_{jww'}\right] \tag{52}$$

$$\dot{\rho} = -\mathrm{i}\left[H_S\left(t\right),\rho\right] - \sum_{ijww'} K_{ijww'}(t)\left(\left[A_i, A_{jww'}\rho\right] - \left[A_i, \rho A^\dagger_{jww'}\right]\right) \tag{53}$$

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* n.dattani@cfa.harvard.edu
† edcchaparroso@unal.edu.co