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:

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

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:

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

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:

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

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

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

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

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

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

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

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

$$= H_B \tag{15}$$

III. FREE-ENERGY MINIMIZATION

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

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

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

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: $\rho_{\mathrm{Total}}(0) = \rho_S(0) \otimes \rho_B(0)$, where $\rho_B(0) \equiv \rho_B^{\mathrm{Thermal}} \equiv \rho_B$. Taking as reference state ρ_B and truncating at second order in $H_I(t)$, we obtain our master equation in the interaction picture:

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

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:

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

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

and expanding the commutators yields:

$$\frac{\mathrm{d}\widetilde{\rho_{\bar{S}}}(t)}{\mathrm{d}t} = -\int_0^t \mathrm{Tr}_B\Bigg(\sum_j C_j(t)\Big(\widetilde{A_j}(t)\otimes\widetilde{B_j}(t)\Big)\sum_i C_i(s)\Big(\widetilde{A_i}(s)\otimes\widetilde{B_i}(s)\Big)\widetilde{\overline{\rho_S}}(t)\rho_B - \sum_j C_j(t)\Big(\widetilde{A_j}(t)\otimes\widetilde{B_j}(t)\Big)\widetilde{\overline{\rho_S}}(t)\rho_B\sum_i C_i(s)\Big(\widetilde{A_i}(s)\otimes\widetilde{B_i}(s)\Big) \tag{28}$$

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

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:

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

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

with the phonon propagator given by:

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

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

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

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:

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

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

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

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:

$$\widetilde{A_j}\left(t\right) = \sum_{w(t)} e^{-\mathrm{i}w(t)\tau} A_j\left(w(t)\right) \tag{38}$$

$$\widetilde{A_j}\left(t-\tau, t\right) = \sum_{w(t), w'(t-\tau)} e^{-\mathrm{i}w(t)t} e^{\mathrm{i}w'(t-\tau)} A'_j\left(w\left(t\right), w'\left(t-\tau\right)\right) \tag{39}$$

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 $w\left(t\right)$ 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:

$$A_i\left(0\right) = \langle+|\, A_i \,|+\rangle\, |+\rangle \langle+| + \langle-|\, A_i \,|-\rangle\, |-\rangle \langle-| \tag{40}$$

$$A_i\left(w\right) = \langle+|\, A_i \,|-\rangle\, |+\rangle \langle-| \tag{41}$$

$$A_i\left(-w\right) = \langle-|\, A_i \,|+\rangle\, |-\rangle \langle+| \,. \tag{42}$$

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

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

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:

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

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

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

We will now show that many useful master equations can be dervied as special cases of the above "mother" of all master equations.

V. TIME-INDEPENDENT VPQME AS A LIMITING CASE

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