

A general non-Markovian master equation for time-dependent Hamiltonians with coupling that is weak, strong, or anything in between

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I. THE HAMILTONIAN

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

$$H_T(t) = H_S(t) + H_I + H_B, \quad (1)$$

$$H_S(t) = \varepsilon_0(t) |0\rangle\langle 0| + \varepsilon_1(t) |1\rangle\langle 1| + V_{10}(t) |1\rangle\langle 0| + V_{01}(t) |0\rangle\langle 1|, \quad (2)$$

$$H_I = |0\rangle\langle 0| \sum_{\mathbf{k}} \left(g_{0\mathbf{k}} b_{\mathbf{k}}^\dagger + g_{0\mathbf{k}}^* b_{\mathbf{k}} \right) + |1\rangle\langle 1| \sum_{\mathbf{k}} \left(g_{1\mathbf{k}} b_{\mathbf{k}}^\dagger + g_{1\mathbf{k}}^* b_{\mathbf{k}} \right), \quad (3)$$

$$H_B = \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}}. \quad (4)$$

II. UNITARY TRANSFORMATION INTO THE VARIATIONALLY OPTIMIZABLE FRAME

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

$$V \equiv |0\rangle\langle 0| \sum_{\mathbf{k}} \left(\frac{v_{0\mathbf{k}}}{\omega_{\mathbf{k}}} b_{\mathbf{k}}^\dagger - \frac{v_{0\mathbf{k}}^*}{\omega_{\mathbf{k}}} b_{\mathbf{k}} \right) + |1\rangle\langle 1| \sum_{\mathbf{k}} \left(\frac{v_{1\mathbf{k}}}{\omega_{\mathbf{k}}} b_{\mathbf{k}}^\dagger - \frac{v_{1\mathbf{k}}^*}{\omega_{\mathbf{k}}} b_{\mathbf{k}} \right) \quad (5)$$

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:

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

We get:

$$\overline{H(t)} = \varepsilon_0(t) |0\rangle\langle 0| + \varepsilon_1(t) |1\rangle\langle 1| + V_{10}(t) |1\rangle\langle 0| B_{1+} B_{0-} + V_{01}(t) |0\rangle\langle 1| B_{0+} B_{1-} + \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} \quad (7)$$

$$+ \sum_{\mathbf{k}} \left(|1\rangle\langle 1| \left(\frac{|v_{1\mathbf{k}}|^2}{\omega_{\mathbf{k}}} - \left(v_{1\mathbf{k}}^* b_{\mathbf{k}} + v_{1\mathbf{k}} b_{\mathbf{k}}^\dagger \right) \right) + |0\rangle\langle 0| \left(\frac{|v_{0\mathbf{k}}|^2}{\omega_{\mathbf{k}}} - \left(v_{0\mathbf{k}}^* b_{\mathbf{k}} + v_{0\mathbf{k}} b_{\mathbf{k}}^\dagger \right) \right) \right) \quad (8)$$

$$+ \sum_{\mathbf{k}} \left(|0\rangle\langle 0| \left(g_{0\mathbf{k}} \left(b_{\mathbf{k}}^\dagger - \frac{v_{0\mathbf{k}}^*}{\omega_{\mathbf{k}}} \right) + g_{0\mathbf{k}}^* \left(b_{\mathbf{k}} - \frac{v_{0\mathbf{k}}}{\omega_{\mathbf{k}}} \right) \right) + |1\rangle\langle 1| \left(g_{1\mathbf{k}} \left(b_{\mathbf{k}}^\dagger - \frac{v_{1\mathbf{k}}^*}{\omega_{\mathbf{k}}} \right) + g_{1\mathbf{k}}^* \left(b_{\mathbf{k}} - \frac{v_{1\mathbf{k}}}{\omega_{\mathbf{k}}} \right) \right) \right) \quad (9)$$

We assume that the bath starts equilibrium with inverse temperature $\beta = 1/k_B T$:

$$\rho_B = \frac{e^{-\beta H_B}}{\text{Tr}(e^{-\beta H_B})} \quad (10)$$

With the following definitions and relations:

$$D(\pm v_{i\mathbf{k}}) \equiv e^{\pm \left(\frac{v_{i\mathbf{k}}}{\omega_{\mathbf{k}}} b_{\mathbf{k}}^\dagger - \frac{v_{i\mathbf{k}}^*}{\omega_{\mathbf{k}}} b_{\mathbf{k}} \right)}. \quad (11)$$

$$B_{i\pm} \equiv e^{\pm \sum_{\mathbf{k}} \frac{v_{i\mathbf{k}}}{\omega_{\mathbf{k}}} (b_{\mathbf{k}}^\dagger - b_{\mathbf{k}})} \quad (12)$$

$$= \prod_{\mathbf{k}} D(\pm v_{i\mathbf{k}}) \quad (13)$$

$$B_i \equiv \langle B_{i\pm} \rangle_{H_B} \quad (14)$$

$$= e^{-(1/2) \sum_{\mathbf{k}} \left(\frac{v_{i\mathbf{k}}}{\omega_{\mathbf{k}}} \right)^2 \coth(\beta \omega_{\mathbf{k}}/2)} \quad (15)$$

$$B_{iz} \equiv \sum_{\mathbf{k}} \left((g_{i\mathbf{k}} - v_{i\mathbf{k}}) b_{\mathbf{k}}^\dagger + (g_{i\mathbf{k}} - v_{i\mathbf{k}})^* b_{\mathbf{k}} \right) \quad (16)$$

$$B_x = \frac{B_+ + B_- - 2B}{2} \quad (17)$$

$$B_y = \frac{B_- - B_+}{2} \quad (18)$$

$$\langle B_z \rangle_{H_B} = 0 \quad (19)$$

$$R_i \equiv \sum_{\mathbf{k}} \left(\frac{|v_{i\mathbf{k}}|^2}{\omega_{\mathbf{k}}} - \left(g_{i\mathbf{k}} \frac{v_{i\mathbf{k}}^*}{\omega_{\mathbf{k}}} + g_{i\mathbf{k}}^* \frac{v_{i\mathbf{k}}}{\omega_{\mathbf{k}}} \right) \right) \quad (20)$$

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

$$\overline{H_T(t)} \equiv \overline{H_{\bar{S}}(t)} + \overline{H_{\bar{I}}} + \overline{H_{\bar{B}}} \quad (21)$$

$$\overline{H_{\bar{S}}(t)} \equiv (\varepsilon_0(t) + R_0) |0\rangle\langle 0| + (\varepsilon_1(t) + R_1) |1\rangle\langle 1| + \frac{B\sigma_x}{2} (V_{10}(t) + V_{01}(t)) + \frac{iB\sigma_y}{2} (V_{10}(t) - V_{01}(t)) \quad (22)$$

$$\overline{H_{\bar{I}}} \equiv B_z |1\rangle\langle 1| + \Re(V_{10}(t)) (B_x \sigma_x + B_y \sigma_y) - \Im(V_{10}(t)) (B_x \sigma_y - B_y \sigma_x) \quad (23)$$

$$\overline{H_{\bar{B}}} \equiv \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} \quad (24)$$

$$= H_B \quad (25)$$

III. FREE-ENERGY MINIMIZATION

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

$$A \leq A_B \equiv -\frac{1}{\beta} \ln \left(\text{Tr} \left(e^{-\beta \overline{H_{\bar{S}}(t)} + H_{\bar{B}}} \right) \right) + \langle \overline{H_{\bar{I}}} \rangle_{\overline{H_{\bar{S}}(t)} + H_{\bar{B}}} + O \left(\langle \overline{H_{\bar{I}}^2} \rangle_{\overline{H_{\bar{S}}(t)} + H_{\bar{B}}} \right) \quad (26)$$

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 $\{v_{\mathbf{k}}\}$:

$$\frac{\partial A_B}{\partial v_{\mathbf{k}}} = 0. \quad (27)$$

This leads us to:

$$v_{\mathbf{k}} = \frac{g_{\mathbf{k}} \left(1 - \frac{\tanh(\frac{\beta \eta}{2})}{\eta} (\varepsilon_1(t) + R_1 - \varepsilon_0(t)) \right)}{1 - \frac{\tanh(\frac{\beta \eta}{2})}{\eta} \left(\varepsilon_1(t) + R_1 - \varepsilon_0(t) - \frac{2|V_{10}(t)|^2 B^2}{\omega_{\mathbf{k}}} \coth \left(\frac{\beta \omega_{\mathbf{k}}}{2} \right) \right)}, \quad (28)$$

with the following definitions:

$$\eta = \sqrt{\left(\text{Tr}\left(\overline{H_S(t)}\right)\right)^2 - 4\text{Det}\left(\overline{H_S(t)}\right)} \quad (29)$$

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 $\rho_{\text{Total}}(0) = \rho_S(0) \otimes \rho_B$, the transformed density operator is equal to:

$$\overline{|0\rangle\langle 0| \otimes \rho_B} = |0\rangle\langle 0| \otimes \rho_B \quad (30)$$

$$\overline{|1\rangle\langle 1| \otimes \rho_B} = |1\rangle\langle 1| \otimes B_+ \rho_B B_- \quad (31)$$

$$\overline{|0\rangle\langle 1| \otimes \rho_B} = |0\rangle\langle 1| \otimes \rho_B B_- \quad (32)$$

$$\overline{|1\rangle\langle 0| \otimes \rho_B} = |1\rangle\langle 0| \otimes B \rho_{+B} \quad (33)$$

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

$$\tilde{O} \equiv U^\dagger(t) O U(t) \quad (34)$$

$$U(t) \equiv \mathcal{T} \exp \left(-i \int_0^t dv \overline{H_S}(v) \right). \quad (35)$$

Therefore:

$$\widetilde{\overline{\rho_S}}(t) = U^\dagger(t) \overline{\rho_S}(t) U(t), \text{ where} \quad (36)$$

We define $A_1 = \sigma_x$, $A_2 = \sigma_y$, $A_3 = \frac{I + \sigma_z}{2} = |1\rangle\langle 1|$, $A_4 = \sigma_x$ and $A_5 = -\sigma_y$. Furthermore we label $B_1(t) = B_x = -B_5(t)$, $B_2(t) = B_y = B_4(t)$ and $B_3(t) = B_z$, also $C_1(t) = \Re(V_{10}(t)) = C_2(t)$, $C_3(t) = 1$ and $C_4(t) = \Im(V_{10}(t)) = -C_5(t)$. Therefore we have:

$$\overline{H_I}(t) = \sum_i C_i(t) (A_i \otimes B_i(t)) \quad (37)$$

$$\widetilde{H_I}(t) = \sum_i C_i(t) \left(\widetilde{A_i}(t) \otimes \widetilde{B_i}(t) \right) \quad (38)$$

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

$$\frac{d\widetilde{\overline{\rho_S}}(t)}{dt} = - \int_0^t \text{Tr}_B \left[\widetilde{H_I}(t), \left[\widetilde{H_I}(s), \widetilde{\overline{\rho_S}}(t) \rho_B \right] \right] ds \quad (39)$$

$$= - \int_0^t \sum_{ij} \left(C_i(t) C_j(s) \left(\Lambda_{ij}(\tau) \left[\widetilde{A_i}(t), \widetilde{A_j}(s) \widetilde{\overline{\rho_S}}(t) \right] + \Lambda_{ji}(-\tau) \left[\widetilde{\overline{\rho_S}}(t) \widetilde{A_j}(s), \widetilde{A_i}(t) \right] \right) \right) ds \quad (40)$$

where:

$$\Lambda(\tau) = \begin{pmatrix} \Lambda_{11}(\tau) & 0 & 0 & 0 & -\Lambda_{11}(\tau) \\ 0 & \Lambda_{22}(\tau) & \Lambda_{23}(\tau) & \Lambda_{22}(\tau) & 0 \\ 0 & \Lambda_{32}(\tau) & \Lambda_{33}(\tau) & \Lambda_{32}(\tau) & 0 \\ 0 & \Lambda_{22}(\tau) & \Lambda_{23}(\tau) & \Lambda_{22}(\tau) & 0 \\ -\Lambda_{11}(\tau) & 0 & 0 & 0 & \Lambda_{11}(\tau) \end{pmatrix}, \quad (41)$$

$$\Lambda_{11}(\tau) = \frac{B(\tau)B(0)}{2} \left(e^{\phi(\tau)} + e^{-\phi(\tau)} - 2 \right) \quad (42)$$

$$\Lambda_{22}(\tau) = \frac{B(\tau)B(0)}{2} \left(e^{\phi(\tau)} + e^{-\phi(\tau)} \right) \quad (43)$$

$$\Lambda_{33}(\tau) = \int_0^\infty d\omega J(\omega) (1 - F(\omega))^2 G_+(\tau) \quad (44)$$

$$\Lambda_{32}(\tau) = B(\tau) \int_0^\infty d\omega \frac{J(\omega)}{\omega} F(\omega) (1 - F(\omega)) iG_-(\tau) \quad (45)$$

$$\Lambda_{23}(\tau) = -B(0) \int_0^\infty d\omega \frac{J(\omega)}{\omega} F(\omega, \tau) (1 - F(\omega, \tau)) iG_-(\tau) \quad (46)$$

with the phonon propagator given by:

$$\phi(\tau) = \int_0^\infty d\omega \frac{J(\omega)}{\omega^2} F(\omega)^2 G_+(\tau), \quad (47)$$

$$G_\pm(\tau) = (n(\omega) + 1) e^{-i\tau\omega} \pm n(\omega) e^{-i\tau\omega} \quad (48)$$

$$n(\omega) = (e^{\beta\omega} - 1)^{-1}. \quad (49)$$

$$\frac{d\overline{\rho_S}(t)}{dt} = -i[H_S(t), \overline{\rho_S}(t)] - \sum_{ij} \int_0^t C_i(t) C_j(t-\tau) \Lambda_{ij}(\tau) \left[A_i, \widetilde{A}_j(t-\tau, t) \overline{\rho_S}(t) \right] + C_j(t) C_i(t-\tau) \Lambda_{ji}(-\tau) \left[\overline{\rho_S}(t) \widetilde{A}_j(t-\tau, t), A_i \right] d\tau. \quad (50)$$

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 :

$$\widetilde{A}_j(\tau) = \sum_w e^{-i\omega\tau} A_j(w) \quad (51)$$

$$\widetilde{A}_j(t) = \sum_{w(t)} e^{-i\omega(t)\tau} A_j(w(t)) \quad (52)$$

$$\widetilde{A}_j(t-\tau, t) = \sum_{w(t), w'(t-\tau)} e^{-i\omega(t)t} e^{i\omega'(t-\tau)} A'_j(w(t), w'(t-\tau)) \quad (53)$$

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:

$$A_i(0) = \langle + | A_i | + \rangle | + \rangle \langle + | + \langle - | A_i | - \rangle | - \rangle \langle - | \quad (54)$$

$$A_i(w) = \langle + | A_i | - \rangle | + \rangle \langle - | \quad (55)$$

$$A_i(-w) = \langle - | A_i | + \rangle | - \rangle \langle + |. \quad (56)$$

We define the following response functions:

$$K_{ijww'}(t) = \int_0^t C_i(t) C_j(t-\tau) \Lambda_{ij}(\tau) e^{i\omega\tau} e^{-it(w-w')} d\tau \quad (57)$$

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

$$\frac{d\overline{\rho_S}(t)}{dt} = -i[H_S(t), \overline{\rho_S}] - \sum_{ijww'} K_{ijww'}(t) \left[A_i, A_{jww'} \overline{\rho_S}(t) - \overline{\rho_S}(t) A_{jww'}^\dagger \right] \quad (58)$$

$$\dot{\rho} = -i[H_S(t), \rho] - \sum_{ijww'} K_{ijww'}(t) \left[A_i, A_{jww'} \rho - \rho A_{jww'}^\dagger \right] \quad (59)$$

$$\dot{\rho} = -i[H_S(t), \rho] - \sum_{ijww'} K_{ijww'}(t) \left([A_i, A_{jww'} \rho] - [A_i, \rho A_{jww'}^\dagger] \right) \quad (60)$$

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