Open quantum systems – lecture 4

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1.4 Generic form of the BMS master equation

Also for fully general system-reservoir couplings, described by $H = H_S + H_I + H_B$ with

$$H_I = \sum_\alpha S_\alpha \otimes B_\alpha \tag{1.1}$$

with system operators S_α and bath operators B_α one can derive the Born-Markov-secular master equation analogous to the previous section. Assuming that for a thermal equilibrium reservoir one works in a frame where $\langle B_\alpha \rangle = 0$, the same steps can be performed. In general, one will have multiple reservoir correlation functions which one can arrange in a matrix

$$C_{\alpha\bar{\alpha}}(\tau) = \mathrm{Tr}\left\{e^{+\mathrm{i}H_B\tau} B_\alpha e^{-\mathrm{i}H_B\tau} B_{\bar{\alpha}} \bar{\rho}_B\right\} , \tag{1.2}$$

and analogously one can compute even and odd Fourier transforms

$$\gamma_{\alpha\bar{\alpha}}(\omega) = \int C_{\alpha\bar{\alpha}}(\tau) e^{+\mathrm{i}\omega\tau} d\tau \, , \qquad \sigma_{\alpha\bar{\alpha}}(\omega) = \int C_{\alpha\bar{\alpha}}(\tau) \mathrm{sgn}(\tau) e^{+\mathrm{i}\omega\tau} d\tau = \frac{\mathrm{i}}{\pi} \mathcal{P} \int \frac{\gamma_{\alpha\bar{\alpha}}(\omega')}{\omega - \omega'} d\omega' \, . \tag{1.3}$$

Using instead of a Fock space representation the system energy eigenbasis

$$H_S \left|a\right\rangle = E_a \left|a\right\rangle \tag{1.4}$$

and the abbreviation $L_{ab} = \left|a\right\rangle \left\langle b\right|$, the Born-Markov-secular (BMS) master equation is given by

Def. 1 (BMS master equation)**.** *For an interaction Hamiltonian $H_I = \sum_\alpha S_\alpha \otimes B_\alpha$, the BMS master equation reads*

$$\begin{aligned}
\dot{\rho}_S &= -\mathrm{i}\left[H_S + \sum_{ab} \sigma_{ab} L_{ab}, \rho_S\right] + \sum_{abcd} \gamma_{ab,cd} \left[L_{ab} \rho_S L_{cd}^\dagger - \frac{1}{2}\left\{L_{cd}^\dagger L_{ab}, \rho_S\right\}\right] , \\
\sigma_{ab} &= \frac{\delta_{E_a,E_b}}{2\mathrm{i}} \sum_{\alpha\bar{\alpha}} \sigma_{\alpha\bar{\alpha}}(E_b - E_c) \left\langle c\right| S_{\bar{\alpha}} \left|b\right\rangle \left\langle c\right| S_\alpha^\dagger \left|a\right\rangle^* , \\
\gamma_{ab,cd} &= \delta_{E_b-E_a,E_d-E_c} \sum_{\alpha\bar{\alpha}} \gamma_{\alpha\bar{\alpha}}(E_b - E_a) \left\langle a\right| S_{\bar{\alpha}} \left|b\right\rangle \left\langle c\right| S_\alpha^\dagger \left|d\right\rangle^* .
\end{aligned} \tag{1.5}$$

- The above master equation is derived using Born-, Markov- and secular approximations. It is of Lindblad form (one can show that $\gamma_{ab,cd}$ is a positive semidefinite matrix, i.e., that $\sum_{ab,cd} x_{ab}^* \gamma_{ab,cd} x_{cd} \geq 0$ and that the Lamb-shift Hamiltonian $H_{\mathrm{LS}} = \sum_{ab} \sigma_{ab} L_{ab}$ is hermitian).

- From the occurrence of the Kronecker δ functions in the dampening coefficients $\gamma_{ab,cd}$ and Lamb-shift matrix elements σ_{ab} one can see that the BMS master equation is discontinuous with respect to degeneracies inside the system: If we tune a parameter of the system such that the system undergoes a transition through a point where its spectrum is degenerate, this maps to observables: For near but not exact degeneracies, we get a different solution than for exact degeneracy. These points should be handled with special care – e.g. by using perturbation theory both in the system-reservoir coupling and the system-local degeneracy-breaking term.

- From the structure of the $\sigma_{ab} \propto \delta_{E_a,E_b}$ it follows that $[H_S, H_{\rm LS}] = 0$.
- The reservoir correlation functions obey the Kubo-Martin-Schwinger (KMS) relation

$$C_{\alpha\bar{\alpha}}(\tau) = C_{\bar{\alpha}\alpha}(-\tau - {\rm i}\beta)\,, \tag{1.6}$$

which transfers to their Fourier transform as

$$\gamma_{\alpha\bar{\alpha}}(-\omega) = \gamma_{\bar{\alpha}\alpha}(+\omega) e^{-\beta\omega}\,, \tag{1.7}$$

and to the dampening coefficients as

$$\gamma_{ab,cd} = \gamma_{dc,ba} e^{\beta(E_b - E_a)}\,. \tag{1.8}$$

With this, one can show that

$$\bar{\rho}_S = \frac{e^{-\beta H_S}}{Z_S} = \sum_n \frac{e^{-\beta E_n}}{Z_S} \left|n\right\rangle \left\langle n\right| \tag{1.9}$$

is one steady-state solution of the BMS master equation.

- To compare this with the previously discussed example, identify $S = a + a^\dagger$ and $B = \sum_k (h_k b_k + h_k^* b_k^\dagger)$, one then finds with $\gamma(\omega) = \Gamma(\omega)[1 + n_B(\omega)]$ with $\Gamma(-\omega) = -\Gamma(+\omega)$ the relation

$$\frac{\gamma(-\omega)}{\gamma(+\omega)} = e^{-\beta\omega}\,, \tag{1.10}$$

which corresponds to the KMS relation. Furthermore, the non-vanishing Lamb-shift matrix elements and dissipative coefficients are given by

$$\begin{aligned} \sigma_{nn} &= \frac{\sigma(+\Omega)}{2{\rm i}} n + \frac{\sigma(-\Omega)}{2{\rm i}}(n+1)\,, \\ \gamma_{nn+1,mm+1} &= \gamma(+\Omega)\sqrt{(n+1)(m+1)}\,, \\ \gamma_{nn-1,mm-1} &= \gamma(-\Omega)\sqrt{nm}\,. \end{aligned} \tag{1.11}$$

Inserting this and using that

$$\begin{aligned} a^\dagger a &= \sum_n n \left|n\right\rangle \left\langle n\right|\,, \qquad & a a^\dagger &= \sum_n (n+1) \left|n\right\rangle \left\langle n\right|\,, \\ a &= \sum_n \sqrt{n+1} \left|n\right\rangle \left\langle n+1\right|\,, \qquad & a^\dagger &= \sum_n \sqrt{n} \left|n\right\rangle \left\langle n-1\right|\,, \end{aligned} \tag{1.12}$$

we find that the BMS master equation is identical to our previous example.

An important property of the BMS master equation arises for the quite common case of a non-degenerate system Hamiltonian, where $\delta_{E_a,E_b} = \delta_{ab}$. If we then consider the populations of the density matrix in the system energy eigenbasis $\rho_{nn} = \left\langle n\right| \rho_S \left|n\right\rangle$, we obtain that the unitary part does not influence these

$$\begin{aligned} \dot{\rho}_{nn} &= \sum_{abcd} \gamma_{ab,cd} \left[\left\langle n|a\right\rangle \rho_{bd} \left\langle c|n\right\rangle - \frac{1}{2} \left\langle n|d\right\rangle \left\langle c|a\right\rangle \rho_{bn} - \frac{1}{2} \rho_{nd} \left\langle c|a\right\rangle \left\langle b|n\right\rangle \right] \\ &= \sum_{bd} \gamma_{nb,nd} \rho_{bd} - \frac{1}{2} \sum_{ab} \gamma_{ab,an} \rho_{bn} - \frac{1}{2} \sum_{ad} \gamma_{an,ad} \rho_{nd}\,. \end{aligned} \tag{1.13}$$

From the structure of the dampening coefficients we can now conclude that for non-degenerate levels, populations only couple to populations, and we obtain in the energy eigenbasis the Pauli rate equation.

Def. 2 (Pauli rate equation)**.** *For a non-degenerate system Hamiltonian H_S, an interaction $H_I = \sum_\alpha S_\alpha \otimes B_\alpha$ with $\langle B_\alpha \rangle = 0$ and Fourier transforms (1.3) of the correlation functions (1.2), the Pauli rate equation reads*

$$\dot{\rho}_{nn} = \sum_m \gamma_{nm,nm} \rho_{mm} - \sum_m \gamma_{mn,mn} \rho_{nn} \,, \tag{1.14}$$

where the transition rate $m \to n$ is given by

$$\gamma_{nm,nm} = \sum_{\alpha\bar{\alpha}} \gamma_{\alpha\bar{\alpha}}(E_m - E_n) \langle n| S_{\bar{\alpha}} |m\rangle \langle n| S_\alpha^\dagger |m\rangle^* \,. \tag{1.15}$$

As the transition rates $\gamma_{nm,nm}$ are just the specialized dampening coefficients of the BMS master equations, they fulfil detailed balance $\gamma_{nm,nm} = \gamma_{mn,mn} e^{-\beta(E_n - E_m)}$, and the Pauli rate equation has a thermal steady state.