Week 9

PHY 435 / 635 Decoherence and Open Quantum Systems
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5 Non-Markovian Open Quantum Systems

In section 1.5.6 we had seen that a stochastic process $X(t)$ can be classified as "Markovian" (Non-Markovian) depending on whether the probabilities for the next step depend only on its currents state at time t (or also the history at times $t' < t$). The same nomenclature applies to the underlying evolution of a probability distribution $P(X,t)$. Since (the diagonal of) a density matrix also represents a probability distribution, we use the terminology for open quantum systems as well: A

Markovian Open Quantum System is one for which the evolution of the reduced density matrix $\frac{\partial}{\partial t}\hat{\rho}_S(t)$ depends only on the present density matrix $\hat{\rho}_S(t)$, and not on its past $\hat{\rho}_S(t')$, $t' < t$.

Consequently a

Markovian Master equation is one in which the right-hand side in $\frac{\partial}{\partial t}\hat{\rho}_S(t) = RHS$, does not contain any explicit dependencies on $\hat{\rho}_S(t')$ at $t' < t$, nor requires knowledge of the environmental history.

- We distinguish the two statements due to some subtleties: For example a seemingly Non-Markovian Master equation where the RHS <u>does</u> contain $\hat{\rho}_S(t')$ at $t' < t$ may still give rise to Markovian dynamics (if those dependencies happen to be negligible or unimportant).
- According to the definitions above, "Non-Markovian" implies the negation of the statement.
- We will now supply some first examples of Non-Markovianity, building on section 4, and then explore a bit more what the definitions above imply.

The starting point for this section is the Quantum Master equation in the second Born approximation (4.16).

- That equations also already deals with only the reduced DM of the system $\hat{\rho}_S^{(I)}(t)$ all information about the environment is neatly encapsulated in the correlation functions $\mathcal{C}_{\alpha,\beta}(t-t')$.

- However since we have not made the Markov approximation, the RHS still explicitly depends on $\hat{\rho}_S(t')$ at $t' < t$ (see time integration limits).
- Conceptually, this constitutes an integro-differential equation, posing additional challenges in its solution.

5.1 Redfield Formalism

As a first example of a fairly simple to use Non-Markovian ME, we revisit the Redfield equations (4.17), which had popped up in section 4.2 mainly as a step in the derivation of the Born-Markov ME. However at this point we had not yet made the Markov approximation. Firstly, note that (4.17) can be rewritten as

Redfield equation in tensor notation,

$$\frac{d}{dt}\rho^{(I)}_{\mathcal{S},ab}(t) = -\sum_{cd} R_{ab;cd}\ \rho^{(I)}_{\mathcal{S},cd}(t) \tag{5.1}$$

where matrix elements are defined as usual $\rho^{(I)}_{\mathcal{S},ab}(t) = \langle\, a\,|\hat{\rho}^{(I)}_{\mathcal{S}}(t)|\, b\,\rangle$. We will use states $|\, n\,\rangle$ to denote basis states of the system, and then define the Redfield Relaxation Tensor

$$R_{ab;cd} = \delta_{a,c}\sum_{e}\Gamma^{*}_{be,de} + \delta_{b,d}\sum_{e}\Gamma_{ae,ec} - \Gamma^{*}_{ca,bd} - \Gamma_{db,ac}. \tag{5.2}$$

where the new symbol $\Gamma_{ab,cd} = \sum_{\alpha}\langle\, a\,|\hat{S}^{(I)}_{\alpha}(t)|\, b\,\rangle\langle\, c\,|\Gamma_{\alpha}(t)|\, d\,\rangle$. We assume $\hat{S}$ is Hermitian but $\hat{\Gamma}$ may not be.

- To show (5.1) from (4.17), we first take matrix elements $\langle\, a\,|\cdots|\, b\,\rangle$ of (4.17) and then insert the system unit operator in the form of $\mathbb{1} = \sum_n |\, n\,\rangle\langle\, n\,|$, between any two of operators ($\hat{\rho}$, $\hat{S}$, $\hat{\Gamma}$).
- In section 5.1.1 we now apply the Redfield formalism to the (first, simplified) Spin-Boson model, for which we had found the complete evolution pictorially in section 2.2.1 and mathematically in assignment 1. We can then compare the open quantum system approach with the full solution in section 5.1.2.

5.1.1 Simplified Spin-Boson model with the Redfield method

To apply Eq. (5.1) to (2.10)-(2.12), we have to go through the tedious task of assembling all the ingredients $\hat{\Gamma}$, $\hat{S}^I(t)$, $\Gamma_{ab,cd}$, $R_{ab;cd}$. Luckily there are only two states in the system basis $|\, n\,\rangle \in \{|\uparrow\rangle, |\downarrow\rangle\}$.

Using (4.59) with $\Delta_0 = 0$ (Simplified SBM), we find $\hat{S}^I(\tau) = \sigma_z(0)$, so the system part of $\hat{H}_{\rm int}$ does not evolve in the interaction picture, and its matrix elements are

$$\langle\, a\,|\hat{S}^I(\tau)|\, b\,\rangle = \delta_{ab}(\delta_{a\uparrow} - \delta_{a\downarrow}). \tag{5.3}$$

Similar to Eq. (4.26) we define $\hat{H}_{\text{int}} = \hat{\sigma_z} \otimes \underbrace{\sum_i \bar{\kappa}_i \left(\hat{a}_i + \hat{a}_i^\dagger\right)}_{=\hat{E}}$, so there is only a single environmental operator $\hat{E}$ and we can also skip the index α. Thus as final piece to find $\Gamma_{ab,cd}$ we look at $\hat{\Gamma}_\alpha(t) = \int_0^t dt' \sum_\beta \mathcal{C}_{\alpha,\beta}(t-t')\hat{S}_\beta^{(I)}(t')$ from Eq. (4.17) and simplify this here to $\hat{\Gamma}(t) = \int_0^t d\tau\ \ \mathcal{C}(\tau)\sigma_z(0)$. Since we have the same oscillator environment as in section 4.4, we can use Eq. (4.32) for the bath correlation, assuming zero temperature $T \to 0$ and taking into account our slightly different definition of $\hat{E}$ here, which involves $\bar{\kappa}_i$ instead of κ_i. We find

$$\mathcal{C}(\tau) = \sum_j \bar{\kappa}_j^2 e^{-i\omega_j \tau}. \tag{5.4}$$

which we can straightforwardly integrate over time to find

$$\hat{\Gamma}(t) = \int_0^t d\tau\ \ \mathcal{C}(\tau)\sigma_z(0) = \underbrace{i\sum_j \frac{\bar{\kappa}_j^2}{\omega_j}\left(e^{-i\omega_j\tau} - 1\right)}_{\equiv\gamma(t)}\sigma_z(0). \tag{5.5}$$

and hence

$$\langle\, c\,|\hat{\Gamma}(t)|\, d\,\rangle = i\gamma(t)\delta_{cd}(\delta_{c\uparrow} - \delta_{c\downarrow}). \tag{5.6}$$

Now we combine (5.3) and (5.6) to write

$$\Gamma_{ab,cd} = i\gamma(t)\delta_{ab}(\delta_{a\uparrow} - \delta_{a\downarrow})\delta_{cd}(\delta_{c\uparrow} - \delta_{c\downarrow}), \tag{5.7}$$

from which we find[6]

$$R_{ab,cd} = -2\,\text{Im}[\gamma(t)]\big[1 - (\delta_{a\uparrow} - \delta_{a\downarrow})(\delta_{b\uparrow} - \delta_{b\downarrow})\big]\delta_{ac}\delta_{bd}. \tag{5.8}$$

Plugging these into (5.1) we finally reach the now surprisingly simple

Redfield equations for the simplified Spin-Boson model in the interaction picture

$$\begin{aligned} \frac{d}{dt}\rho_{\uparrow\uparrow}(t) &= 0, & \frac{d}{dt}\rho_{\uparrow\downarrow}(t) &= 4\text{Im}[\gamma(t)]\rho_{\uparrow\downarrow}(t), \\ \frac{d}{dt}\rho_{\downarrow\downarrow}(t) &= 0, & \frac{d}{dt}\rho_{\downarrow\uparrow}(t) &= 4\text{Im}[\gamma(t)]\rho_{\downarrow\uparrow}(t). \end{aligned} \tag{5.9}$$

Note: we have simplified notation $\rho^{(I)}_{\mathcal{S},\uparrow\uparrow}(t) \to \rho_{\uparrow\uparrow}(t)$

[6] Use e.g. $(\delta_{a\uparrow} - \delta_{a\downarrow})(\delta_{a\uparrow} - \delta_{a\downarrow}) = 1$.

Variation of constants/parameters: From mathematics courses we know that the ODE $f'(t) = g(t)f(t)$ has the general solution

$$f(t) = Ce^{\int dt\ g(t)} \tag{5.10}$$

where C is set by the initial conditions.

Using the result above, we can solve (5.9) to give $\rho_{\uparrow\uparrow}(t) = \rho_{\uparrow\uparrow}(0)$, $\rho_{\downarrow\downarrow}(t) = \rho_{\downarrow\downarrow}(0)$ and

$$\rho_{\uparrow\downarrow}(t) = \rho_{\uparrow\downarrow}(0)e^{-4\sum_j \frac{\bar{\kappa}_j^2}{\omega_j^2}\left(1-\cos{(\omega_j t)}\right)} \tag{5.11}$$

while $\rho_{\uparrow\downarrow}(t) = \rho_{\downarrow\uparrow}(t)^*$.

- Let's keep this result aside for a while and first revisit our earlier solution of the full problem (without using open system techniques / Master equations).

5.1.2 Reduced dynamics of the Spin

The simplified Spin-Boson model with $\Delta_0 = 0$ can be analytically solved (see section 2.2.1, assignment 1 and SD). In assignment one, you have found the solution

$$|\,\Psi(t)\,\rangle = c_1|\downarrow\rangle|\,\mathcal{E}_-\,\rangle + c_2|\uparrow\rangle|\,\mathcal{E}_+\,\rangle, \tag{5.12}$$

for the time dependent wave function following from the initial state $|\,\Psi(0)\,\rangle = (c_1|\downarrow\rangle + c_2|\uparrow\rangle)|\,0,\cdots,0\,\rangle$, where $|\,0,\cdots,0\,\rangle$ denotes all oscillators in the ground-state (hence the environment is at $T = 0$). Here $|\,\mathcal{E}_+\,\rangle$ is an environment state that is a tensor product of coherent states $|\,\mathcal{E}_+\,\rangle = |\,\lambda_1(t)/2\,\rangle \otimes |\,\lambda_2(t)/2\,\rangle \otimes \ldots$, where each amplitude

$$\lambda_i(t) \equiv 2\frac{\bar{\kappa_i}}{\omega_i}(1 - e^{i\omega_i t}) \tag{5.13}$$

will in general be different for the various environment oscillators. For $|\,\mathcal{E}_-\,\rangle$ we flip the sign of all $\lambda_i(t) \to -\lambda_i(t)$.

Since we managed to solve the whole model (4.58) for the simple case $\Delta_0 = 0$, we can construct the density matrix $\hat{\rho}(t) = |\,\Psi(t)\,\rangle\langle\,\Psi(t)\,|$, and then calculate the reduced density matrix for the spin only, using Eq. (3.13). Since Eq. (5.12) takes the bi-partite form Eq. (3.18) (treating the environment as just one"part" which is fine), we can directly use Eq. (3.19) for this and reach:

$$\hat{\rho}_S = |c_1|^2|\downarrow\rangle\langle\downarrow| + |c_2|^2|\uparrow\rangle\langle\uparrow| + c_1^*c_2|\downarrow\rangle\langle\uparrow|\underbrace{\langle\,\mathcal{E}_-\,|\,\mathcal{E}_+\,\rangle}_{=r(t)} + c_2^*c_1|\uparrow\rangle\langle\downarrow|\langle\,\mathcal{E}_+\,|\,\mathcal{E}_-\,\rangle\Big). \tag{5.14}$$

We call $r(t)$ the decoherence factor. Since we have an explicit expression for $|\,\mathcal{E}_\pm\,\rangle$ we can evaluate $r(t)$ directly. We use that the overlap of two coherent states

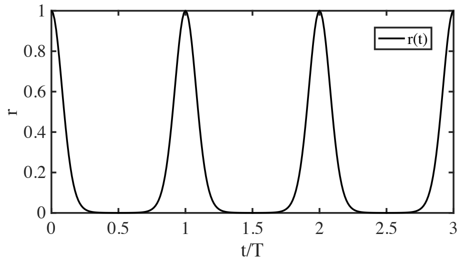
$$\langle\,\lambda\,|\,\mu\,\rangle = \exp{[-|\lambda|^2/2 - |\mu|^2/2 + \lambda^*\mu]}, \tag{5.15}$$

which can be shown from the definition (1.26), and find:

$$r(t) = \langle\, \mathcal{E}_- \,|\, \mathcal{E}_+ \,\rangle = \prod_i \langle\, -\lambda_i(t)/2 \,|\, \lambda_i(t)/2 \,\rangle \overset{Eq.~(5.15)}{=} \prod_i \exp\left[-|\lambda_i(t)|^2/2\right]$$

$$\overset{Eq.~(5.13)}{=} \exp\left[-4\sum_i \frac{\bar{\kappa}_i{}^2}{\omega_i^2}\big(1-\cos(\omega_i t)\big)\right]. \tag{5.16}$$

Example: Compare full and ME solutions of the Spin Boson model: We can now directly extract the coherence factor $r(t)$ from (5.16) with that obtained in (5.11) ($\rho_{\uparrow\downarrow}(0) = c_1^* c_2$ so $r(t)$ is just the part with the exponential). We find the same expression in both cases. For just a *single* environmental oscillator (not really a bath), this is plotted in the figure below. We see strong periodic revivals of coherence, corresponding to the times where the oscillator has returned to its initial state. Since whether this happens depends on exactly when the oscillator has "started" its motion, this now *depends* on the history of the bath. Revival features of coherence as shown are characteristic of non-Marovian systems.



left: Coherence factor $r(t)$ for a single environmental oscillator with $\kappa = \omega = 2\pi$, and period $T = 2\pi/\omega$.

- We have now explicitly validated the general idea to derive an evolution equation for the system only, taking into account the environment effectively via its correlation functions, by comparison with the complete solution.
- The non-Markovian Redfield equation is capable to capture the revival features shown in the graph above, which would not be the case for a Markov treatment.
- See SD for some additional discussion of decoherence in the Spin-Boson model, such as a non-zero temperature environment.

5.1.3 Full Spin-Boson model with the Redfield method

We finally drop the simplification $\Delta_0 = 0$, solving the complete Spin-Boson model. We thus have to re-evaluate $\hat{S}^I(\tau)$ and all quantities where it appears, since the system evolution will now be different. As in section 4.5.1 we use $\omega_0 = 0$ however, and thus again can write

$$\hat{S}^{(I)}(\tau) = \hat{\sigma}_z(0)\cos(\Delta_0\tau) - \hat{\sigma}_y(0)\sin(\Delta_0\tau), \tag{5.17}$$

with

$$\langle\, a \,|\hat{S}^I(\tau)|\, b \,\rangle = \delta_{ab}(\delta_{a\uparrow} - \delta_{a\downarrow})\cos(\Delta_0\tau) - (i\delta_{c\uparrow}\delta_{d\downarrow} - i\delta_{c\downarrow}\delta_{d\uparrow})\sin(\Delta_0\tau). \tag{5.18}$$

This changes (5.5) according to Eq. (4.59) into

$$\hat{\Gamma}(t) = \int_0^t d\tau\ \mathcal{C}(\tau)\hat{S}^{(I)}(\tau) = \int_0^t d\tau\ \sum_j \bar{\kappa}_j^2 e^{-i\omega_j\tau}\left(\hat{\sigma}_z(0)\cos\left(\Delta_0\tau\right) - \hat{\sigma}_y(0)\sin\left(\Delta_0\tau\right)\right)$$

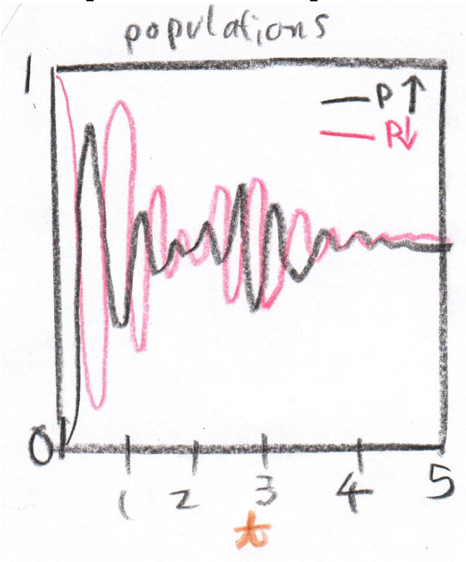
$$= \underbrace{\sum_j \bar{\kappa}_j^2 \frac{i\omega_j + e^{-i\omega_j\tau}\left(\Delta_0\sin\left(\Delta_0\tau\right) - i\omega_j\cos\left(\Delta_0\tau\right)\right)}{\Delta_0^2-\omega_j^2}\hat{\sigma}_z(0)}_{=\gamma_z(t)}$$

$$+ \underbrace{\sum_j \bar{\kappa}_j^2 \frac{-\Delta_0 + e^{-i\omega_j\tau}\left(\Delta_0\cos\left(\Delta_0\tau\right) + i\omega_j\sin\left(\Delta_0\tau\right)\right)}{\Delta_0^2-\omega_j^2}\hat{\sigma}_y(0)}_{=\gamma_y(t)}. \tag{5.19}$$

Matrix elements are thus $\langle c|\hat{\Gamma}(t)|d\rangle = \gamma_z(t)\delta_{cd}(\delta_{c\uparrow} - \delta_{c\downarrow}) + \gamma_y(t)(i\delta_{c\uparrow}\delta_{d\downarrow} - i\delta_{c\downarrow}\delta_{d\uparrow})$. We again assemble $\Gamma_{ab,cd}$ and $R_{ab,cd}$ and convert back to the Schrödinger picture as in section 4.2.

This time the equations would be much more complicated than Eq. (5.9), where each equation for ρ_{ab} contains most of the other ρ_{cd} on the rhs., together with time dependent functions stemming from the interplay of bath and system evolution, such as $\sin(\Delta t)$, $\sin(\omega_j t)$ [implementation: project].

Example: Redfield equations for the full Spin-Boson model:



left: We sketched the expected dynamics on the left hands side. The time dependence of the Redfield rate coefficients on the rhs. yields to oscillations that are damped faster during some times than others, and can even show partial revivals of coherent oscillations. Compare this with the monotonous damping in section 4.5.2.