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## NON-MARKOVIAN DYNAMICS IN OPEN QUANTUM SYSTEMS

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# 1 The Lindblad theory for open quantum systems and its extension

**Abstract**

We recall the Lindblad structure of the master equation for an open quantum system, which describes the dynamics in the Markovian case. We will consider in particular the issue of complete positivity, pointing to extensions of the Lindblad theory which describe non-Markovian systems and still ensure a well-defined dynamics. Examples will be provided of this generalized Lindblad structure.

## 1.1 Dynamics of open quantum systems

As basic setting we consider a system with state $\rho_S$ and Hamiltonian $H_S$ in interaction through $V$ with an environment having state $\rho_E$ and Hamiltonian $H_E$. The total state is given by $\rho \in \mathcal{TC}(\mathcal{H}_S \otimes \mathcal{H}_E)$, with $\rho = \rho^\dagger$, $\rho \geqslant 0$, $\mathrm{Tr}_{S+E}\rho = 1$ so that

$$\mathrm{Tr}_S \rho = \rho_E \qquad \mathrm{Tr}_E \rho = \rho_S.$$

Our basic aim is to eliminate the degrees of freedom of the environment to obtain effective equations of motion, let us say master equations, for the system only.

Working hypotheses:

i) factorized initial state

$$\rho \;=\; \rho_S \otimes \rho_E,$$

an hypothesis which essentially cannot be released to obtain a physically well-defined closed effective dynamics;

ii) overall unitary dynamics

$$\rho(t) \;=\; \mathcal{U}(t)\rho(0) = \mathrm{e}^{-iHt}\rho(0)\mathrm{e}^{+iHt},$$

hypothesis which could be released allowing e.g. for a semigroup dynamics $\rho(t) = \mathrm{e}^{t\mathcal{L}}\rho(0)$ for the whole system.

For fixed $\rho_E$ we then have the commutative diagram

$$\begin{tikzcd}
\rho_S(0) \otimes \rho_E \arrow[r, "\mathcal{U}(t)"] \arrow[d, shift left, "Tr_E"] & \rho(t) \arrow[d, "Tr_E"] \\
\rho_S(0) \arrow[r, "\Phi(t)"] \arrow[u, shift left, "\mathcal{A}"] & \rho_S(t)
\end{tikzcd}$$

where $\mathcal{A}$ is called assignment map

$$\begin{aligned} \mathcal{A}\colon \mathcal{TC}(\mathcal{H}_S) &\mapsto \mathcal{TC}(\mathcal{H}_S \otimes \mathcal{H}_E) \\ \rho_S &\rightsquigarrow \rho_S \otimes \rho_E \end{aligned}$$

linear, positive, and such that $\mathrm{Tr}_E \circ \mathcal{A} = \mathbb{1}_{\mathcal{TC}(\mathcal{H}_S)}$. Indeed for fixed $\rho_E$ the assignment

$$\rho_S(0) \;\mapsto\; \rho_S(t) = \Phi(t)\rho_S(0) = \mathrm{Tr}_E\{U(t)\rho_S(0) \otimes \rho_E U^\dagger(t)\}$$

is a linear map which preserves hermiticity and trace, further sending positive operators to positive operators, therefore in particular sending states to states: let us call it quantum dynamical map. Actually $\Phi(t)$ for any $t$ is a completely positive and trace preserving (CPT) map or quantum channel, since it can be written in Kraus form as

$$\Phi(t)\sigma \;=\; \sum_{\alpha\beta} W_{\alpha\beta}(t)\sigma W_{\alpha\beta}^\dagger(t)$$

with $\sum_{\alpha\beta} W^{\dagger}_{\alpha\beta}(t) W_{\alpha\beta}(t) = \mathbb{1}$, $W_{\alpha\beta}(t) = \sqrt{\lambda_\beta}\langle\varphi_\alpha|U(t)|\varphi_\beta\rangle$ with $\lambda_\beta \geqslant 0$, $\sum_\beta \lambda_\beta = 1$ and $\{\varphi_\beta\}$ SONC in $\mathcal{H}_S$.

`Exercise: verify these relations, are the` $W_{\alpha\beta}(t)$ `unique?`
`Exercise: verify that` $\Phi(t)$ `is CPT even when` $\mathcal{U}(t)$ `is CPT but not necessarily unitary`

The Kraus form implies complete positivity (CP) according to the definition:

$$\Phi: \mathcal{TC}(\mathcal{H}_S) \;\mapsto\; \mathcal{TC}(\mathcal{H}_S)$$

is CP provided

$$\Phi \otimes \mathbb{1}: \mathcal{TC}(\mathcal{H}_S \otimes \mathbb{C}_n) \;\mapsto\; \mathcal{TC}(\mathcal{H}_S \otimes \mathbb{C}_n)$$

is positive for all $n \in \mathbb{N}$ (or up to the dimension of $\mathcal{H}_S$ in the finite dimensional case). The difference between postivity and CP can be detected considering entangled states.

The map $\Phi$ acting on the states is CP iff is CP the adjoint map $\Phi'$ acting on observables according to the duality form $\mathrm{Tr}\{B^\dagger\sigma\}$ with $B \in \mathcal{B}(\mathcal{H}_S)$ and $\rho \in \mathcal{TC}(\mathcal{H}_S)$

$$\mathrm{Tr}\{B\Phi[\sigma]\} \;=\; \mathrm{Tr}\{\Phi'[B]\sigma\}.$$

`Exercise: write the adjoint map of` $\Phi[\sigma] = \sum_i A_i \sigma A_i^\dagger$
`Exercise: what does trace preservation of` $\Phi$ `implies for` $\Phi'$ `?`

Equivalent formulations of the CP condition are:
i) $\Phi' \otimes \mathbb{1}$ is positive for all $n \in \mathbb{N}$
ii) the condition

$$\sum_{i,j=1}^{n} \langle\psi_i|\Phi'\Big(B_i^\dagger B_j\Big)|\psi_j\rangle \geqslant 0 \quad \forall n \in \mathbb{N}, \forall\{\psi_i\} \subset \mathcal{H}_S, \forall\{B_i\} \subset \mathcal{B}(\mathcal{H}_S)$$

holds.
`Exercise: prove that the two formulations of the CP condition are equivalent`
`Exercise: check that a unitary evolution is CP`
Note the equivalence between the following statements:

1. $\Phi$ is CP according to either of the two equivalent definitions
2. $\Phi$ can be written in Kraus form: $\Phi[\sigma] = \sum_i A_i \sigma A_i^\dagger$
3. $\Phi$ can be obtained from an overall unitary evolution for certain $\mathcal{H}_E$, $\rho_E$ and $U$: $\Phi[\sigma] = \mathrm{Tr}_E\{U\sigma \otimes \rho_E U^\dagger\}$

## 1.2 Quantum dynamical semigroups

An explicit general characterization of quantum dynamical map is known only for special cases. An important and general class is obtained assuming a semigroup composition law for the quantum dynamical map as a function of the time argument

$$\Phi(t+s) \;=\; \Phi(t) \circ \Phi(s) \qquad \forall t, s \geqslant 0$$

where each $\Phi(t)$ is a CPT map. This is called the (time-homogeneous) Markovian case. A one-parameter group of unitary operators according to Stone's theorem is described by its generator given by a self-adjoint operator. Likewise for a semigroup of contraction operators a generator characterized by the Hille-Yosida theorem exists such that

$$\Phi(t) \;=\; \mathrm{e}^{t\mathcal{L}}.$$

If for any $t$ the map is CP then the collection of these maps is called a quantum dynamics semigroup (QDS).

Physical conditions allowing for semigroup dynamics are typically given by

$$\tau_E \ll \tau_S$$

i.e. environment correlation time (decay time of correlation function) much shorter than relaxation time of reduced system. Equivalently, in the notation to be used later on,

$$\gamma_0 \ll \lambda$$

i.e. relaxation rate much less than bandwidth of the bath or width of its spectral density.

This separation of time scales (so called Markov condition) together with weak coupling (so called Born approximation), which also justifies the choice of a factorized intial state, typically allows for a description of the dynamics in terms of a QDS.

The characterization of the structure of the generators of QDS is given by the famous Gorini Kossakowski Sudarshan Lindblad theorem. Its finite dimensional version reads:

**Theorem (GKSL)** Let $\dim \mathcal{H}_S = N$, a linear operator $\mathcal{L}\colon \mathcal{TC}(\mathcal{H}_S) \mapsto \mathcal{TC}(\mathcal{H}_S)$ is the generator of a QDS, that is to say a one-parameter continuous semigroup of CPT maps $\Phi(t) = \mathrm{e}^{t\mathcal{L}}$ iff it is of the form

$$\mathcal{L}[\rho] \;=\; -i[H,\rho] + \sum_{k=1}^{N^2-1} \gamma_k \left[ L_k \rho L_k^\dagger - \frac{1}{2}\left\{ L_k^\dagger L_k, \rho \right\} \right]$$

with $\gamma_k \geqslant 0$; $H = H^\dagger$, $L_k \in \mathcal{B}(\mathcal{H}_S)$.

The result extends to infinite dimensional Hilbert spaces provided one asks for norm continuity of $\Phi(t)$. Most importantly it is a necessary and sufficient condition. We give an idea of the proof, pointing to extensions of the sufficient condition to account for more general situations.

*Necessary condition*

If $\Phi(t)$ is CPT, according to the Kraus representation at any time it can be written as $\Phi(t)[\rho] = \sum_i A_i(t) \rho A_i^\dagger(t)$ with $\sum_i A_i^\dagger(t) A_i(t) = \mathbb{1}$. Writing the $A_i(t)$ in terms of an orthonormal basis $\{F_i\}_{i=1,\ldots,N^2}$, with $F_{N^2} = \frac{\mathbb{1}}{\sqrt{N}}$, such that $\mathrm{Tr}_{\mathcal{H}_S} F_i F_j = \delta_{ij}$, one has

$$\Phi(t)[\rho] \;=\; \sum_{i,j=1}^{N^2} c_{ij}(t) F_i \rho F_j^\dagger$$

with $c_{ij}(t)$ a positive matrix. We know that the generator exists and is given by

$$\lim_{\varepsilon \to 0^+} \frac{\Phi(\varepsilon) - \mathbb{1}}{\varepsilon}[\rho] \;=\; \mathcal{L}[\rho].$$

Relying on the existence of the limit and imposing trace preservation one obtains the following form for the generator

$$\mathcal{L}[\rho] \;=\; -i[H,\rho] + \sum_{k,l=1}^{N^2-1} a_{kl} \left[ F_k \rho F_l^\dagger - \frac{1}{2}\left\{ F_l^\dagger F_k, \rho \right\} \right],$$

where $H = H^\dagger$, and $a_{kl} = \lim_{\varepsilon \to 0} \frac{c_{kl(\varepsilon)}}{\varepsilon}$ is a positive matrix known as Kossakowski matrix ($a_{kl} = \lim_{\varepsilon \to 0} c_{kl(\varepsilon)}/\varepsilon$).

Diagonalization of the positive matrix leads to an explicit Lindblad form. In Schrödinger picture

$$\mathcal{L}[\rho] \;=\; -i[H,\rho] + \sum_{k=1}^{N^2-1} \gamma_k \left[ L_k \rho L_k^\dagger - \frac{1}{2}\left\{ L_k^\dagger L_k, \rho \right\} \right]$$

corresponding to the Heisenberg picture

$$\mathcal{L}'[X] \;=\; +i[H,X] + \sum_{k=1}^{N^2-1} \gamma_k \left[ L_k^\dagger X L_k - \frac{1}{2}\left\{ L_k^\dagger L_k, X \right\} \right],$$

which can be equivalently be written in socalled standard form by means of the CP map

$$\Psi[X] \;=\; \sum_{k=1}^{N^2-1} \gamma_k L_k^\dagger X L_k$$

as follows

$$\mathcal{L}'[X] \;=\; +i[H,X] + \Psi[X] - \frac{1}{2}\{\Psi[\mathbb{1}], X\}.$$

The $\{L_k\}$ are typically called Lindblad operators.

*Sufficient condition I*

We want to see that a generator in Lindblad form leads to a CP map. Preservation of hermiticity and trace is immediately checked, we show CP pointing to a perturbation expansion of the solution. Let us put $\mathcal{L} = \mathcal{L}_R + \mathcal{L}_J$, sum of a relaxing and jump part, according to

$$\begin{aligned}
\mathcal{L}_R[\rho] \;&=\; -i[H,\rho] - \frac{1}{2}\left\{\sum_k \gamma_k L_k^\dagger L_k, \rho\right\} \\
&=\; -i\Big(H_{\text{eff}}\rho - \rho H_{\text{eff}}^\dagger\Big) \\
\mathcal{L}_J[\rho] \;&=\; \sum_k \gamma_k L_k \rho L_k^\dagger
\end{aligned}$$

with $\mathcal{L}_J$ a CP map. We know that

$$\frac{\mathrm{d}}{\mathrm{dt}}\rho(t) \;=\; \mathcal{L}\rho(t)$$

and therefore due to $\rho(t) = \Phi(t)\rho(0)$ also

$$\frac{\mathrm{d}}{\mathrm{dt}}\Phi(t) \;=\; \mathcal{L}\Phi(t) \qquad \Phi(0) = \mathbb{1}.$$

Denoting by $\mathcal{R}(t)$ the solution of the relaxing part

$$\frac{\mathrm{d}}{\mathrm{dt}}\mathcal{R}(t) \;=\; \mathcal{L}_R\mathcal{R}(t) \qquad \mathcal{R}(0) = \mathbb{1}$$

given by

$$\mathcal{R}(t)[\rho] \;=\; \mathrm{e}^{\mathcal{L}_R t}[\rho] = \mathrm{e}^{-iH_{\text{eff}}t}\rho\,\mathrm{e}^{+iH_{\text{eff}}^\dagger t}$$

one has

$$\begin{aligned}
\Phi(t) \;&=\; \mathcal{R}(t) + \int_0^t \mathrm{d}\tau \mathcal{R}(t-\tau)\mathcal{L}_J\Phi(\tau) \\
&=\; \mathrm{e}^{\mathcal{L}_R t} + \int_0^t \mathrm{d}\tau \mathrm{e}^{\mathcal{L}_R(t-\tau)}\mathcal{L}_J\Phi(\tau) \\
&=\; \mathcal{R}(t) + (\mathcal{R}\star\mathcal{L}_J\Phi)(t).
\end{aligned}$$

This equation is of the form $G = G^0 + G^0VG$ and is solved by the Dyson series

$$\Phi(t) \;=\; \mathcal{R}(t) + (\mathcal{R}\star\mathcal{L}_J\mathcal{R})(t) + (\mathcal{R}\star\mathcal{L}_J\mathcal{R}\star\mathcal{L}_J\mathcal{R})(t) + \ldots$$

which is a CP map by construction, because such are $\mathcal{R}(t)$ and $\mathcal{L}_J$. Appearently it is enough to ask $\mathcal{R}(t)$ and $\mathcal{L}_J\mathcal{R}(t)$ to be CP, but the inverse of $\mathcal{R}(t)$ is also CP, so that this requirement is not weaker. The solution of the master equation can thus be explicitly written as a jump expansion as follows

$$\begin{aligned}
\rho(t) \;&=\; \Phi(t)\rho(0) \\
&=\; \mathcal{R}(t)\rho(0) + \sum_{n=1}^{\infty} \int_0^t \mathrm{d}t_n \ldots \int_0^{t_2} \mathrm{d}t_1 \mathcal{R}(t-t_n)\mathcal{L}_J\mathcal{R}(t_n - t_{n-1})\ldots\mathcal{L}_J\mathcal{R}(t_1)\rho(0).
\end{aligned}$$

`Exercise:verify explicitly that the Dyson expansion is solution of the Lindblad master equation`

*Sufficient condition II*

The proof still works if we allow the operators appearing in the Lindblad structure as well as the decay rates $\gamma_k$ to become time dependent, provided the latter always stay positive. This situation corresponds to a time-inhomogeneous Markovian case. Starting from

$$\frac{\mathrm{d}}{\mathrm{dt}}\Phi(t) = \mathcal{L}(t)\Phi(t)$$

with $\Phi(t) \equiv \Phi(t,\,0)$ and the initial condition $\Phi(t,\,t) = \mathbb{1}$, we can still consider a relaxing part $\mathcal{L}_R(t)$ and a jump part $\mathcal{L}_J(t)$, where the latter still is a CP map thanks to the positivity of the $\gamma_k(t)$. As done before starting from the solution of the time-local master equation

$$\frac{\mathrm{d}}{\mathrm{dt}}\mathcal{R}(t,s) = \mathcal{L}_R(t)\mathcal{R}(t,s)$$

where $\mathcal{R}(t) \equiv \mathcal{R}(t,0)$, $\mathcal{R}(t,t) = \mathbb{1}$ and $t \geqslant s \geqslant 0$, given by

$$\mathcal{R}(t,s) = \vec{T}\exp\left(\int_s^t \mathrm{d}\tau\mathcal{L}_{\mathcal{R}}(\tau)\right)$$

where $\vec{T}$ denotes the chronological time ordering. This is a CP map satisfying the two-time composition law

$$\mathcal{R}(t,\tau)\circ\mathcal{R}(\tau,s) = \mathcal{R}(t,s) \qquad \forall t \geqslant \tau \geqslant s.$$

As a result we can still write a Dyson expansion for the time evolution map, whose very structure ensures CP of the time evolution. One has

$$\begin{aligned}\rho(t) &= \Phi(t)\rho(0)\\ &= \mathcal{R}(t)\rho(0)\\ &\quad+\sum_{n=1}^{\infty}\int_0^t \mathrm{d}t_n ... \int_0^{t_2}\mathrm{d}t_1\mathcal{R}(t,t_n)\mathcal{L}_J(t_n)\mathcal{R}(t_n,t_{n-1})...\mathcal{R}(t_2,t_1)\mathcal{L}_J(t_1)\mathcal{R}(t_1)\rho(0),\end{aligned}$$

and therefore a time evolution map characterized by two time indexes, satisfying the composition law

$$\Phi(t,\tau)\circ\Phi(\tau,s) = \Phi(t,s) \qquad \forall t \geqslant \tau \geqslant s$$

where each of the maps $\Phi(t,s)$ is CP and can be written as

$$\Phi(t,s) = \vec{T}\exp\left(\int_s^t \mathrm{d}\tau\mathcal{L}(\tau)\right).$$

This kind of time local master equations arise e.g. in the time-convolutionless projection operator technique.

*Sufficient condition III*

A further extension of the validity of this sufficient condition can be obtained considering master equations of integrodifferential form. Let us consider an equation of the form

$$\frac{\mathrm{d}}{\mathrm{dt}}\rho(t) = \int_0^t \mathrm{d}\tau\mathcal{L}(t-\tau)\rho(\tau)$$

where again the operator part has the typical structure ensuring preservation of hermiticity and trace

$$\mathcal{L}(\tau)\rho = -i[H(\tau),\rho]+\sum_k \gamma_k(\tau)\Big[L_k(\tau)\rho L_k^\dagger(\tau)-\frac{1}{2}\Big\{L_k^\dagger(\tau)L_k(\tau),\rho\Big\}\Big].$$

Considering the usual splitting $\mathcal{L}(\tau) = \mathcal{L}_R(\tau) + \mathcal{L}_J(\tau)$, we have the evolution equations

$$\frac{\mathrm{d}}{\mathrm{dt}}\Phi(t) = \int_0^t \mathrm{d}\tau\mathcal{L}(t-\tau)\Phi(\tau) \qquad \Phi(0) = \mathbb{1}$$

for the whole dynamics and

$$\frac{\mathrm{d}}{\mathrm{dt}}\mathcal{R}(t) = \int_0^t \mathrm{d}\tau\mathcal{L}_R(t-\tau)\mathcal{R}(\tau) \qquad \mathcal{R}(0) = \mathbb{1}$$

for the relaxing part. The Laplace transformed equations

$$\hat{\Phi}(u) = \frac{\mathbb{1}}{u - \left(\hat{\mathcal{L}}_R(u) + \hat{\mathcal{L}}_J(u)\right)}$$

and

$$\hat{\mathcal{R}}(u) = \frac{\mathbb{1}}{u - \hat{\mathcal{L}}_R(u)}$$

lead to the Dyson equation

$$\hat{\Phi}(u) = \hat{\mathcal{R}}(u) + \hat{\mathcal{R}}(u)\hat{\mathcal{L}}_J(u)\hat{\Phi}(u)$$

or going back in the time domain

$$\Phi(t) = \mathcal{R}(t) + (\mathcal{R} \star \mathcal{L}_J \star \Phi)(t),$$

which is solved once again by a Dyson series expansion

$$\Phi(t) = \mathcal{R}(t) + (\mathcal{R} \star \mathcal{L}_J \star \mathcal{R})(t) + (\mathcal{R} \star \mathcal{L}_J \star \mathcal{R} \star \mathcal{L}_J \star \mathcal{R})(t) + \ldots.$$

Note that at this point we can still say nothing about CP of $\Phi(t)$. However this formal expansion of the solution tells us that if we can show that $\mathcal{R}(t)$ and $\mathcal{L}_J(t)$ are CP, then $\Phi(t)$ is CP. The same holds under the weaker condition that $\mathcal{R}(t)$ and $(\mathcal{R} \star \mathcal{L}_J)(t)$ are CP.

This kind of generalized master equations arise in the Nakajima-Zwanzig projection operator technique.

### 1.2.1 Example

Two-level atom interacting with radiation field at given temperature. The system is described in $\mathcal{H}_S = \mathbb{C}^2$, with Hamiltonian $H_S = \omega_0 \sigma_+ \sigma_-$ and Lindblad generator

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{dt}}\rho &= -i[H_S, \rho] + \gamma_0(N_\beta + 1)\left[\sigma_- \rho \sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-, \rho\}\right] \\ &\quad + \gamma_0 N_\beta \left[\sigma_+ \rho \sigma_- - \frac{1}{2}\{\sigma_-\sigma_+, \rho\}\right]\end{aligned}$$

where $\gamma_0$ is the spontaneous emission rate, $N_\beta$ the mean number of photons in the electromagnetic field at inverse temperature $\beta$ at the resonant frequency $\omega_0$. The first term describes induced and spontaneous emission, the second induced absorption. There are only two Lindblad operators

$$\begin{aligned}\gamma_1 L_1 &= \sqrt{\gamma_0(N_\beta + 1)}\sigma_- \\ \gamma_2 L_2 &= \sqrt{\gamma_0 N_\beta}\sigma_+.\end{aligned}$$

This master equation can describe dynamics of populations and coherences, spectrum of emitted radiation, statistics of photon detection.

### 1.2.2 Example

Massive test particle interacting with background gas. The system is described in $\mathcal{H}_S = L^2(\mathbb{R}^3)$, with Hamiltonian $H_S = \frac{\hat{p}^2}{2M}$ and Lindblad generator

$$\frac{\mathrm{d}}{\mathrm{dt}}\rho(t) = -i[H_S, \rho] + \Gamma \int \mathrm{d}q \mathcal{P}(q)\left[\mathrm{e}^{iq\hat{x}}\rho \mathrm{e}^{iq\hat{x}} - \rho\right]$$

where $\Gamma$ is the collision rate, $\mathcal{P}(q)$ the probability distribution of momentum exchanges, which in Born approximation reads $\Gamma \mathcal{P}(q) = (2\pi)^4 n_{\mathrm{gas}}\left|\tilde{V}(q)\right|^2$, with $V(x - y)$ the interaction potential. There is a continuum of Lindblad operators

$$\gamma(q)L(q) = \sqrt{\Gamma \mathcal{P}(q)}\mathrm{e}^{iq\hat{x}}$$

This master equation can describe collisional decoherence. If extended to account for energy transfer it also describes quantum Brownian motion and thermalization effects, giving a quantum counterpart of the classical linear Boltzmann equation.

## 1.3 Generalized Lindblad structure

Consider a situation in which one has a tripartite Hilbert space, so that you have some freedom in setting the border between system and environment, including the ancillary degrees of freedom in either of the two. As a result the interaction between what you consider as system and environment is mediated by unobserved degrees of freedom, which can be exploited to provide a finer characterization of the bath. Building on the latter example of collisional decoherence, let us consider a massive particle with internal degrees of freedom interacting through collisions with a gas, so that the Hilbert space for the overall system is given by

$$\mathcal{H}_{\mathrm{CM}} \otimes \mathcal{H}_{\mathrm{INT}} \otimes \mathcal{H}_{\mathrm{GAS}} = L^2\big(\mathbb{R}^3\big) \otimes \mathbb{C}^n \otimes \mathcal{F}_B\big(L^2\big(\mathbb{R}^3\big)\big).$$

Taken

$$\mathcal{H}_S = \mathcal{H}_{\mathrm{CM}} = L^2\big(\mathbb{R}^3\big)$$

consider a quantum-classical description on $\mathcal{H}_{\mathrm{CM}} \otimes \mathcal{H}_{\mathrm{INT}}$, that is to say among all the possible states in $\mathcal{TC}(\mathcal{H}_{\mathrm{CM}} \otimes \mathcal{H}_{\mathrm{INT}})$ consider block diagonal ones $\varrho \in \mathcal{TC}_{\mathrm{diag}}(\mathcal{H}_{\mathrm{CM}} \otimes \mathcal{H}_{\mathrm{INT}})$ of the form

$$\varrho = \sum_{\alpha=1}^{n} \rho_\alpha \otimes |\alpha\rangle\langle\alpha|,$$

with $\rho_\alpha \in \mathcal{TC}(\mathcal{H}_{\mathrm{CM}})$, corresponding to a classical description for the internal degrees of freedom, which have decohered more quickly or have been prepared in a state which does not exhibit coherences. The dual space is given by $B \in \mathcal{B}_{\mathrm{diag}}(\mathcal{H}_{\mathrm{CM}} \otimes \mathcal{H}_{\mathrm{INT}})$ of the form

$$B = \sum_{\alpha=1}^{n} \mathrm{B}_\alpha \otimes |\alpha\rangle\langle\alpha|,$$

with $\mathrm{B}_\alpha \in \mathcal{B}(\mathcal{H}_{\mathrm{CM}})$. These are the observables whose statistics can be described according to

$$\langle B \rangle_\varrho = \sum_{\alpha=1}^{n} \mathrm{Tr}_{\mathrm{CM}}\{\mathrm{B}_\alpha \rho_\alpha\}.$$

Now we consider a Markovian master equation on $\mathcal{H}_{\mathrm{CM}} \otimes \mathcal{H}_{\mathrm{INT}}$ which provides a CP dynamics given by a QDS on this space, however preserving the block diagonal structure of the states. Otherwise stated we look for a dynamics of the operators $\rho_\alpha$ (with $\rho_\alpha \geqslant 0$, $\mathrm{Tr}_{\mathrm{CM}}\rho_\alpha \leqslant 1$, $\sum_\alpha \mathrm{Tr}_{\mathrm{CM}}\rho_\alpha = 1$), which can be embedded into a Lindblad dynamics on the extended space.

**Theorem (Breuer)** The generator $\mathcal{L}$ of a QDS on $\mathcal{H}_{\mathrm{CM}} \otimes \mathcal{H}_{\mathrm{INT}}$ which sends block diagonal states into block diagonal states, that is such that

$$\mathrm{e}^{\mathcal{L}t}\left(\sum_{\alpha=1}^{n} \rho_\alpha(0) \otimes |\alpha\rangle\langle\alpha|\right) = \sum_{\alpha=1}^{n} \rho_\alpha(t) \otimes |\alpha\rangle\langle\alpha|$$

can be written as

$$\mathcal{L}\left[\sum_{\alpha=1}^{n} \rho_\alpha \otimes |\alpha\rangle\langle\alpha|\right] = \sum_{\alpha=1}^{n} \mathcal{L}_\alpha(\rho_1, \ldots, \rho_n) \otimes |\alpha\rangle\langle\alpha|$$

where the operators $\mathcal{L}_\alpha$ determine the coupled dynamics of the $\rho_\alpha$ according to

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{dt}}\rho_\alpha &= \mathcal{L}_\alpha(\rho_1, \ldots, \rho_n)\rho_\alpha \\ &= -i[\mathrm{H}^\alpha, \rho_\alpha] + \sum_\lambda \sum_{\beta=1}^{n} \left[\mathrm{R}_\lambda^{\alpha\beta}\rho_\beta \mathrm{R}_\lambda^{\alpha\beta\dagger} - \frac{1}{2}\left\{\mathrm{R}_\lambda^{\beta\alpha\dagger}\mathrm{R}_\lambda^{\beta\alpha}, \rho_\alpha\right\}\right],\end{aligned}$$

with $\mathrm{H}^\alpha = \mathrm{H}^{\alpha\dagger}$ and $\mathrm{R}_\lambda^{\beta\alpha}$ operators on $\mathcal{H}_{\mathrm{CM}}$.

*Necessary condition*

Suppose given a Lindblad master equation on $\mathcal{H}_{\mathrm{CM}} \otimes \mathcal{H}_{\mathrm{INT}}$, then it has to be of the form

$$\mathcal{L}[\rho] \;=\; -i[H, \rho] + \sum_\lambda \left[ R_\lambda \rho R_\lambda^\dagger - \frac{1}{2}\left\{ R_\lambda^\dagger R_\lambda, \rho \right\} \right]$$

where without loss of generality

$$\begin{aligned} H &= \sum_{\alpha\beta} H^{\alpha\beta} \otimes |\alpha\rangle\langle\beta| \\ R_\lambda &= \sum_{\alpha\beta} R_\lambda^{\alpha\beta} \otimes |\alpha\rangle\langle\beta| \end{aligned}$$

are operators on $\mathcal{H}_{\mathrm{CM}} \otimes \mathcal{H}_{\mathrm{INT}}$ with $H$ self-adjoint. Inserting this expression into the generator it can be written as

$$\mathcal{L}\varrho \;=\; \sum_{\alpha\beta} \mathcal{D}^{\alpha\beta}(\rho_1, \ldots, \rho_n) \otimes |\alpha\rangle\langle\beta|$$

with

$$\begin{aligned} \mathcal{D}^{\alpha\beta}(\rho_1, \ldots, \rho_n) \;=\; & -i\big(H^{\alpha\beta}\rho_\alpha - \rho_\beta H^{\alpha\beta}\big) \\ & + \sum_\lambda \sum_\gamma \left[ R_\lambda^{\alpha\gamma} \rho_\gamma R_\lambda^{\beta\gamma\dagger} - \frac{1}{2} R_\lambda^{\gamma\alpha\dagger} R_\lambda^{\gamma\beta} \rho_\beta - \frac{1}{2} \rho_\alpha R_\lambda^{\gamma\alpha\dagger} R_\lambda^{\gamma\beta} \right] \end{aligned}$$

and the constraint to preserve block diagonal states implies $\mathcal{D}^{\alpha\beta} = 0$ for $\alpha \neq \beta$, together with $\mathcal{D}^{\alpha\beta} = \mathcal{L}_\alpha$, with $H^\alpha = H^{\alpha\alpha}$ self-adjoint.

*Sufficient condition*

Given $\mathcal{L}_\alpha$ as above the operators

$$\begin{aligned} H &= \sum_\alpha H^\alpha \otimes |\alpha\rangle\langle\alpha| \\ S_\lambda^{\alpha\beta} &= R_\lambda^{\alpha\beta} \otimes |\alpha\rangle\langle\beta| \end{aligned}$$

allow us to build a Lindblad generator

$$\mathcal{L}[\rho] \;=\; -i[H, \rho] + \sum_\lambda \sum_{\alpha\beta} \left[ S_\lambda^{\alpha\beta} \rho S_\lambda^{\alpha\beta\dagger} - \frac{1}{2}\left\{ S_\lambda^{\alpha\beta\dagger} S_\lambda^{\alpha\beta}, \rho \right\} \right]$$

which leaves the space of block diagonal states invariant.

As a result this generalized Lindblad structure provides a Markovian dynamics at the level of the subcollections $\{\rho_1, \ldots, \rho_\alpha, \ldots, \rho_n\}$, but a non-Markovian one for the overall state $w$ obtained by tracing over the internal degrees of freedom considered as part of the environment and undetected in the final measurement. One has a well-defined dynamics

$$w(0) = \sum_{\alpha=1}^n \rho_\alpha(0) = \mathrm{Tr}_{\mathrm{INT}}\left( \sum_{\alpha=1}^n \rho_\alpha(0) \otimes |\alpha\rangle\langle\alpha| \right) \;\rightarrow\; w(t) = \sum_{\alpha=1}^n \rho_\alpha(t)$$

which is non-Markovian and cannot be obtained through a closed evolution equation for $w$ alone according to the non commutativity of the following diagram

$$\begin{tikzcd} \varrho(0) = (\rho_1(0), \ldots, \rho_n(0)) \arrow[r, "\exp(t\mathcal{L})"] \arrow[d, shift left, "Tr_{INT}"] & \varrho(t) = (\rho_1(t), \ldots, \rho_n(t)) \arrow[d, "Tr_{INT}"] \\ w(0) = \sum_{\alpha=1}^n \rho_\alpha(0) \arrow[u, shift left, "/" marking] \arrow[r, "/" marking] & w(t) = \sum_{\alpha=1}^n \rho_\alpha(t) \end{tikzcd}$$

The diagram is non commutative because the initial state on the extended space $\mathcal{H}_{\mathrm{CM}} \otimes \mathcal{H}_{\mathrm{INT}}$ is not factorized, rather classically correlated.

This is an istance of a general fact: reducing the considered/observed number of degreees of freedom leads from a Markovian to a non-Markovian dynamics and viceversa.

This kind of generalized master equations arise in projection operator techniques if one considers projections on classically correlated states.

### 1.3.1 Example

Consider a massive particle with internal degrees of freedom and the collisional decoherence dynamics arising when the scattering cross section depends on the internal state, and the initial preparation is diagonal in the internal states. Then the generalized Lindblad structure takes the form

$$\frac{\mathrm{d}}{\mathrm{dt}}\rho_i = \sum_j \int \mathrm{d}q \mathcal{P}^{ij}(q)\left[\Gamma^{ij}\mathrm{e}^{iq\hat{x}}\rho_j\mathrm{e}^{iq\hat{x}} - \Gamma^{ji}\rho_i\right]$$

where $\Gamma^{ij}$ denote the collision rate for the transition $j \to i$ and $\mathcal{P}^{ij}(q)$ denote the probability density of momentum transfer for the transition $j \to i$.

*n=1*

Standard Lindblad

$$\frac{\mathrm{d}}{\mathrm{dt}}\langle x|\rho(t)|y\rangle = -\Gamma[1-\Phi_{\mathcal{P}}(x-y)]\langle x|\rho(t)|y\rangle$$

where

$$\Phi_{\mathcal{P}}(x-y) = \int \mathrm{d}q\mathcal{P}(q)\mathrm{e}^{iq(x-y)}$$

with solution

$$\langle x|\rho(t)|y\rangle = \mathrm{e}^{-\Gamma[1-\Phi_{\mathcal{P}}(x-y)]t}\langle x|\rho(0)|y\rangle = \Psi(x-y,t)\langle x|\rho(0)|y\rangle$$

suppression of off-diagonal matrix elements exponential in time determined by characteristic function of compound Poisson process.

*n>1*

Assuming no degeneracy and elastic scattering, for $\rho_i(0) = p_i w(0)$ the generalized Lindblad structure leads to

$$\langle x|w(t)|y\rangle = \sum_i p_i\mathrm{e}^{-\Gamma^{ii}[1-\Phi_{\mathcal{P}_{ii}}(x-y)]t}\langle x|w(0)|y\rangle = \Psi(x-y,t)\langle x|w(0)|y\rangle$$

and simple Markovian exponential behaviour in time is immediately lost, allowing for oscillations and more pronounced decoherence beavior.

The ancillary degrees of freedom naturally provide a classical label over which one takes the trace, since this classical label helps in characterizing the initial state but is not observed in the final measurement. One can thus keep into account the modification of the interaction between system and environment due to a classical intermediate degrees of freedom or fine structure of the reservoir (e.g. band structure).

## 1.4 References

For this part see mainly [Breuer2007, Holevo2001, Gorini1976a, Lindblad1976a, Esposito2003a, Esposito2007a, Budini2006a, Breuer2007a, Vacchini2008a, Vacchini2009a, Vacchini2010a, Smirne2010a]

# 2 Non-Markovian dynamics and memory kernels

**Abstract**

We construct a class of master equations with memory kernel, for which sufficient conditions to ensure complete positivity of the dynamics can be formulated. A probabilistic interpretation of these kernels will be given, showing that they provide the quantum counterpart of classical semi-Markov processes, which describe memory effects and include Markov processes as a special case.

## 2.1 Classical semi-Markov processes

Given a master equation in Lindblad form

$$\mathcal{L}[\rho] = -i[H,\rho]+\sum_k \gamma_k\left[L_k\rho L_k^\dagger-\frac{1}{2}\left\{L_k^\dagger L_k,\rho\right\}\right]$$

if the populations in a given basis obey closed evolution equations, the diagonal matrix elements $P_n=\langle n|\rho|n\rangle$ obey the following Pauli master equation for a classical jump Markov process

$$\frac{\mathrm{d}}{\mathrm{dt}}P_n(t) = \sum_m [\Gamma_{nm}P_m-\Gamma_{mn}P_n],$$

where the positive rates can be expressed as

$$\Gamma_{nm} = \sum_k \gamma_k|\langle n|L_k|m\rangle|^2.$$

Remaining first at classical level one can ask whether a similar result is available for a wider class of processes including non-Markovian ones. Quantum mechanics actually is a probability theory, and it is certainly worth to further exploit ideas coming from classical probability theory. Indeed a generalized master equation given by an integrodifferential rate equation can be considered for a class of classical processes known as semi-Markov processes. They arise merging Markov chains and renewal processes. In a Markov jump process one has certain transition probabilities among sites $\pi_{ij}$ ($\sum_i \pi_{ij}=1$) and a waiting time distribution in between jumps given by an exponential distribution $f(\tau)=\lambda \mathrm{e}^{-\lambda\tau}$. The latter distribution has the memoryless property, which denoting by $\tau_n$ the time of the $n$-th jump can be written as

$$P\{\tau_n>t+s|\tau_n>s\} = \frac{P\{\tau_n>t+s\}}{P\{\tau_n>s\}}=\mathrm{e}^{-\lambda_n t}$$

so that the time already spent in a given state is immaterial. If one allows for a generic waiting time distribution, as appears in a renewal process, one obtains a class of non-Markovian jump processes in continuous time known as semi-Markov processes. They obey the socalled semi-Markov property

$$P\{X_{n+1}=j,T_{n+1}-T_n\leq\tau|X_0,T_0,X_1,T_1,...X_n,T_n\} = P\{X_{n+1}=j,T_{n+1}-T_n\leq\tau|X_n\}$$

with $X_n$ state entered at the $n$-th jump and $T_n$ time of the $n$-th jump. The process is characterized by the probability density to make the jump $n\rightarrow m$

$$q_{mn}(\tau) = \pi_{mn}f_n(\tau)$$

normalized according to

$$\sum_m \int_0^{+\infty} d\tau\ q_{mn}(\tau)=1$$

with state dependent waiting time distributions $f_n(\tau)$ and related survival probability

$$g_n(\tau)=1-\int_0^\tau \mathrm{ds}\ f_n(s).$$

The Markovian case is recovered for $f_n(\tau)=\lambda_n\mathrm{e}^{-\lambda_n\tau}$ and $g_n(\tau)=\mathrm{e}^{-\lambda_n\tau}$. The transition probabilities of the process can still be shown to obey a generalized master equation given by

$$\frac{\mathrm{d}}{\mathrm{dt}}P_n(t) = \int_0^t d\tau\sum_m [W_{nm}(\tau)P_m(t-\tau)-W_{mn}(\tau)P_n(t-\tau)]$$

with $W_{mn}(t)=\pi_{mn}k_n(t)$. The $k_n(t)$ are memory functions without a direct physical meaning, but related to waiting time distribution and survival probability according to

$$f_n(\tau)=\int_0^\tau \mathrm{ds}\ k_n(s)g_n(\tau-s)=(k_n*g_n)(\tau)$$
$$\dot{g}_n(\tau)=-\int_0^\tau \mathrm{ds}\ k_n(s)g_n(\tau-s)=-(k_n*g_n)(\tau)$$

or in Laplace transform

$$\begin{aligned}\hat{k}_n(u) &= \frac{\hat{f}_n(u)}{\hat{g}_n(u)}\\ \hat{k}_n(u) &= \frac{u\hat{f}_n(u)}{1-\hat{f}_n(u)}\end{aligned}$$

### 2.1.1 Examples

*1)* Consider a waiting time distribution corresponding to the sum of i.i.d. random variables with equal/different parameters $\lambda_n$ corresponding to socalled Erlang/generalized Erlang distributions.

For $n=1$, parameter $\lambda_1=\lambda$, we have an exponential waiting time distribution, so that

$$k_n(t) \;\rightarrow\; 2\lambda_n\delta(t),$$

a Markov process is recovered and the generalized master equation becomes a standard master equation with $\Gamma_{nm}=\pi_{nm}\lambda_n \geqslant 0$, so that they can be interpreted as transition probabilities per unit time.

For $n=2$, parameters $\lambda_1$, $\lambda_2$, we have from the convolution of two exponential distributions

$$f(\tau)=\frac{\lambda_1\lambda_2}{\lambda_2-\lambda_1}(\mathrm{e}^{-\lambda_1\tau}-\mathrm{e}^{-\lambda_2\tau}) \qquad k(t)=\lambda_1\lambda_2\mathrm{e}^{-(\lambda_1+\lambda_2)t},$$

where the latter kernel can be written as

$$k(t) = \kappa\mathrm{e}^{-\gamma t}$$

provided we have

$$\gamma^2-4\kappa\geqslant 0,$$

so that

$$\lambda_{1,2} = \frac{\gamma}{2}\pm\frac{1}{2}\sqrt{\gamma^2-4\kappa}$$

are positive parameters, and correspondingly

$$f(\tau) = \mathrm{e}^{-\gamma t/2}\left[\cosh\left(\frac{\gamma t}{2}\delta\right)+\frac{1}{\delta}\sinh\left(\frac{\gamma t}{2}\delta\right)\right]$$

with

$$\delta = \sqrt{1-4\frac{\kappa}{\gamma^2}}.$$

For greater $n$ one typically has kernels $k(t)$ which take on negative values. Indeed $k(t)$ need not be always positive in order to ensure the survival probability to be monotonically non-increasing.

*2)* Consider a waiting time distribution given by the convex mixture of exponential distributions.

For $n=2$, parameters $\lambda_1$, $\lambda_2$, weights $p, 1-p$

$$f(\tau)=p\lambda_1\mathrm{e}^{-\lambda_1\tau}+(1-p)\lambda_2\mathrm{e}^{-\lambda_2\tau} \qquad k(t)=\langle\lambda\rangle\left[2\delta(t)-\frac{\Delta\lambda^2}{\langle\lambda\rangle}\mathrm{e}^{-(p\lambda_2+(1-p)\lambda_1)t}\right].$$

## 2.2 Quantum semi-Markov processes

We now export these ideas to the quantum framework, building on the classical input to understand the memory kernel and on the previously introduced sufficient condition to ensure a CP dynamics. The point is to extend the generalized master equation to cope not only with populations but also with coherences.

Consider as before the structure

$$\frac{\mathrm{d}}{\mathrm{dt}}\rho(t) = \int_0^t \mathrm{d}\tau\mathcal{L}(t-\tau)\rho(\tau)$$

with

$$\mathcal{L}(\tau)\rho \;=\; -i[H(\tau),\rho]+\sum_k \gamma_k(\tau)\Big[L_k(\tau)\rho L_k^\dagger(\tau)-\frac{1}{2}\Big\{L_k^\dagger(\tau)L_k(\tau),\rho\Big\}\Big].$$

and the usual splitting $\mathcal{L}(\tau)=\mathcal{L}_R(\tau)+\mathcal{L}_J(\tau)$.

Suppose that the relaxing part can be diagonalized in a fixed basis

$$H(\tau) \;=\; \sum_n \varepsilon_n(\tau)|n\rangle\langle n|$$
$$\sum_k \gamma_k(\tau)L_k^\dagger(\tau)L_k(\tau) \;=\; \sum_n k_n(\tau)|n\rangle\langle n|$$

and $\gamma_k(\tau)\geqslant 0$ so that $\mathcal{L}_J(\tau)$ is a CP map and $k_n(\tau)\geqslant 0$. We can now write the explicit solution for the relaxing part in terms of matrices of functions

$$\mathcal{R}(t)\rho(0)=\sum_{nm} g_{nm}(t)|n\rangle\langle n|\rho(0)|m\rangle\langle m|$$

solutions of

$$\dot{g}_{nm}(t)=-\int_0^t d\tau[z_n(\tau)+z_m^*(\tau)]g_{nm}(t-\tau) \qquad z_n(\tau)=\frac{1}{2}k_n(\tau)+i\varepsilon_n(\tau)$$

with initial condition $g_{nm}(0)=1$. The map $\mathcal{R}(t)$ can be written in Kraus form provided

$$G(t) \;=\; (g_{nm}(t))\geqslant 0.$$

`Exercise: verify this CP condition`

But this requirement implies in particular that the diagonal matrix elements are positive, so that $g_{nn}(t)\geqslant 0$, which together with $k_n(t)\geqslant 0$ allows to read the $g_{nn}(t)$ as survival probability associated thorugh $k_n(t)$ to a well-defined waiting time distribution, thus fixing a classical semi-Markov process. The requirement $G(t)\geqslant 0$ is a natural extension of the classical condition to cope with coherences.

If this condition is satisfied, then according to

$$\Phi(t) \;=\; \mathcal{R}(t)+(\mathcal{R}\star\mathcal{L}_J\star\mathcal{R})(t)+(\mathcal{R}\star\mathcal{L}_J\star\mathcal{R}\star\mathcal{L}_J\star\mathcal{R})(t)+\ldots.$$

the dynamics is CP and therefore well-defined.

`Exercise: see what happens in the Markovian case`

### 2.2.1 Example

If $k_n=k\ \forall n$ the anticommutator part is proportional to the identity and we are left with

$$\mathcal{L}(\tau)\rho \;=\; k(\tau)[\mathcal{E}\rho-\rho]$$

where $\mathcal{E}$ is a CPT map. Coming back to the previous decoherence example we consider

$$\mathcal{E}\rho \;=\; \int \mathrm{d}q\mathcal{P}(q)\mathrm{e}^{iq\hat{x}}\rho\mathrm{e}^{iq\hat{x}}$$

and CP is granted provided the function $g(t)$, related to the memory kernel according to $\dot{g}(\tau)=-(k*g)(\tau)$ allows for a probabilistic reading. At any jump we apply the same operation $\mathcal{E}$, so that the underlying classical process is a renewal process, characterized by the waiting time distribution $f(\tau)$ obtained from

$$\hat{f}(u) \;=\; \frac{\hat{k}(u)}{u+\hat{k}(u)}.$$

The master equation reads

$$\frac{\mathrm{d}}{\mathrm{dt}}\rho(t) \;=\; \int_0^t \mathrm{d}\tau k(t-\tau)[\mathcal{E}\rho(\tau)-\rho(\tau)],$$

and its solution obeys the Dyson equation

$$\rho(t) \;=\; g(t)\rho(0)+\int_0^t \mathrm{d}\tau f(t-\tau)\mathcal{E}\rho(\tau),$$

with jump expansion

$$\begin{aligned}\rho(t) &= p_0(t)\rho(0)+\sum_{n=1}^{\infty}\int_0^t \mathrm{d}t_n\ldots\int_0^{t_2}\mathrm{d}t_1 f(t-t_n)\mathcal{E}f(t_n-t_{n-1})\ldots f(t_2-t_1)\mathcal{E}p_0(t_1)\rho(0)\\ &= \sum_{n=1}^{\infty} p_n(t)\mathcal{E}^n\rho(0)\end{aligned}$$

with $p_n(t)$ number of events up to time $t$, $p_0(t)=g(t)$ and for a general renewal process

$$p_n(t)=\int_0^t \mathrm{d}\tau f(t-\tau)p_{n-1}(\tau).$$

For a Poisson distribution $p_n(t)=\frac{(\lambda t)^n}{n!}\mathrm{e}^{-\lambda t}$, and one recovers the Markovian case.

For the position matrix elements this leads to

$$\langle x|\rho(t)|y\rangle \;=\; \sum_n p_n(t)\Phi_{\mathcal{P}}^n(x-y)\langle x|\rho(0)|y\rangle=\Psi(x-y,t)\langle x|\rho(0)|y\rangle$$

with $\Psi(x-y,t)$ characteristic function of renewal-reward process.

`Exercise: verify the above solution working in Laplace transform, and consider the position matrix elements`

The suppression of off-diagonal matrix elements has two typical regimes. For $\Psi(d,\,t)$ with $d\gg d_0$, where $d_0$ is the relevant scale settled by $\mathcal{P}(q)$, we have strong decoherence, a single interaction event already suppresses the off-diagonal matrix element

$$\Psi(d,t)\cong p_0(t)=g(t)$$

and the relevant quantity is the survival probability, exponential in time for the Markovian case. For $\Psi(d,t)$ with $d\ll d_0$ we have weak decoherence, many interaction events build up the overall effect and exploiting the central limit theorem for renewal processes we have

$$\Psi(d,t)\cong\exp\left[-\frac{1}{2}\left(\Delta q^2+\frac{\sigma^2}{\mu^2}\langle q\rangle^2\right)\frac{t}{\mu}d^2+i\langle q\rangle\frac{t}{\mu}d\right]$$

with $\mu,\sigma$ mean and variance of the waiting time distribution (related by $\sigma^2=\mu^2$ for the Markovian case), while $\langle q\rangle,\Delta q$ denote mean and variance of $\mathcal{P}(q)$.

### 2.2.2 Example

Consider a master equation for a two-level system of the form

$$\mathcal{L}(\tau)\rho \;=\; -i\varepsilon(\tau)[\sigma_+\sigma_-,\rho]+k(\tau)\left[\sigma_-\rho\sigma_+-\frac{1}{2}\{\sigma_+\sigma_-,\rho\}\right]$$

so that $k_+=k$, $k_-=0$, $\varepsilon_+=\varepsilon$, $\varepsilon_-=0$. The matrix reads

$$G(t)=\begin{pmatrix} g_{++}(t) & g_{+-}(t)\\ g_{+-}^*(t) & 1\end{pmatrix}$$

and therefore the sufficient condition for CP becomes

$$g_{++}(t)\geq|g_{+-}(t)|^2,$$

which actually turns out to be also necessary, as seen from an exact solution.

**Exponential memory kernel**

For $\varepsilon(\tau)=0$ and $k(\tau)=\kappa\mathrm{e}^{-\gamma\tau}$

$$\mathcal{L}(\tau)\rho \;=\; \kappa\mathrm{e}^{-\gamma\tau}\left[\sigma_-\rho\sigma_+-\frac{1}{2}\{\sigma_+\sigma_-,\rho\}\right]$$

the sufficient condition is satisfied for $\gamma^2 - 4\kappa \geqslant 0$, which is the classical condition to read a semi-Markov process from the diagonal matrix elements, but this condition now is both necessary and sufficient. A similar condition $\gamma^2 - 4n\kappa \geqslant 0$ applies for the convolution of the Lindblad master equation for the damped harmonic oscillator with an exponential memory kernel

$$\mathcal{L}(\tau)\rho \;=\; \kappa \mathrm{e}^{-\gamma\tau}\left[a\rho a^\dagger - \frac{1}{2}\{a^\dagger a, \rho\}\right]$$

but now due to the infinite dimensionality of the Hilbert space the condition is never satisfied.

**Negative memory kernel still granting CP**

Assume the relaxation part is diagonalized as before, but the $\gamma_k$ and therefore the $k_n$ are no more necessarily positive. As a consequence $\mathcal{L}_J(\tau)$ is no more CP. We can then exploit the weaker requirement $\mathcal{R}\star\mathcal{L}_J$ to be CP. Setting

$$\mathcal{L}_J(\tau) \;=\; \sum_l k_l(\tau)\mathcal{J}_l$$

with $\mathcal{J}_l$ CP the condition can be explicitated. Due to

$$\begin{aligned}(\mathcal{R}\star\mathcal{L}_J)(t)\rho(0) &= \int_0^t \mathrm{d}\tau \mathcal{R}(t-\tau)\sum_l k_l(\tau)\mathcal{J}_l\rho(0) \\ &= \sum_l \sum_{nm} \underbrace{\int_0^t \mathrm{d}\tau g_{nm}(t-\tau)k_l(\tau)}_{f^l_{nm}(t)}|n\rangle\langle n|\mathcal{J}_l\rho(0)|m\rangle\langle m|\end{aligned}$$

the conditions

$$\begin{aligned} F^l(t) = \big(f^l_{nm}(t)\big) \geqslant 0 \qquad \forall l \\ G(t) = (g_{nm}(t)) \geqslant 0 \end{aligned}$$

together ensure CP, granting in particular a classical probabilistic reading for the diagonals $f^l_{nn}(t)$ and $g_{nn}(t)$.

**Necessary and sufficient condition for CP**

Consider now $\varepsilon_n = 0$ and

$$\mathcal{J}_n\rho \;=\; \sum_m \pi_{mn}|m\rangle\langle n|\rho|n\rangle\langle m|$$

so that

$$\mathcal{L}(\tau)\rho \;=\; \sum_{mn} \pi_{mn}k_n(\tau)|m\rangle\langle n|\rho|n\rangle\langle m| - \frac{1}{2}\sum_n k_n(\tau)\{|n\rangle\langle n|, \rho\}.$$

For this kernel populations and coherences decouple, so that the coherences are given as before by

$$\rho_{nm}(t) = g_{nm}(t)\rho_{nm}(0), \qquad n \neq m$$

while assuming the populations follow a classical semi-Markov process the diagonal matrix elements are given by

$$\rho_{nn}(t) = \sum_m T_{nm}(t)\rho_{mm}(0)$$

with $T_{nm}(t)$ classical transition probability. We thus have

$$\begin{aligned}\rho(t) &= \sum_{n\neq m} g_{nm}(t)|n\rangle\langle n|\rho(0)|m\rangle\langle m| + \sum_{mn} T_{nm}(t)|n\rangle\langle m|\rho(0)|m\rangle\langle n| \\ &= \sum_{nm} \tilde{g}_{nm}(t)|n\rangle\langle n|\rho(0)|m\rangle\langle m| + \sum_{n\neq m} T_{nm}(t)|n\rangle\langle m|\rho(0)|m\rangle\langle n|\end{aligned}$$

with $\tilde{g}_{nm}(t) = (T_{nn}(t) - g_{nn}(t))\delta_{nm} + g_{nm}(t)$. Given that $T_{nm}(t) \geqslant 0$ the necessary and sufficient requirement for CP now becomes

$$\tilde{G}(t) = (\tilde{g}_{nm}(t)) \geq 0$$

indeed weaker than

$$G(t) \;=\; (g_{nm}(t)) \geqslant 0$$

since it differs on the diagonals and the transition probability is greater or equal than the survival probability, unless one only has jumps in one direction.

This necessary and sufficient condition also helps in understanding phenomenological Ansatz. Indeed an example in this framework is given by

$$\mathcal{K}(\tau)\rho \;=\; \kappa_+ \mathrm{e}^{-\gamma\tau}\left[\sigma_-\rho\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-,\rho\}\right] + \kappa_- \mathrm{e}^{-\gamma\tau}\left[\sigma_+\rho\sigma_- - \frac{1}{2}\{\sigma_-\sigma_+,\rho\}\right],$$

the classical condition now reads $\frac{\gamma^2}{4} \geq \max\{\kappa_+,\kappa_-\}$. A natural parametrization is given by

$$\kappa_+ \;=\; \gamma\gamma_0(N_\beta + 1)$$
$$\kappa_- \;=\; \gamma\gamma_0 N_\beta$$

so that $\kappa_+ \geqslant \kappa_- \geqslant 0$. Exploiting the necessary and sufficient condition one sees that for $\kappa_- = 0$ corresponding to $T = 0$ one never has CP, due to violation at short times, for $T \neq 0$ a well defined CP dynamics is granted for not too low temperatures. Thus the analysis gives information on the region of validity of the phenomenological Ansatz.

### 2.3 References

For this part see mainly [Breuer2007, Barnett2001a, Budini2004a, Shabani2005a, Budini2006a, Maniscalco2006a, Maniscalco2007a, Breuer2008a, Breuer2009a, Kossakowski2009a, Chruscinski2010a, Mazzola2010a, Haikka2010a]

## 3 Projection operator techniques

**Abstract**

We consider a general approach to the non-Markovian dynamics of open quantum systems. This is based on projection operator techniques of nonequilibrium statistical mechanics, which allow to recast the equations of motion of the system as a perturbation expansion. Both the Nakajima-Zwanzig and the time-convolutionless approaches will be considered, focusing on the model of a qubit coupled to a Bosonic reservoir.

### 3.1 Projection operators

The basic idea comes from nonequilibrium statistical mechanics: we have a complex system and try to obtain a manageable dynamics by eliminating degrees of freedom by means of some projection operator, thus considering the dynamics or relevant variables only, to be described in terms of effective master equations.

A projection operator is a map which sends states into states

$$\mathcal{P}\colon \rho \mapsto \rho' = \mathcal{P}\rho$$

which is linear, idempotent $\mathcal{P}^2 = \mathcal{P}$, positive and trace preserving. Having in mind that $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_E$ we consider projection operators of the form

$$\mathcal{P} \;=\; \mathbb{1}_S \otimes \Lambda$$

with $\Lambda$ a CPT idempotent map on $\mathcal{H}_E$. This choice implies in particular that separable (product) states are sent to separable (product) states, so that the space of separable (product) states is invariant under $\mathcal{P}$, no artificial entanglement is introduced. One exploits furthermore the crucial property

$$\rho_S = \mathrm{Tr}_E\rho = \mathrm{Tr}_E\mathcal{P}\rho$$

so that knowledge of the dynamics of the relevant part is enough to recover the reduced state $\rho_S$. A representation theorem can be formulated for a projection operator as above.

**Theorem (Breuer)** A projection operator with the above properties can be written as

$$\mathcal{P}\rho \;=\; \sum_i \mathrm{Tr}_E\{A_i\rho\}\otimes B_i$$

with $\{A_i\},\{B_i\}$ linear independet sets of observables with the properties

1. $\mathrm{Tr}_E\{A_iB_i\}=\delta_{ij}$
2. $\sum_i \mathrm{Tr}_E\{B_i\}A_i=\mathbb{1}_E$
3. $\sum_i A_i^T\otimes B_i\geqslant 0$

### 3.1.1 Standard projection

Standard projection operator onto a factorized state is obtained for

$$A=\mathbb{1}_E \qquad B=\rho_E$$

for a fixed environmental state

$$\mathcal{P}\rho \;=\; \mathrm{Tr}_E\rho\otimes\rho_E=\rho_S\otimes\rho_E$$

### 3.1.2 Correlated projection

Correlated projection operator is obtained considering an orthogonal decomposition of unity in $\mathcal{H}_E$ according to $\Pi_i=\Pi_i^\dagger$, $\Pi_i\Pi_j=\delta_{ij}\Pi_i$, $\sum_i \Pi_i=\mathbb{1}_E$, and defining

$$A_i=\Pi_i \qquad B_i=\frac{\Pi_i\rho_E\Pi_i}{\mathrm{Tr}_E\{\Pi_i\rho_E\}}=\rho_E^i$$

with $\rho_E^i$ collection of statistical operators obtained from fixed environmental state $\rho_E$

$$\mathcal{P}\rho \;=\; \sum_i \mathrm{Tr}_E\{\Pi_i\rho_E\}\otimes\frac{\Pi_i\rho_E\Pi_i}{\mathrm{Tr}_E\{\Pi_i\rho_E\}}.$$

## 3.2 Projected equations of motion

For the overall complex system one has the Liouville von Neumann equation with $H=H_0+\alpha V$ and therefore in interaction picture with $V(t)=\mathrm{e}^{iH_0t}V\mathrm{e}^{-iH_0t}$

$$\frac{\mathrm{d}}{\mathrm{dt}}\rho(t) \;=\; -i\alpha[V(t),\rho(t)]\equiv\mathcal{L}(t)\rho(t).$$

We now use $\mathcal{P}$ and the complementary projection operator $\mathbb{1}-\mathcal{Q}$ to write the statistical operator in terms of a relevant and irrelevat part $\rho=\mathcal{P}\rho+\mathcal{Q}\rho$ obeying

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{dt}}\mathcal{P}\rho(t) &= \mathcal{P}\mathcal{L}(t)\mathcal{P}\rho(t)+\mathcal{P}\mathcal{L}(t)\mathcal{Q}\rho(t)\\ \frac{\mathrm{d}}{\mathrm{dt}}\mathcal{Q}\rho(t) &= \mathcal{Q}\mathcal{L}(t)\mathcal{P}\rho(t)+\mathcal{Q}\mathcal{L}(t)\mathcal{Q}\rho(t).\end{aligned}$$

The second equation can be solved as

$$\mathcal{Q}\rho(t) \;=\; \mathcal{G}_{\mathcal{Q}}(t,0)\mathcal{Q}\rho(0)+\int_0^t \mathrm{dt}_1\mathcal{G}_{\mathcal{Q}}(t,t_1)\mathcal{Q}\mathcal{L}(t_1)\mathcal{P}\rho(t_1)$$

with

$$\mathcal{G}_{\mathcal{Q}}(t,t_1) \;=\; \vec{T}\exp\left(\int_{t_1}^t \mathrm{dt}_2\mathcal{Q}\mathcal{L}(t_2)\right),$$

where $\vec{T}$ denotes chronological time ordering.

Substituting in the first equation and using the natural simplifying assumptions
i) $\mathcal{Q}\rho(0)$
ii) $\mathcal{P}\mathcal{L}(t_1)...\mathcal{L}(t_{2n+1})\mathcal{P}=0$
one has

$$\frac{\mathrm{d}}{\mathrm{dt}}\mathcal{P}\rho(t) \;=\; \int_0^t \mathrm{dt}_1\mathcal{P}\mathcal{L}(t)\mathcal{G}_{\mathcal{Q}}(t,t_1)\mathcal{L}(t_1)\mathcal{P}\rho(t_1)$$

and we want to obtain perturbation expansions of this equation, allowing for approximate solutions, recalling that $\mathrm{Tr}_E\mathcal{P}\rho(t) = \rho_S(t)$. This equation is exact and different choices of $\mathcal{P}$ lead to equations for different relevant states, which all lead to the same exact equation for $\rho_S$, though rearranged in a non perturbative way. There are two ways to express the exact equations of motion for the dynamics of $\rho(t) = \Phi(t)\rho(0)$:

*Integrodifferential*

$$\frac{\mathrm{d}}{\mathrm{dt}}\rho(t) = (\mathcal{K}_{\mathrm{NZ}} \star \rho)(t) = (\mathcal{K}_{\mathrm{NZ}} \star \Phi)(t)\rho(0)$$

which in Laplace transform leads to

$$\hat{\mathcal{K}}_{\mathrm{NZ}}(u) = u\mathbb{1} - \hat{\Phi}^{-1}(u)$$

*Time local*

$$\frac{\mathrm{d}}{\mathrm{dt}}\rho(t) = \mathcal{K}_{\mathrm{TCL}}(t)\rho(t) = \mathcal{K}_{\mathrm{TCL}}(t)\Phi(t)\rho(0)$$

with

$$\mathcal{K}_{\mathrm{TCL}}(t) = \dot{\Phi}(t)\Phi^{-1}(t).$$

Let us explore these two possibilities.

## 3.3 Nakajima-Zwanzig master equation

Our master equation for $\mathcal{P}\rho(t)$ is already of the form

$$\frac{\mathrm{d}}{\mathrm{dt}}\mathcal{P}\rho(t) = \int_0^t \mathrm{dt}_1 \mathcal{K}_{\mathrm{NZ}}(t,t_1)\mathcal{P}\rho(t_1)$$

where the memory kernel is given by

$$\mathcal{K}_{\mathrm{NZ}}(t,t_1) = \mathcal{P}\mathcal{L}(t)\mathcal{G}_{\mathcal{Q}}(t,t_1)\mathcal{L}(t_1)\mathcal{P}$$

and admits an expansion relying on the one of $\mathcal{G}_{\mathcal{Q}}(t,t_1)$

$$\begin{aligned}\mathcal{G}_{\mathcal{Q}}(t,t_1) &= \vec{T}\exp\left(\int_{t_1}^t \mathrm{dt}_2 \mathcal{Q}\mathcal{L}(t_2)\right)\\ &= \mathbb{1} + \int_{t_1}^t \mathrm{dt}_2\mathcal{Q}\mathcal{L}(t_2) + \int_{t_1}^t \mathrm{dt}_2 \int_{t_1}^{t_2} \mathrm{dt}_3 \mathcal{Q}\mathcal{L}(t_2)\mathcal{Q}\mathcal{L}(t_3) + \ldots\end{aligned}$$

so that we can write $\mathcal{K}_{\mathrm{NZ}} = \mathcal{K}_{\mathrm{NZ}}^{(2)} + \mathcal{K}_{\mathrm{NZ}}^{(4)} + \ldots$ with

$$\begin{aligned}\mathcal{K}_{\mathrm{NZ}}^{(2)}(t,t_1) &= \mathcal{P}\mathcal{L}(t)\mathcal{L}(t_1)\mathcal{P}\\ \mathcal{K}_{\mathrm{NZ}}^{(4)}(t,t_1) &= \int_{t_1}^t \mathrm{dt}_2 \int_{t_1}^{t_2} \mathrm{dt}_3 [\mathcal{P}\mathcal{L}(t)\mathcal{L}(t_2)\mathcal{L}(t_3)\mathcal{L}(t_1)\mathcal{P} - \mathcal{P}\mathcal{L}(t)\mathcal{L}(t_2)\mathcal{P}\mathcal{L}(t_3)\mathcal{L}(t_1)\mathcal{P}]\end{aligned}$$

The Nakajima-Zwanzig master equation to second order for $\rho_S(t)$, obtained by taking the partial trace reads

$$\frac{\mathrm{d}}{\mathrm{dt}}\rho_S(t) = -\int_0^t \mathrm{dt}_1 \mathrm{Tr}_E\{\mathcal{P}[V(t),[V(t_1),\mathcal{P}\rho(t_1)]]\}$$

and for $\mathcal{P}\rho \to \sum_i \mathrm{Tr}_E\{A_i\rho\} \otimes B_i$

$$\frac{\mathrm{d}}{\mathrm{dt}}\rho_S(t) = -\int_0^t \mathrm{dt}_1 \sum_j \mathrm{Tr}_E\{B_j\}\mathrm{Tr}_E\left\{A_j\left[V(t),\left[V(t_1),\sum_i \mathrm{Tr}_E\{A_i\rho(t_1)\}\otimes B_i\right]\right]\right\}.$$

*Standard projection*

$A \to \mathbb{1}_E$, $B \to \rho_E$

$$\frac{\mathrm{d}}{\mathrm{dt}}\rho_S(t) = -\int_0^t \mathrm{dt}_1 \mathrm{Tr}_E\{[V(t),[V(t_1),\rho_S(t_1)\otimes\rho_E]]\}$$

*Correlated projection*

$A_i \to \Pi_i$, $B_i \to \rho_E^i$

$$\frac{\mathrm{d}}{\mathrm{dt}} w_j(t) = -\int_0^t \mathrm{dt}_1 \mathrm{Tr}_E \left\{ \Pi_j \left[ V(t), \left[ V(t_1), \sum_i w_i(t_1) \otimes \rho_E^i \right] \right] \right\}.$$

where $w_i(t) = \mathrm{Tr}_E\{\Pi_i \rho\}$ so that $\rho_S(t) = \sum_i w_i(t)$.

## 3.4 Time-convolutionless master equation

To obtain a master equation for $\mathcal{P}\rho(t)$ local in time as suggested we have to consider a backward in time propagator for the full dynamics, so that

$$\rho(t_1) = \mathcal{G}(t, t_1)\rho(t)$$

for $t_1 < t$, given by

$$\mathcal{G}(t, t_1) = \overleftarrow{T} \exp\left( - \int_{t_1}^t \mathrm{dt}_2 \mathcal{L}(t_2) \right)$$

with antichronological time ordering. Inserting in the equation for $\mathcal{P}\rho(t)$ we have

$$\frac{\mathrm{d}}{\mathrm{dt}} \mathcal{P}\rho(t) = \mathcal{P}\mathcal{L}(t) \underbrace{\int_0^t \mathrm{dt}_1 \mathcal{G}_{\mathcal{Q}}(t, t_1) \mathcal{L}(t_1) \mathcal{P} \mathcal{G}(t, t_1)}_{\Sigma(t)} (\mathcal{P} + \mathcal{Q})\rho(t)$$

With this definition of $\Sigma(t)$ the previously obtained expression of $\mathcal{Q}\rho(t)$ becomes

$$\mathcal{Q}\rho(t) = \Sigma(t)(\mathcal{P} + \mathcal{Q})\rho(t)$$

and provided the inverse of $\mathbb{1} - \Sigma(t)$ exists (always true for short times since $\Sigma(0) = 0$ and weak coupling since $\Sigma(t)_{|\alpha=0} = 0$) one has

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{dt}} \mathcal{P}\rho(t) &= \left\{ \mathcal{P}\mathcal{L}(t) \frac{\mathbb{1}}{\mathbb{1} - \Sigma(t)} \mathcal{P} \right\} \mathcal{P}\rho(t) \\ &= \mathcal{K}_{\mathrm{TCL}}(t) \mathcal{P}\rho(t) \end{aligned}$$

but according to

$$\frac{\mathbb{1}}{\mathbb{1} - \Sigma(t)} = \sum_{n=0}^{\infty} \Sigma^n(t)$$

and

$$\Sigma(t) = \int_0^t \mathrm{dt}_1 \mathcal{G}_{\mathcal{Q}}(t, t_1) \mathcal{L}(t_1) \mathcal{P} \mathcal{G}(t, t_1)$$

one obtains a perturbation expansion $\mathcal{K}_{\mathrm{TCL}} = \mathcal{K}_{\mathrm{TCL}}^{(2)} + \mathcal{K}_{\mathrm{TCL}}^{(4)} + \ldots$with

$$\begin{aligned} \mathcal{K}_{\mathrm{TCL}}^{(2)}(t) &= \int_0^t \mathrm{dt}_1 \mathcal{P}\mathcal{L}(t)\mathcal{L}(t_1)\mathcal{P} \\ \mathcal{K}_{\mathrm{TCL}}^{(4)}(t) &= \int_0^t d t_1 \int_0^{t_1} d t_2 \int_0^{t_2} d t_3 [\mathcal{P}\mathcal{L}(t)\mathcal{L}(t_1)\mathcal{L}(t_2)\mathcal{L}(t_3)\mathcal{P} - \mathcal{P}\mathcal{L}(t)\mathcal{L}(t_1)\mathcal{P}\mathcal{L}(t_2)\mathcal{L}(t_3)\mathcal{P} \\ &\quad - \mathcal{P}\mathcal{L}(t)\mathcal{L}(t_2)\mathcal{P}\mathcal{L}(t_1)\mathcal{L}(t_3)\mathcal{P} - \mathcal{P}\mathcal{L}(t)\mathcal{L}(t_3)\mathcal{P}\mathcal{L}(t_1)\mathcal{L}(t_2)\mathcal{P}]. \end{aligned}$$

An important fact is that for the TCL expansion one has an explicit though cumbersome recipe to directly express the $n$-th contribution

$$\mathcal{K}_{\mathrm{TCL}}^{(n)} = \int_0^t \mathrm{dt}_1 \int_0^{t_1} \mathrm{dt}_2 \ldots \int_0^{t_{n-2}} \mathrm{dt}_{n-1} \langle \mathcal{L}(t) \ldots \mathcal{L}(t_{n-1}) \rangle_{\mathrm{oc}}$$

in terms of socalled ordered cumulants.

The time-convolutionless master equation to second order for $\rho_S(t)$, obtained by taking the partial trace, reads

$$\frac{\mathrm{d}}{\mathrm{dt}} \rho_S(t) = -\int_0^t \mathrm{dt}_1 \mathrm{Tr}_E\{\mathcal{P}[V(t), [V(t_1), \mathcal{P}\rho(t)]]\}$$

and for $\mathcal{P}\rho \rightarrow \sum_i \mathrm{Tr}_E\{A_i\rho\} \otimes B_i$

$$\frac{\mathrm{d}}{\mathrm{dt}}\rho_S(t) = -\int_0^t \mathrm{dt}_1 \sum_j \mathrm{Tr}_E\{B_j\}\mathrm{Tr}_E\left\{A_j\left[V(t),\left[V(t_1),\sum_i \mathrm{Tr}_E\{A_i\rho(t)\} \otimes B_i\right]\right]\right\}.$$

*Standard projection*
$A \rightarrow \mathbb{1}_E$, $B \rightarrow \rho_E$

$$\frac{\mathrm{d}}{\mathrm{dt}}\rho_S(t) = -\int_0^t \mathrm{dt}_1 \mathrm{Tr}_E\{[V(t),[V(t_1),\rho_S(t)\otimes\rho_E]]\}$$

*Correlated projection*
$A_i \rightarrow \Pi_i$, $B_i \rightarrow \rho_E^i$

$$\frac{\mathrm{d}}{\mathrm{dt}}w_j(t) = -\int_0^t \mathrm{dt}_1 \mathrm{Tr}_E\left\{\Pi_j\left[V(t),\left[V(t_1),\sum_i w_i(t)\otimes\rho_E^i\right]\right]\right\}.$$

where $w_i(t) = \mathrm{Tr}_E\{\Pi_i\rho\}$, so that $\rho_S(t) = \sum_i w_i(t)$

## 3.5 Explicit treatment of damped Jaynes-Cummings model

We consider the exact explicit expression of time-convolutionless (TCL) and Nakajima-Zwanzig (NZ) master equation for a specific instructive model, the damped Jaynes-Cummings. We have $H_S = \omega_0\sigma_+\sigma_-$, $H_E = \omega b^\dagger b$ with interaction

$$H_I = \sigma_+ \otimes \sum_k g_k b_k + h.c. = \sigma_+ \otimes B + h.c.$$

thanks to the rotating wave approximation in the coupling the model can be solved analytically for Boson bath initially in the vacuum.

**Born approximation**

Let us first look at the Born, second order approximation in projection operator technique, assuming a standard projection with $\rho_E = |0\rangle\langle 0|$. NZ to second order in iteraction picture reads

$$\frac{\mathrm{d}}{\mathrm{dt}}\rho(t) = \int_0^t \mathrm{dt}_1 2f(t-t_1)\left[\sigma_-\rho(t_1)\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-,\rho(t_1)\}\right]$$

and therefore TCL to second order

$$\frac{\mathrm{d}}{\mathrm{dt}}\rho(t) = \int_0^t \mathrm{dt}_1 2f(t-t_1)\left[\sigma_-\rho(t)\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-,\rho(t)\}\right].$$

The function $f(t)$ is the relevant correlation function of the model, given by the vacuum expectation value of product of field operators

$$\begin{aligned} f(t-t_1) &= e^{i\omega_0(t-t_1)}\langle 0|B(t)B^\dagger(t_1)|0\rangle \\ &= \sum_k |g_k|^2 e^{i(\omega_0-\omega_k)(t-t_1)} \\ &= \int \mathrm{d}\omega J(\omega) e^{i(\omega_0-\omega)(t-t_1)} \end{aligned}$$

with $J(\omega) = \sum_k |g_k|^2\delta(\omega-\omega_k)$ the spectral density given by sum of (coupling strength)$^2$ $\times$ (density of modes). The typical expression is Lorentzian

$$J(\omega) = \frac{1}{2\pi}\frac{\gamma_0\lambda^2}{(\omega_0-\omega-\Delta)+\lambda^2}$$

where $\Delta$ denotes detuning from resonance. Here $1/\tau_E = \lambda$ the spectral width, $1/\tau_S = \gamma_0$ the relaxation time, and the coupling strength or expansion parameter is $\alpha = \tau_E/\tau_S = \gamma_0/\lambda$. The corresponding correlation function is an exponential

$$f(t-t_1) = \frac{1}{2}\gamma_0\lambda \mathrm{e}^{-\lambda|t-t_1|}\mathrm{e}^{i\Delta(t-t_1)}.$$

In the Markov approximation $\gamma_0 \ll \lambda$, one has $f(t-t_1) \to \gamma_0 \delta(t-t_1)$ and one obtains the Lindblad master equation

$$\frac{\mathrm{d}}{\mathrm{dt}}\rho(t) = \gamma_0 \left[\sigma_- \rho(t)\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-, \rho(t)\}\right].$$

**Exact solution**

Due to conservation of the number of excitations $N = \sigma_+\sigma_- + \sum_k b_k^\dagger b_k$ the model can be exactly solved, since for initial vacuum state the dynamics is restricted to a finite dimensional subspace. We can solve the Schrödinger equation

$$\frac{\mathrm{d}}{\mathrm{dt}}|\Psi(t)\rangle = -i\, H_I(t)|\Psi(t)\rangle$$

observing that initial states with the structure

$$|\Psi(0)\rangle = c_0|0\rangle \otimes |0\rangle_E + c_1(0)|1\rangle \otimes |0\rangle_E + \sum_k c_k(0)|0\rangle \otimes |k\rangle_E$$

are preserved in form with time. For $c_k(0) = 0$ so that the initial state is factorized one is lead upon substitution in the Schrödinger equation to solve the coupled equations

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{dt}} c_1(t) &= -i \sum_k g_k e^{i(\omega_0 - \omega_k)t} c_k(t) \\ \frac{\mathrm{d}}{\mathrm{dt}} c_k(t) &= -i\, g_k^* e^{-i(\omega_0 - \omega_k)t} c_1(t) \end{aligned}$$

and therefore $\dot{c}_1(t) = -(f \star c_1)(t)$. Let $G(t)$ be the solution of

$$\dot{G}(t) = -(f \star G)(t)$$

with initial condition $G(0) = 1$, so that $c_1(t) = G(t)c_1(0)$. Then one has

$$\begin{aligned} \rho(t) &= \mathrm{Tr}_E\{|\Psi(t)\rangle\langle\Psi(t)|\} \\ &= \begin{pmatrix} |G(t)|^2 \rho_{11}(0) & G(t)\rho_{10}(0) \\ G^\star(t)\rho_{01}(0) & \rho_{00}(0) + (1 - |G(t)|^2)\rho_{11}(0) \end{pmatrix} \end{aligned}$$

which actually is the general solution since any state can be expressed as mixture of pure states, and $G(t)$ does not depend on the initial condition.

**Exact TCL and NZ equations**

Given now the exact time evolution mapping

$$\Phi(t)\colon \rho(0) \to \rho(t) = \Phi(t)\rho(0)$$

we can construct the exact TCL and NZ equation, exploiting the above introduced relations

$$\mathcal{K}_{\mathrm{TCL}}(t) = \dot{\Phi}(t)\Phi^{-1}(t)$$

and

$$\hat{\mathcal{K}}_{\mathrm{NZ}}(u) = u\mathbb{1} - \hat{\Phi}^{-1}(u).$$

This can be done considering a matrix representation of $\Phi(t)$. The latter can be obtained considering its action on a basis of operators in $\mathbb{C}^2$, given by $\{X_i\} = \left\{\frac{1}{\sqrt{2}}\mathbb{1}, \frac{1}{\sqrt{2}}\sigma_i\right\}_{i=1,2,3}$, orthonormal according to $\mathrm{Tr}_S\{X_i X_j\} = \delta_{ij}$. We then have

$$\Phi[\rho] = \sum_{kl} F_{kl} \mathrm{Tr}_S\left\{X_l^\dagger \rho\right\} X_k$$

with $F_{kl} = \mathrm{Tr}_S\left\{X_k^\dagger \Phi[X_l]\right\}$. In terms of the matrix $F = (F_{kl})$ our relations become

$$\mathcal{K}_{\mathrm{TCL}}(t) = \dot{F}(t) F^{-1}(t)$$

and

$$\hat{\mathcal{K}}_{\mathrm{NZ}}(u) = u\mathbb{1} - \hat{F}^{-1}(u).$$

Given the expression of these matrices providing the action of $\Phi$ on $\rho$ though its coefficients in a given operator basis, we can obtain a corresponding expression of $\Phi$ as superoperator acting on $\rho$ as an operator. For the case at hand the TCL result is

$$\mathcal{K}_{\mathrm{TCL}}(t) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -\frac{\gamma}{2} & -\frac{\varepsilon}{2} & 0 \\ 0 & +\frac{\varepsilon}{2} & +\frac{\gamma}{2} & 0 \\ \gamma & 0 & 0 & -\gamma \end{pmatrix}$$

with

$$\varepsilon(t) + i\gamma(t) = -2\left[\frac{\dot{G}(t)}{G(t)}\right]$$

so that

$$\varepsilon(t) = -2\mathrm{Im}\left[\frac{\dot{G}(t)}{G(t)}\right]$$
$$\gamma(t) = -2\mathrm{Re}\left[\frac{\dot{G}(t)}{G(t)}\right]$$

which in operator form reads

$$\mathcal{K}_{\mathrm{TCL}}(t)\rho = -\frac{i}{2}\varepsilon(t)[\sigma_+\sigma_-, \rho] + \gamma(t)\left[\sigma_-\rho\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-, \rho\}\right].$$

Similarly though with more calculations for the NZ case

$$\hat{\mathcal{K}}_{\mathrm{NZ}}(u) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -\widehat{\mathrm{Re}\, f}(u) & -\widehat{\mathrm{Im}\, f}(u) & 0 \\ 0 & \widehat{\mathrm{Im}\, f}(u) & -\widehat{\mathrm{Re}\, f}(u) & 0 \\ \hat{k}_1(u) & 0 & 0 & \hat{k}_1(u) \end{pmatrix}$$

where the function

$$\hat{k}_1(u) = \frac{1 - u\widehat{|G|^2}(u)}{\widehat{|G|^2}(u)}$$

is the solution of the convolution equation

$$\frac{\mathrm{d}}{\mathrm{dt}}|G(t)|^2 = -\left(k_1 * |G|^2\right)(t)$$

so that in operator form one has

$$\frac{\mathrm{d}}{\mathrm{dt}}\rho(t) = (\mathcal{K}_{\mathrm{NZ}} \star \rho)(t)$$

with

$$\begin{aligned} \mathcal{K}_{\mathrm{NZ}}(\tau)\rho = & -i\,\mathrm{Im}\, f(\tau)[\sigma_+\sigma_-, \rho] \\ & + k_1(\tau)\left[\sigma_-\rho\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-, \rho\}\right] \\ & + \frac{1}{4}k_2(\tau)[\sigma_z\rho\sigma_z - \rho] \end{aligned}$$

and

$$k_1(\tau) + k_2(\tau) = 2\,\mathrm{Re}\, f$$

One already notices the different operator structures in the two master equations.

**Exact evolution for Lorentzian spectral density**

Recall that according to

$$\rho(t) \;=\; \begin{pmatrix} |G(t)|^2\rho_{11}(0) & G(t)\rho_{10}(0) \\ G^\star(t)\rho_{01}(0) & \rho_{00}(0)+(1-|G(t)|^2)\rho_{11}(0) \end{pmatrix}$$

the overall dynamics is know upon knowledge of $G$ obeying

$$\dot{G}(t) \;=\; -(f\star G)(t)$$

which for our Lorentzian spectral density reads

$$G(t) \;=\; \mathrm{e}^{-\lambda t/2}\left[\cosh\left(\frac{\lambda t}{2}\delta\right)+\frac{1}{\delta}\sinh\left(\frac{\lambda t}{2}\delta\right)\right],$$

with $\delta=\sqrt{1-2\gamma_0/\lambda}$. In the weak coupling regime $\gamma_0/\lambda<2$ one has $\delta\in\mathbb{R}$, so that $G(t)$ is always positive. In the strong coupling regime $\gamma_0/\lambda>2$ one has $\delta\in i\mathbb{R}$, so that $G(t)$ oscillates between positive and negative values going through zero.

**TCL for Lorentzian spectral density**

For a typical spectral density and therefore correlation function we can provide explicit expressions, which upon expansion in the coupling coefficient $\alpha=\gamma_0/\lambda$ allow to recover the perturbation expansion and compare it with the exact result.

For a Lorentzian spectral density on resonance for the TCL case one has

$$\begin{aligned}\varepsilon(t) &= 0\\ \gamma(t) &= 2\gamma_0\frac{\sinh\left(\frac{\lambda t}{2}\delta\right)}{\delta\cosh\left(\frac{\lambda t}{2}\delta\right)+\sinh\left(\frac{\lambda t}{2}\delta\right)}\end{aligned}$$

with $\delta=\sqrt{1-2\gamma_0/\lambda}$, so that correctly in the Markov approximation for $\lambda\gg\gamma_0$ one has $\gamma\to\gamma_0$. The master equation reads

$$\frac{\mathrm{d}}{\mathrm{dt}}\rho(t) \;=\; \gamma(t)\left[\sigma_-\rho(t)\sigma_+-\frac{1}{2}\{\sigma_+\sigma_-,\rho(t)\}\right].$$

In the weak coupling regime $\gamma_0/\lambda<2$ one has $\delta\in\mathbb{R}$, so that $\gamma(t)$ is always positive and grows monotonically to the Markovian value (for $\gamma_0/\lambda\ll1$). In the strong coupling regime $\gamma_0/\lambda>2$ one has $\delta\in i\mathbb{R}$, so that $\gamma(t)$ oscillates between positive and negative values, actually diverging at given points when strictly on resonance, reaching for long times a Markovian approximation for finite detuning. Considering an expansion in the coupling coefficient $\alpha=\gamma_0/\lambda$ one has

$$\begin{aligned}\gamma^{(2)}(t) &= \gamma_0\big(1-e^{-\lambda t}\big)\\ &= 2\mathrm{Re}\int_0^t \mathrm{dt}_1 f(t_1)\end{aligned}$$

and

$$\begin{aligned}\gamma^{(4)}(t) &= \frac{\gamma_0^2}{\lambda}[\sinh(\lambda t)-\lambda t]e^{-\lambda t}\\ &= 2\mathrm{Re}\int_0^t \mathrm{dt}_1\int_0^{t_!}\mathrm{dt}_2\int_0^{t_2}\mathrm{dt}_3[f(t-t_2)f(t_1-t_3)-f(t-t_3)f(t_1-t_2)]\end{aligned}$$

where we have also indicated the expression for the corresponding term of the perturbation expansion of the TCL series. Notice that these functions always stay positive so that the approximation given by second or fourth order grant CP. The overall dynamics however is not in Lindblad form for strong coupling, since $\gamma(t)$ goes through negative values. As already said for the TCL series we can give the expression of the $2n$-th order contribution as

$$\begin{aligned}\varepsilon(t)+i\gamma(t) &= -2\left[\frac{\dot{G}(t)}{G(t)}\right]\\ &= 2\int_0^t\mathrm{dt}_1\int_0^{t_1}\mathrm{dt}_2\ldots\int_0^{t_{2n-2}}\mathrm{dt}_{2n-1}(-)^{n+1}\langle f(t-t_1)f(t_2-t_3)\ldots f(t_{2n-2}-t_{2n-1})\rangle_{\mathrm{oc}}\end{aligned}$$

**NZ for Lorentzian spectral density**

For a Lorentzian spectral density on resonance for the NZ case one has

$$\begin{aligned}
\varepsilon(t) &= 0\\
k_1(t) &= \gamma_0\lambda e^{-3\lambda t/2}\left[\cosh\left(\frac{\lambda t}{2}\delta'\right)+\frac{1}{\delta'}\sinh\left(\frac{\lambda t}{2}\delta'\right)\right]\\
k_2(t) &= 2\mathrm{Re}\, f(t)-k_1(t)\\
&= \gamma_0\lambda e^{-\lambda t}\left\{1-e^{-\lambda t/2}\left[\cosh\left(\frac{\lambda t}{2}\delta'\right)+\frac{1}{\delta'}\sinh\left(\frac{\lambda t}{2}\delta'\right)\right]\right\}
\end{aligned}$$

with $\delta'=\sqrt{1-4\gamma_0/\lambda}$. The master equation reads

$$\frac{\mathrm{d}}{\mathrm{dt}}\rho(t) = \int_0^t d\tau\left\{k_1(t-\tau)\left[\sigma_-\rho(\tau)\sigma_+-\frac{1}{2}\{\sigma_+\sigma_-,\rho(\tau)\}\right]+\frac{1}{4}k_2(t-\tau)[\sigma_z\rho(\tau)\sigma_z-\rho(\tau)]\right\}$$

Considering an expansion in the coupling coefficient $\alpha=\gamma_0/\lambda$ one has

$$k_1^{(2)}(t) = \gamma_0\lambda e^{-\lambda t}$$

and

$$k_2^{(2)}(t) = 0$$

and for higher orders $k_2^{(2n)}(t) = -k_1^{(2n)}(t)$, so that the Nakajima-Zwanzig master equation to second order reads

$$\frac{\mathrm{d}}{\mathrm{dt}}\rho(t) = \gamma_0\lambda\int_0^t d\tau \mathrm{e}^{-\lambda(t-\tau)}\left[\sigma_-\rho(\tau)\sigma_+-\frac{1}{2}\{\sigma_+\sigma_-,\rho(\tau)\}\right].$$

As seen discussing quantum semi-Markov processes, to second order CP is not preserved in the NZ approach unless in weak coupling approximation corresponding to $1-4\gamma_0/\lambda\geqslant 0$. At fourth order one has

$$\begin{aligned}
k_1^{(4)}(t) &= \gamma_0^2\left[\mathrm{e}^{-\lambda t}(1-\lambda t)-\mathrm{e}^{-2\lambda t}\right]\\
k_2^{(4)}(t) &= -k_1^{(4)}(t)
\end{aligned}$$

and therefore a different operator structure.

Also in the NZ case the expression of the memory kernel at various orders can be obtained directly from the perturbation series, according to the expressions

$$\begin{aligned}
k_1^{(2)}(t) &= 2\mathrm{Re}\, f(t)\\
k_1^{(4)}(t) &= -2\mathrm{Re}\int_{t_1}^t \mathrm{d}t_2\int_{t_1}^{t_2}\mathrm{d}t_3[f(t-t_3)f(t_1-t_2)+f(t-t_1)f(t_3-t_2)]
\end{aligned}$$

although in this case an explicit expression for the $2n$-th order contribution is not available.

## 3.6 References

For this part see mainly [Breuer2007, Vacchini2010b, Smirne2010b, Breuer2010a]

**A word of warning:**

The bibliography is very incomplete, we only quote papers directly related to the exposition. A wider and more reasonable panorama of the activity on the subject can be gained looking at the papers quoted in the given references, where more justice is made to the work of other authors.

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"One of the principal objects of theoretical research in any department of knowledge is to find the point of view from which the subject appears in the greatest simplicity" (Josiah Willard Gibbs)