Dynamics of open quantum systems: Role of correlation

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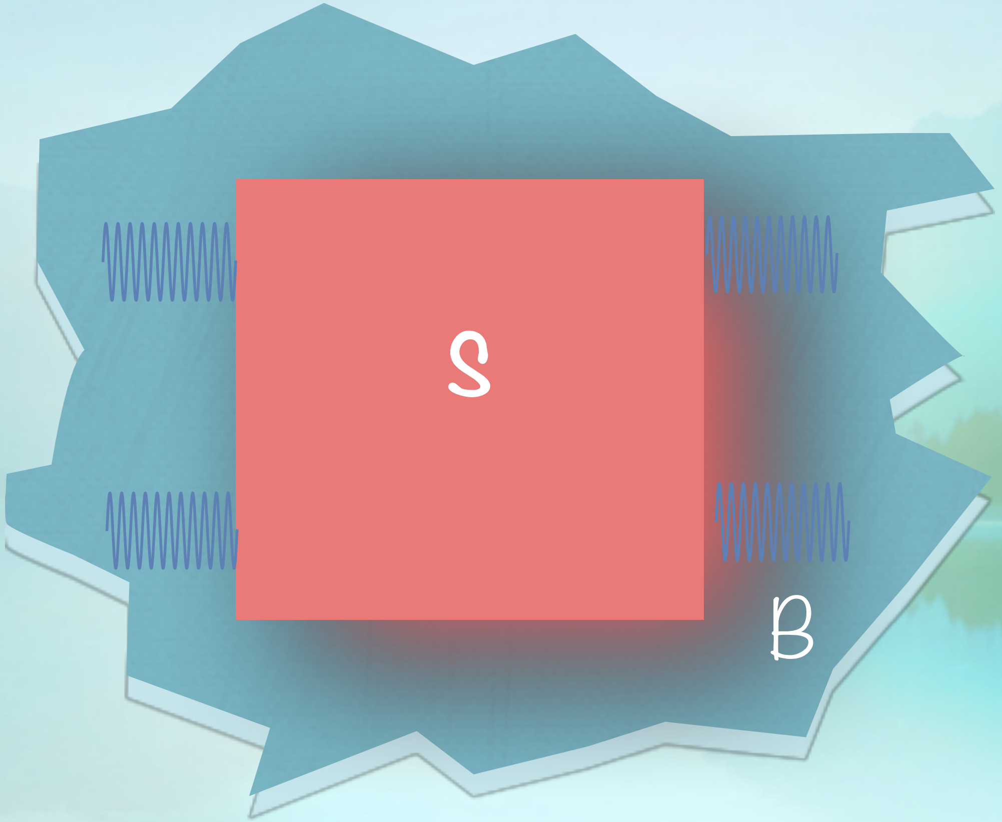
A postulate of quantum mechanics: Closed system evolves unitarily



$$H_{\rm tot} = H_S + H_B + H_{\rm int}$$

$$\dot{\varrho}_{SB}(t) = -i[H_{\rm tot}, \varrho_{SB}(t)]$$

What about the system alone?

measuring a local observable: $A \otimes \mathbb{I}$

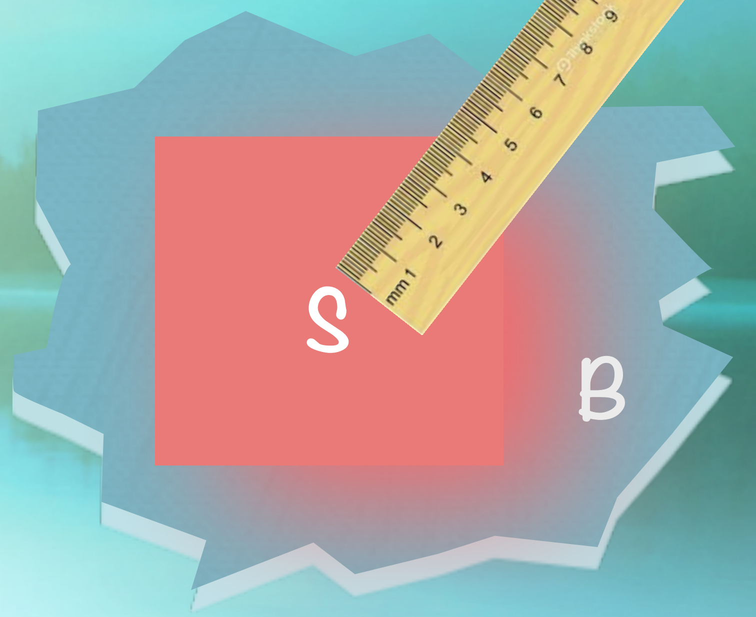
the Born rule

$$\begin{aligned}\langle A \rangle &= \mathrm{Tr}[A \otimes \mathbb{I} \varrho_{SB}] \\ &= \mathrm{Tr}_S[\mathrm{Tr}_B[A \varrho_{SB}]] \\ &= \mathrm{Tr}_S[A\, \mathrm{Tr}_B[\varrho_{SB}]]\end{aligned}$$

ϱ_S

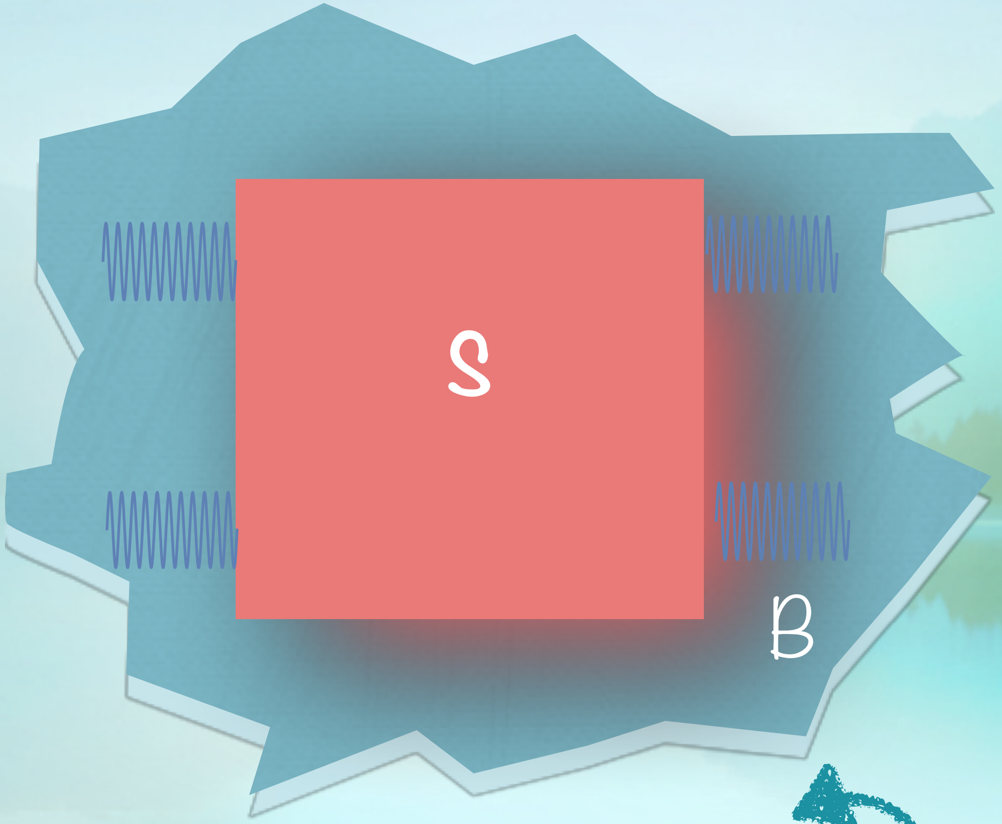
reduced density matrix

$$\varrho_S = \mathrm{Tr}_B[\varrho_{SB}]$$



what is the dynamical equation which governs evolution of ϱ_S ?

$$\varrho_{SB} \neq \varrho_S \otimes \varrho_B$$



$$\varrho_{SB} = \varrho_S \otimes \varrho_B + \chi$$

correlation

$$\mathrm{Tr}_S[\chi] = \mathrm{Tr}_B[\chi] = 0$$

χ contains all kinds of correlation in the system

quantum correlations

free entanglement $|\psi_{SB}\rangle = \frac{1}{\sqrt{d}} \sum_{i=1}^{d} |ii'\rangle$

bound entanglement

quantum discord $\varrho_{SB} = \sum_i p_i \Pi_i \otimes \varrho_i$

classical correlations $\varrho_{SB} = \sum_i p_i \Pi_i \otimes \tilde{\Pi}_i$

to measure a local observable at an instant of time we did not need to know correlation

Does subsystem dynamics depend on correlations?

subsystem dynamics extracted from unitary evolution

$\varrho_{SB}(0) = \varrho_S(0) \otimes \varrho_B(0) \quad \equiv \quad \chi(0) = 0$ no initial correlation

$H_{\text{tot}} = H_S + H_B + H_{\text{int}}$

$\varrho_S(\tau) = \mathrm{Tr}_B[U(\tau)\varrho_S(0) \otimes \varrho_B(0)U^\dagger(\tau)]$

$A_{n(i,j)} = \sqrt{\lambda_i}\langle e_j|U(t)|\lambda_i\rangle$

$\varrho_B(0) = \sum_i \lambda_i |\lambda_i\rangle\langle\lambda_i|$

$\varrho_S(\tau) = \mathcal{E}_S(\tau)[\varrho_S(0)] = \sum_n A_n(\tau)\varrho_S(0)A_n^\dagger(\tau)$ Kraus representation

$\sum_n A_n^\dagger A_n = \mathbb{I}$

$U_{SB}(t)$

Quantum channel $\equiv$ CPT map $\equiv$ dynamical map

semigroup property of the channel & derivation of Markovian master equation

time homogeneous dynamical semigroup property, i.e, divisibility of dynamical map

$$\mathcal{E}_S(\tau_1+\tau_2)=\mathcal{E}_S(\tau_2)\mathcal{E}_S(\tau_1) \qquad \forall \tau_1,\tau_2 \geqslant 0$$

inverse maps are not dynamical maps

$$\mathcal{E}_S(\tau)=e^{\mathcal{L}_S\tau}$$

$\mathcal{L}_S$ is time-independent generator

starting from Kraus representation $\frac{d}{d\tau}\varrho_S(\tau)=\mathcal{L}_S\varrho_S(\tau)$ Markovian quantum master equation

$$\mathcal{L}_S\varrho_S(\tau)=-i[\widetilde{H}_S,\varrho_S(\tau)]+\sum_m \gamma_m\left(2L_m\varrho_S L_m^\dagger-\{L_m^\dagger L_m,\varrho_S\}\right)$$

Gorini, Kossakowski, Sudarshan, Lindblad equation

γ_m: positive, time-independent

L_m: time-independent

microscopic derivation of Markovian master equation

in the week coupling regime:

—Born approximation $\varrho_{SB}(\tau) = \varrho_S(\tau) \otimes \varrho_B(0)$ $(\tau_S \gg \tau_B)$

—Markov approximation killing the dependence of time evolution of the state on the state at earlier times

$$\frac{d}{d\tau}\varrho_S(\tau) = -\int_0^\tau \mathrm{Tr}_B[H_{\mathrm{int}}(\tau), [H_{\mathrm{int}}(s), \varrho_S(\tau) \otimes \varrho_B(0)]]ds$$

→ Redfield equation (time local master equation) with memory effects

—Rotating wave approximation (RWA)

→ leads to the generator of a dynamical semigroup

$$\mathcal{L}_S\varrho_S(\tau) = -i[\widetilde{H}_S, \varrho_S(\tau)] + \sum_m \gamma_m \left(2L_m\varrho_S L_m^\dagger - \{L_m^\dagger L_m, \varrho_S\}\right)$$

What if the system runs in a regime beyond Born-Markov and RWA?

Projection operator techniques

Nakajima—Zwanzig projection operator technique

$$\frac{d}{dt}\mathcal{P}\tilde{\rho}(t) = \mathcal{P}\mathcal{V}(t)\mathcal{P}\tilde{\rho}(t) + \mathcal{P}\mathcal{V}(t)\mathcal{G}(t,0)\mathcal{Q}\tilde{\rho}(0) + \int_0^t du \mathcal{P}\mathcal{V}(t)\mathcal{G}(t,u)\mathcal{Q}\mathcal{V}(u)\mathcal{P}\tilde{\rho}(u)$$

$$\mathcal{P}\rho = \mathrm{Tr}_B(\rho)\otimes\rho_B \qquad \tilde{\rho}(t) = e^{i(H_A+H_B)t}\rho(t)e^{-i(H_A+H_B)t}$$

$$\mathcal{Q}\rho = (\mathbb{1}-\mathcal{P})\rho \qquad \mathcal{G}(t,s) = \mathcal{T}e^{\int_s^t dt'\mathcal{Q}\mathcal{V}(t')}$$

$$\mathcal{V}(t)\cdot \equiv -i[\tilde{V}(t),\cdot]$$

Path integral techniques

Monte Carlo techniques

etc...

Time-local master equation in the presence of memory effects (without semigroup property)?

Gorini-Kossakowski-Sudarshan theorem

Any linear map with Hermiticity and trace preserving properties can be associated to a time-local generator as

$$\mathcal{L}_S \varrho_S(\tau) = -i[\widetilde{H}_S, \varrho_S(\tau)] + \sum_m \gamma_m \left(2L_m \varrho_S L_m^\dagger - \{L_m^\dagger L_m, \varrho_S\}\right)$$

— Theorem is just about existence (non-constructive)

— No clue on how to derive rates and jump operators

dynamics of an open quantum system?

Schrödinger equation: $\mathrm{d}\varrho_S(\tau) = -i\mathrm{Tr}_B[H_{\mathrm{tot}}, \varrho_{SB}(\tau)]d\tau$

$$\varrho_{SB}(\tau) = \varrho_S(\tau) \otimes \varrho_B(\tau) + \chi(\tau)$$

?

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\varrho_S(\tau) = -i\left[H_S + \mathrm{Tr}_B[H_{\mathrm{int}}\varrho_B(\tau)], \varrho_S(\tau)\right] - i\sum_i \left[\mathcal{S}_i, \mathrm{Tr}_B[\chi(\tau)\mathcal{B}_i]\right]$$

environment-induced correction

correlation

$\{\mathcal{S}_i\}$ orthonormal operator basis of the system $\quad H_{\mathrm{int}} = \sum \mathcal{S}_i \otimes \mathcal{B}_i$

Going to appropriate picture:

virtual interaction H_χ

$\varrho_S(\tau) \quad \otimes \quad \varrho_B(\tau)$

$\chi(\tau)$

$\varrho_{SB}(\tau)$

$$\varrho_{SB}(\tau) \approx e^{-i\tau_\chi(\tau)H_\chi(\tau)}\varrho_S(\tau) \otimes \varrho_B(\tau) e^{i\tau_\chi(\tau)H_\chi^\dagger(\tau)}$$

correlation picture

$$\chi(\tau) = -i\tau_\chi [\![H_\chi(\tau), \varrho_S(\tau) \otimes \varrho_B(\tau)]\!]$$

definition:

$[\![A, B]\!] = AB - B^\dagger A^\dagger$

Good news:

D. S. Djordjević, J. Comput. Appl. Math. **200**, 701 (2007)

Theorem 2.2. *Let $A \in \mathscr{L}(H, K)$ have a closed range and $B \in \mathscr{L}(H)$. Then the following statements are equivalent:*

(a) *There exists a solution $X \in \mathscr{L}(H, K)$ of Eq.* $A^*X + X^*A = B$

(b) $B = B^*$ *and* $(I - A^\dagger A)B(I - A^\dagger A) = 0$.

pseudo inverse

If (a) *or* (b) *is satisfied, then any solution of Eq.* (1) *has the form*

$$X = \frac{1}{2}(A^*)^\dagger B A^\dagger A + (A^*)^\dagger B(I - A^\dagger A) + (I - AA^\dagger)Y + AA^\dagger Z A,$$

where $Z \in \mathscr{L}(K)$ satisfies $A^*(Z + Z^*)A = 0$, and $Y \in \mathscr{L}(H, K)$ is arbitrary.

$$\chi(\tau) = -i\tau_\chi [\![H_\chi(\tau), \varrho_S(\tau) \otimes \varrho_B(\tau)]\!] \equiv \left(\varrho_S(\tau) \otimes \varrho_B(\tau)\right)\left(i\tau_\chi H_\chi^\dagger(\tau)\right) + \left(i\tau_\chi H_\chi^\dagger(\tau)\right)^\dagger \left(\varrho_S(\tau) \otimes \varrho_B(\tau)\right) = \chi(\tau)$$

$$P_0(\tau)\chi(\tau)P_0(\tau) = 0$$

projector onto the null-space of $\varrho_S(\tau) \otimes \varrho_B(\tau)$

$$\chi(\tau) = -i\tau_\chi [\![H_\chi(\tau), \varrho_S(\tau) \otimes \varrho_B(\tau)]\!]$$

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\varrho_S(\tau) = -i\Big[H_S + \mathrm{Tr}_B[H_{\mathrm{int}}\varrho_B(\tau)], \varrho_S(\tau)\Big] - i\sum_i \Big[\mathcal{S}_i, \mathrm{Tr}_B[\chi(\tau)\mathcal{B}_i]\Big]$$

expansion in $\{\mathcal{S}_i\}$ basis

$$H_\chi(\tau) = \sum_j \mathcal{S}_j \otimes \mathcal{B}_j^\chi(\tau)$$

environment correlation functions

$$c_{ij}(\tau) = \mathrm{Tr}[\varrho_B(\tau)\mathcal{B}_i\mathcal{B}_j^\chi(\tau)]$$

Hermitian

$$\boldsymbol{b}(\tau) := \big(\boldsymbol{c}(\tau) - \boldsymbol{c}^\dagger(\tau)\big)/2i$$

$$\boldsymbol{a}(\tau) := \big(\boldsymbol{c}(\tau) + \boldsymbol{c}^\dagger(\tau)\big)/2$$

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\varrho_S(\tau) = -i\Big[\widetilde{H}_S, \varrho_S(\tau)\Big] + \tau_\chi \sum_{ij} a_{ij}(\tau)\Big(2\mathcal{S}_j\varrho_S\mathcal{S}_i - \{\mathcal{S}_i\mathcal{S}_j, \varrho_S\}\Big)$$

in which

$$\widetilde{H}_S = H_S + \mathrm{Tr}_B[H_{\mathrm{int}}\,\varrho_B(\tau)] + \tau_\chi \sum_{ij} b_{ij}(\tau)\mathcal{S}_i\mathcal{S}_j$$

putting into standard form:

diagonalization → $U\boldsymbol{a}U^\dagger = \boldsymbol{\Gamma}$

defining $L_m = \sum_i U_{mi} S_i$

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\varrho_S(\tau) = -i[\widetilde{H}_S, \varrho_S(\tau)] + \tau_\chi \sum_m \gamma_m \left(2L_m \varrho_S L_m^\dagger - \{L_m^\dagger L_m, \varrho_S\}\right)$$

γ_m is real but can be negative

example: Jaynes-Cummings model with initial system-bath correlation

$$H_S = (\omega_0/2)\sigma_z + \omega a^\dagger a + \lambda(\sigma_+ \otimes a + \sigma_- \otimes a^\dagger)$$

correlated initial state $\quad |\psi(0)\rangle = r_1|\mathrm{e}, 0\rangle + r_2|\mathrm{g}, 1\rangle$

$$\dot{\varrho}_S = -i[H_S + \widetilde{\omega}_0\sigma_z, \varrho_S] + \gamma_1^\chi(2\sigma_-\varrho_S\sigma_+ - \{\sigma_+\sigma_-, \varrho_S\}) - \gamma_2^\chi(2\sigma_+\varrho_S\sigma_- - \{\sigma_-\sigma_+, \varrho_S\})$$

$$\gamma_1^\chi = -\lambda\alpha_2/\big(2(1-\alpha_1)\big)$$

$$\gamma_2^\chi = \lambda\alpha_2/\big(2(1+\alpha_1)\big)$$

$$\widetilde{\omega}_0 = 4\lambda r_1 r_2 \alpha_1/\big(1 + 4r_1^2 - 4r_1^4 - (\alpha_1^2 - \alpha_2^2)\big)$$

Reduction to Markovian master equation

Expanding $\chi(\tau)$ around a zero-correlation point up to the **first order** (no need to Born, Markov, RWA)

$$\chi(\tau_0+\delta\tau) = -i\delta\tau[\widetilde{H}_{\text{int}}(\tau_0+\delta\tau), \varrho_S(\tau_0+\delta\tau)\otimes\varrho_B(\tau_0+\delta\tau)] + O(\delta\tau^2)$$

$$\rightarrow \quad H_\chi \equiv \widetilde{H}_{\text{int}} = \sum_i (\mathcal{S}_i - \langle\mathcal{S}_i\rangle_S)\otimes(\mathcal{B}_i - \langle\mathcal{B}_i\rangle_B) \rightarrow \mathcal{B}_j^\chi$$

$c_{ij} \propto \mathrm{Cov}(\mathcal{B}_i, \mathcal{B}_j) \rightarrow$ $\boldsymbol{a}$ positive, $\boldsymbol{b}=0$

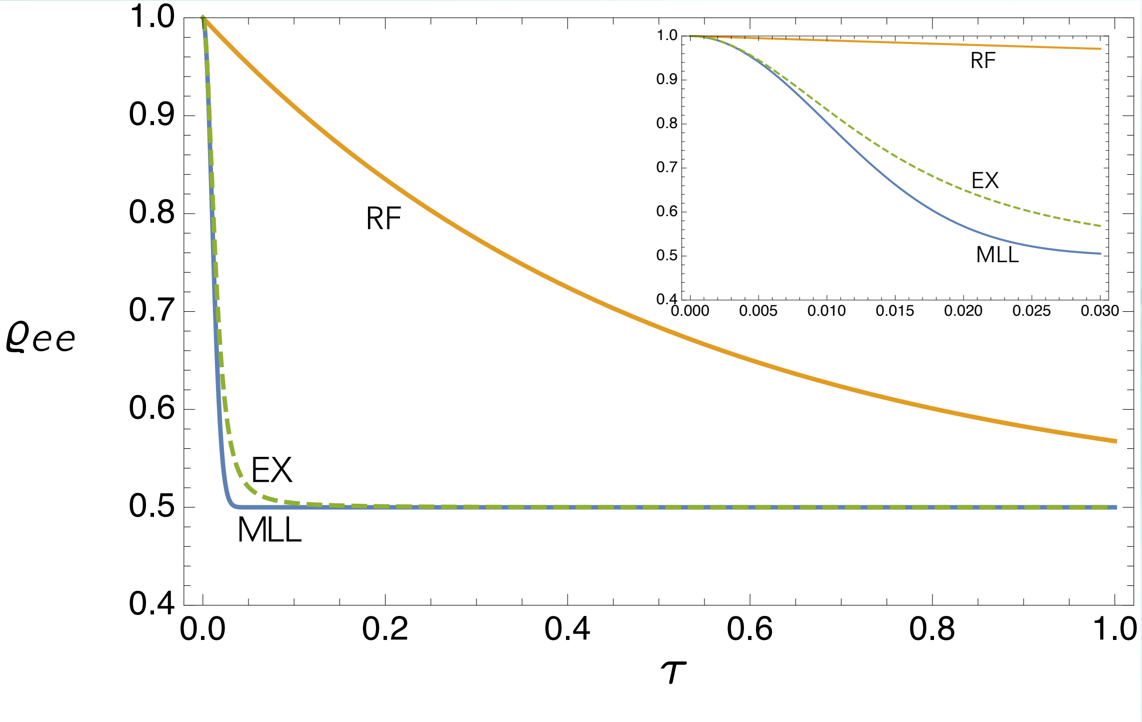
$$\frac{\mathrm{d}}{\mathrm{d}\tau}\varrho_S(\tau) = -i\left[\widetilde{H}_S, \varrho_S(\tau)\right] + \tau_\chi \sum_{ij} a_{ij}(\tau)\Big(2\mathcal{S}_j\varrho_S\mathcal{S}_i - \{\mathcal{S}_i\mathcal{S}_j, \varrho_S\}\Big)$$

$\rightarrow \gamma_m \geqslant 0$

example: Atom in a bosonic bath

$$H_{SB} = \omega_0 \sigma_+ \sigma_- + \sum_n \omega_n a_n^\dagger a_n - \sigma_x \otimes O_B \quad ; \quad O_B = \sum_n \kappa_n (a_n + a_n^\dagger)$$

$$\dot{\varrho}_S(\tau) = -i[H_S, \varrho_S(\tau)] + \gamma(\tau)\big(\sigma_x \varrho_S(\tau)\sigma_x - \varrho_S(\tau)\big) \quad ; \quad \gamma(\tau) = 2\tau\, \mathrm{Cov}_{B_0}(O_B, O_B)$$



$$\beta = 1, \eta = 0.5, \omega_c = 100, \omega_0 = 0$$

Exact solution: Braun et al. PRL (2001)

Summary

- I claimed that any general open system dynamics can be written in the form of Lindblad equation
- I indirectly justified existence of such equation, based on a Gorini, Kossakowski, Sudarshan theorem
- I then constructively derived this equation and obtained rate and jump operators explicitly
- Markovianity condition for the dynamics obtained simply by expansion of correlation