

A few puzzles in open quantum dynamics

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Joint ongoing work with D. Chruściński, R. Floreanini and G. Nichele

Outline I

- 1 Lack of Complete Positivity: only a short-time problem?**
 - 1 qubit systems
 - 2-qubit systems

- 2 Super-activation of back-flow of information**
 - Non-Markovian dynamics
 - Back-flow of information

- 3 Conclusions and outlook**

Redfield vs Davis

Redfield vs Davis

Non-Positivity vs Complete Positivity

Redfield vs Davis

Non-Positivity vs Complete Positivity

- Total Hamiltonian: $H_T = H_S + H_B + \lambda H_{int}$
- System-bath unitary evolution:

$$\rho_T(t) = U_T(t)\rho_S \otimes \rho_B U_T^\dagger(t), \quad U_T(t) = \exp(-itH_T)$$

- Open system **reduced** dynamics:

$$\rho_S \mapsto \rho_S(t) = \text{Tr}_B \rho_T(t)$$

- **Weak-coupling limit**: extraction of a semigroup

$$\rho_S \mapsto \rho_S(t) = \gamma_t[\rho_S], \quad \gamma_t \circ \gamma_s = \gamma_s \circ \gamma_t = \gamma_{t+s}, \quad 0 \leq s, t$$

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Slipped initial conditions **DO NOT** eliminate all problems:
others emerge that are related to **entanglement**,
through the **local open dynamics**

$$\Gamma_t := \text{id} \otimes \gamma_t$$

1-qubit

F.B., D. Chruściński, R. Floreanini, OSID 29, 2022

- Hamiltonians and bath equilibrium state:

$$H_S = \omega \sigma_3, \quad H_{int} = \sum_{i=1}^3 \sigma_i \otimes B_i, \quad \rho_B = \frac{e^{-\beta H_B}}{Z_\beta}$$

- Diagonal bath correlation functions:

$$G_{ii}(s) = \text{Tr}_B [\rho_B B_i(s) B_i] = [G_{ii}(-s)]^\dagger \neq 0$$

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Redfield weak-coupling limit

- Master equation: $\partial_t \rho_S(t) = \mathbb{L}[\rho_S(t)] = -i[H_S, \rho_S(t)] + \mathbb{D}[\rho_S(t)]$

$$\rho_S(t) = \gamma_t[\rho_S] = \exp(t\mathbb{L})[\rho_S]$$

$$\mathbb{D}[\rho] = -\lambda^2 \int_0^\infty ds \text{Tr}_B \left(\left[H_{int}(s), \left[H_{int}, \rho \otimes \rho_B \right] \right] \right)$$

- Interaction representation:

$$H_{int}(s) = \sum_{i=1}^3 \sigma_i(s) \otimes B_i(s)$$

$$\sigma_i(s) = e^{isH_S} \sigma_i e^{-isH_S} = \sum_{j=1}^3 U_{ij}(s) \sigma_j, \quad B_i(s) = e^{isH_B} B_i e^{-isH_B}$$

$$U_{ij}(s) = n_i n_j + (\delta_{ij} - n_i n_j) \cos(2\omega s) - \varepsilon_{ijk} n_k \sin(2\omega s)$$

Generator in GKSL form

$$\mathbb{D}[\rho_S(t)] = -i[H_{LS}, \rho] + \sum_{i,j=1}^3 C_{ij} \left(\sigma_j \rho \sigma_i - \frac{1}{2} \{ \sigma_i \sigma_j, \rho \} \right)$$

- **Lamb-shift correction:**

$$H_{LS} = \frac{\lambda^2}{2} \delta\omega \sigma_3$$

$$\delta\omega = \int_0^\infty ds \sin(2\omega s) \left(G_{11}(s) + G_{11}(-s) + G_{22}(s) + G_{22}(-s) \right)$$

- **Kossakowski matrix:** $C = \begin{pmatrix} C_{11} & C_{12} & 0 \\ C_{21} & C_{22} & 0 \\ 0 & 0 & C_{33} \end{pmatrix}$

$$C_{11} = \frac{\lambda^2}{2} \int_{-\infty}^{\infty} ds e^{2i\omega s} \left(G_{11}(s) + G_{11}(-s) \right),$$

$$C_{22} = \frac{\lambda^2}{2} \int_{-\infty}^{\infty} ds e^{2i\omega s} \left(G_{22}(s) + G_{22}(-s) \right),$$

$$C_{12} = \lambda^2 \int_0^\infty ds \sin(2\omega s) \left(G_{22}(s) - G_{11}(-s) \right) = [C_{21}]^*,$$

$$C_{33} = \lambda^2 \int_{-\infty}^{\infty} ds G_{33}(s)$$

Bloch vector representation

$$\rho = \frac{1}{2}(\sigma_0 + \vec{\rho} \cdot \vec{\sigma}), \quad \text{Det}[\rho] = \frac{1}{4} \left(1 - \sum_{j=1}^3 \rho_j^2 \right) \geq 0,$$

- the state ρ as a 4-vector $|\rho\rangle \equiv (1, \rho_1, \rho_2, \rho_3)$
- Reduced dynamics in Schrödinger-like form

$$\partial_t |\rho(t)\rangle = -2\mathcal{L} |\rho(t)\rangle, \quad \mathcal{L} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & a & b + \tilde{\omega} & 0 \\ 0 & b - \tilde{\omega} & \alpha & 0 \\ w & 0 & 0 & \gamma \end{pmatrix}$$

$$\begin{aligned} a &= \mathcal{C}_{22} + \mathcal{C}_{33}, & b &= -\text{Re}(\mathcal{C}_{12}), \\ \alpha &= \mathcal{C}_{11} + \mathcal{C}_{33}, & w &= -2\text{Im}(\mathcal{C}_{12}), \\ \gamma &= \mathcal{C}_{11} + \mathcal{C}_{22}, & \tilde{\omega} &:= \omega + \frac{\lambda^2}{2}\delta\omega \end{aligned}$$

Tendency to equilibrium

- **KMS conditions:**

$$G_{ij}(t) = G_{ji}(-t-i\beta) \implies \gamma - w = e^{-2\beta w} (\gamma + w) \implies \frac{w}{\gamma} = \frac{1 - e^{-2\beta w}}{1 + e^{-2\beta w}}$$

- **Unique equilibrium state:**

$$\mathbb{L}[\rho] = 0 \implies \rho_1 = \rho_2 = 0, \rho_3 = -\frac{w}{\gamma} \implies \rho = \frac{e^{-\beta H_S}}{\text{Tr}[e^{-\beta H_S}]}$$

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Lack of positivity

- Determinants can be **negative at small times:**

$$\left. \frac{d}{dt} \text{Det}[\rho(t)] \right|_{t=0} = 2 \left[a\rho_1^2 + \alpha\rho_2^2 + 2b\rho_1\rho_2 + \rho_3(w + \gamma\rho_3) \right]$$

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$$\boxed{\rho_3 = 0, \rho_1^2 + \rho_2^2 = 1 \implies \text{Det}[\rho] = 0}, \quad \boxed{a\rho_1^2 + \alpha\rho_2^2 + 2b\rho_1\rho_2 \neq 0}$$

An inert qubit statistically coupled to a qubit evolving with the Redfield dynamics γ_t

- **Local compound reduced dynamics:** $\Gamma_t = \text{id} \otimes \gamma_t$

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- Local compound reduced dynamics: $\Gamma_t = \text{id} \otimes \gamma_t$

- X -states:

$$\rho_X = \begin{pmatrix} \rho_{11} & 0 & 0 & \rho_{14} \\ 0 & \rho_{22} & \rho_{23} & 0 \\ 0 & \rho_{23}^* & \rho_{33} & 0 \\ \rho_{14}^* & 0 & 0 & \rho_{44} \end{pmatrix}$$

- Γ_t maps X -states into themselves
- Reduced density matrix of the second qubit:

$$\rho_2(t) = \text{Tr}_1 [\rho(t)] \geq 0$$

Choi-Jamiołkowski matrix $\Gamma_t[\Pi]$: γ_t CP after some time

$$\Pi = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} \mapsto \Gamma_t[\Pi] = \begin{pmatrix} \rho_{11}(t) & 0 & 0 & \rho_{14}(t) \\ 0 & \rho_{22}(t) & \rho_{23}(t) & 0 \\ 0 & \rho_{23}^*(t) & \rho_{33}(t) & 0 \\ \rho_{14}^*(t) & 0 & 0 & \rho_{44}(t) \end{pmatrix}$$

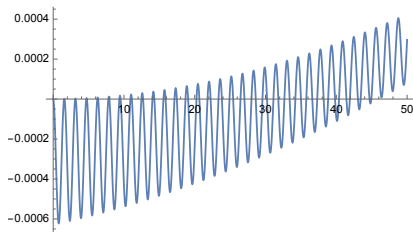


Figure: Central matrix determinant: $a/\omega = 0.005$, $b/\omega = 0.05$, $\alpha/\omega = 0.001$, $\gamma/\omega = 0.001$, $w = \gamma$

Entanglement of X -states via concurrence

$$\mathfrak{C}[\rho] = 2 \max \left\{ 0, |\rho_{23}| - \sqrt{\rho_{11}\rho_{44}}, |\rho_{14}| - \sqrt{\rho_{22}\rho_{33}} \right\}$$

- A 4-parameter family of X -states:

$$\tilde{\rho} = \begin{pmatrix} \mu & 0 & 0 & u \\ 0 & \nu & iv & 0 \\ 0 & -iv & 1 - 2\mu - \nu & 0 \\ u & 0 & 0 & \mu \end{pmatrix}, \quad \mu, \nu, u, v \in \mathbb{R}$$

$$\mu \geq 0, \quad \nu \geq 0, \quad 0 \leq 2\mu + \nu \leq 1$$

$$u^2 \leq \mu^2, \quad v^2 \leq \nu(1 - 2\mu - \nu).$$

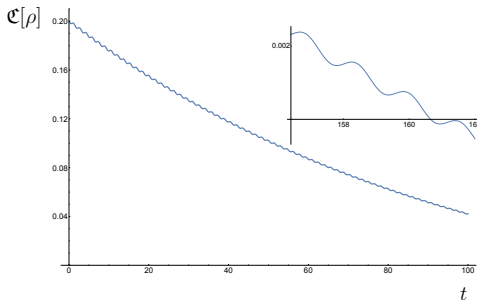


Figure: Concurrence as a function of time in units $1/\omega$, with $a/\omega = 0.005$, $b/\omega = 0.05$, $\alpha/\omega = 0.001$, $\gamma/\omega = 0.001$, $w = \gamma$, for an initial state with $\mu = 0.025$, $\nu = 0.1$, $u = 0.02$ and $v = 0.125$

Local (tensorized) reduced dynamics

$$\gamma_t \text{ CP} \Leftrightarrow \text{id} \otimes \gamma_t \text{ P}$$

More physically: two open quantum systems with same local interactions with a common environment

What about $\gamma_t^{(1)} \otimes \gamma_t^{(2)}$?

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More physically: two open quantum systems with same local interactions with a common environment

What about $\gamma_t^{(1)} \otimes \gamma_t^{(2)}$?

- $\gamma_t \otimes \gamma_t$ **positive (P)** $\Leftrightarrow \gamma_t$ **CP**

F.B., R. Floreanini, R. Romano, JPA 35, 2002

- $\gamma_t^{(1)} \otimes \gamma_t^{(2)}$ can be **P** without $\gamma_t^{(1,2)}$ being both **CP**

F.B., R. Floreanini, M. Piani, OSID 11, 2004

Time-dependent generators: $\partial_t \rho_S(t) = \mathbb{L}_t[\rho_S(t)]$

$$\mathbb{L}_t[\rho_S] = -i[H(t), \rho_S(t)] + \mathbb{D}_t[\rho_S(t)]$$

$$\mathbb{D}_t[\rho_S] = -i[H_{LS}(t), \rho_S] + \sum_{i,j=1}^3 C_{ij}(t) \left(\sigma_j \rho \sigma_i - \frac{1}{2} \{ \sigma_i \sigma_j, \rho \} \right)$$

- $\gamma_t : \rho_S \mapsto \rho_S(t)$ can be **CP** without $C(t) = [C_{ij}(t)] \geq 0$
- $C(t) = [C_{ij}(t)] \geq 0 \Leftrightarrow \gamma_t$ **CP-divisible**

A. Rivas, S. Huelga: Open Quantum Systems: an Introduction, Springer 2012

$$\gamma_t = \gamma_{t,s} \circ \gamma_s,$$

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$$\gamma_t = \gamma_{t,s} \circ \gamma_s,$$

$$\gamma_{t,s} \text{ CP } t \geq s \geq 0$$

$\gamma_t \otimes \gamma_t$ **P-divisible** $\Leftrightarrow \gamma_t$ **CP-divisible**

F.B., D.Chruściński, S.Filippov, PRA 95, 2017

1-qubit non-Markovianity

$$\begin{aligned}\partial_t \rho_S(t) &= \frac{1}{2} \left(\sigma_1 \rho_S(t) \sigma_1 - \rho_S(t) \right) + \frac{1}{2} \left(\sigma_2 \rho_S(t) \sigma_2 - \rho_S(t) \right) \\ &\quad - \frac{\tanh t}{2} \left(\sigma_3 \rho_S(t) \sigma_3 - \rho_S(t) \right)\end{aligned}$$

- **Pauli map:**

$$\gamma_t[\sigma_1] = e^{-t} \cosh t \sigma_1, \quad \gamma_t[\sigma_2] = e^{-t} \cosh t \sigma_2, \quad \gamma_t[\sigma_3] = e^{-2t} \sigma_3$$

- **Intertwiner:** $\gamma_{t,s} = \gamma_t \circ \gamma_s^{-1}$,

$$\gamma_{t,s}[\sigma_{1,2}] = e^{-(t-s)} \frac{\cosh t}{\cosh s} \sigma_{1,2}, \quad \gamma_{t,s}[\sigma_3] = e^{-2(t-s)} \sigma_3$$

- Choi-Jamiołkowski matrix:

$$\text{id} \otimes \gamma_t[\mathcal{P}] = \frac{1}{4} \begin{pmatrix} 1 + e^{-2t} & 0 & 0 & 2e^{-t} \cosh t \\ 0 & 1 - e^{-2t} & 0 & 0 \\ 0 & 0 & 1 - e^{-2t} & 0 \\ 2e^{-t} \cosh t & 0 & 0 & 1 + e^{-2t} \end{pmatrix}$$

$$(1 + e^{-2t})^2 - 4e^{-2t} \cosh^2 t = 0 \implies \gamma_t \text{ CP } \forall t \geq 0$$

- Kossakowski matrix: $C_t = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -\tanh t \end{pmatrix}$

- $\gamma_t : \rho_S \mapsto \gamma_t[\rho_S]$ never CP-divisible
- $\gamma_t : \rho_S \mapsto \gamma_t[\rho_S]$ always P-divisible:

D. Chruściński, F.A. Wudarski, PLA 377, 2013.

$$1 - \tanh t \geq 1 \quad \forall t \geq 0 \implies \gamma_{t,s} \text{ P}$$

Back-flow of information (BFI)

γ_t P-divisible, NOT CP-divisible

\implies

$\gamma_t \otimes \gamma_t$ NOT P-divisible



NO BFI



BFI

Back-flow of information

from environment to system due to an open dynamics Γ_t between $t \geq s \geq 0$ if

$$\|\Gamma_t[\Delta]\|_1 > \|\Gamma_s[\Delta]\|_1, \quad \|X\|_1 := \text{Tr}(\sqrt{X^\dagger X})$$

for a Hellstrom matrix

$$\Delta = \mu\rho_1 - (1 - \mu)\rho_2, \quad 0 \leq \mu \leq 1$$

- Γ_t **P** iff **contractive**

$$\|\Gamma_t[X]\|_1 \leq \|X\|_1 \quad \forall X$$

- γ_t **P-divisible** \implies **NO backflow of information:**

$$\gamma_{t,s} \text{ **P** } \implies \|\gamma_t[\Delta]\|_1 = \|\gamma_{t,s} \circ \gamma_s[\Delta]\|_1 \leq \|\gamma_s[\Delta]\|_1$$

Super-activation of back-flow of information

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$\gamma_t \otimes \gamma_t$ NOT P-divisible

1 qubit: no back-flow

2 qubits: back-flow under local reduced dynamics

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- Super-activation of BFI is a quantum phenomenon:
In a commutative setting (diagonal states and observables):

$$\gamma_t \text{ P-divisible} \implies \gamma_t \otimes \gamma_t \text{ P-divisible}$$

- Super-activation of BFI requires quantum discord

- Since $\gamma_{t,s} \otimes \gamma_{t,s}$ is **NOT P**:

$$\|\gamma_{t,s} \otimes \gamma_{t,s}[\Pi]\|_1 > \|\Pi\|_1$$

- Suppose a Hellstrom matrix Δ exists such that $\gamma_s \otimes \gamma_s[\Delta] = \lambda \Pi$, $\lambda > 0$, then

$$\|\gamma_t \otimes \gamma_t[\Delta]\|_1 = \lambda \|\gamma_{t,s} \otimes \gamma_{t,s}[\Pi]\|_1 > \lambda \|\Pi\|_1 = \|\gamma_s \otimes \gamma_s[\Delta]\|_1$$

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Is $\Delta = \lambda^{-1} \gamma_s^{-1} \otimes \gamma_s^{-1}[\Pi]$ a Hellstrom matrix for two separable states?

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Is $\Delta = \lambda^{-1} \gamma_s^{-1} \otimes \gamma_s^{-1}[\Pi]$ a Hellstrom matrix for two separable states?

- From **separable isotropic states** $\rho_r := (1-r)\frac{1}{4} + r\Pi$, $0 \leq r \leq 1$,

$$\Pi = \frac{1}{r}\rho_r - \frac{1-r}{r}\frac{1}{4} \implies \gamma_s^{-1} \otimes \gamma_s^{-1}[\Pi] = \frac{1}{r}\gamma_s^{-1} \otimes \gamma_s^{-1}[\rho_r] - \frac{1-r}{r}\frac{1}{4}$$

- For sufficiently small r , $\gamma_s^{-1} \otimes \gamma_s^{-1}[\rho_r]$ is **separable** by continuity.

Example

Isotropic state (Fano's form):

$$\rho_r = \frac{1}{4} [1_4 + r(\sigma_1 \otimes \sigma_1 - \sigma_2 \otimes \sigma_2 + \sigma_3 \otimes \sigma_3)]$$

- **Preimage:**

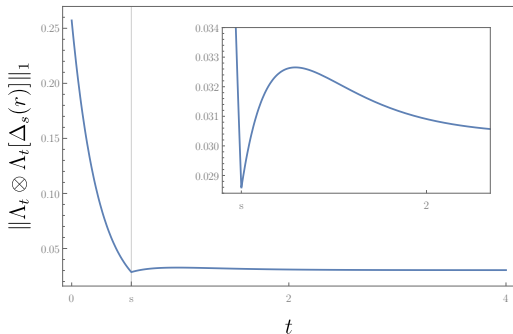
$$\begin{aligned} \tilde{\rho}_{r,s} &:= \Lambda_s^{-1} \otimes \Lambda_s^{-1} [\rho_r] \\ &= \frac{1}{4} \left[1_4 + r \frac{e^{2s}}{\cosh^2 s} (\sigma_1 \otimes \sigma_1 - \sigma_2 \otimes \sigma_2) + r e^{4s} \sigma_3 \otimes \sigma_3 \right] \end{aligned}$$

- For $s = \operatorname{arctanh}(\frac{1}{2}) \approx 0.55$, $r < 1/9$ yields

$$\tilde{\rho}_{r,s} = \frac{1}{4} \begin{pmatrix} 1+9r & 0 & 0 & \frac{9r}{2} \\ 0 & 1-9r & 0 & 0 \\ 0 & 0 & 1-9r & 0 \\ \frac{9r}{2} & 0 & 0 & 1+9r \end{pmatrix} \geq 0$$

- **Separability:** for $r \leq 2/27 \equiv r^*$

$$T \otimes \text{id}[\rho_{r,s}] = \frac{1}{4} \begin{pmatrix} 1+9r & 0 & 0 & 0 \\ 0 & 1-9r & \frac{9r}{2} & 0 \\ 0 & \frac{9r}{2} & 1-9r & 0 \\ 0 & 0 & 0 & 1+9r \end{pmatrix} \geq 0$$



Conclusions and Outlook

- Even if *lack of positivity* of Redfield reduced dynamics can be eliminated at short times by advocating an ad hoc *slippage of initial conditions mechanism*, problems persist *at all times* in the form of *local generation of entanglement*
- *Super-activation of back-flow of information*: when tensorized, a *1-qubit non-Markovian dynamics without BFI*, can lead to *BFI for 2 qubits*
- *Outlook*: microscopic origin of Super-activation of BFI: collisional models