Non-Markovian Quantum Dynamics of Open Systems

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Non-Markovianity and Strong Coupling Effects in Thermodynamics

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Contents

Recent Review:

H.P.B., E.-M. Laine, J. Piilo, B. Vacchini, Rev. Mod. Phys. 88, 021002 (2016)

Open quantum systems

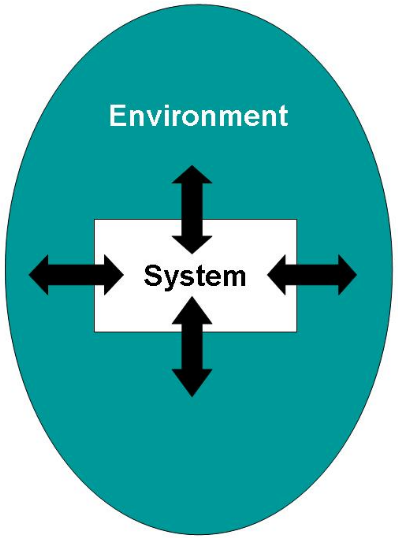
Open system S: density matrix $\rho_S = \mathrm{tr}_E \rho$

Environment E: density matrix $\rho_E = \mathrm{tr}_S \rho$

Total system S+E:

Density matrix matrix ρ_{SE}

Hamiltonian $H = H_S + H_E + H_I$



Applications:

- Atomic physics/quantum optics
- Condensed matter
- Quantum chemistry
- Quantum information
- Quantum thermodynamics
- Relaxation and dissipation
- Decoherence
- Quantum theory of measurement and control
- Transport processes
- ...

Quantum dynamical maps

$$
\begin{array}{ccc}
\rho_{SE}(0) = \rho_S(0) \otimes \rho_E & \xrightarrow{\text{unitary evolution}} & \rho_{SE}(t) = U_t\big[\rho_S(0) \otimes \rho_E\big]U_t^\dagger \\
\mathrm{tr}_E \big\downarrow & & \big\downarrow \mathrm{tr}_E \\
\rho_S(0) & \xrightarrow{\text{dynamical map}} & \rho_S(t) = \Phi_t \rho_S(0)
\end{array}
$$

Quantum dynamical map (quantum channel) Φ_t:

$$\rho_S(0) \longrightarrow \rho_S(t) = \Phi_t \rho_S(0) = \mathrm{tr}_E \left\{ U_t\big[\rho_S(0) \otimes \rho_E\big]U_t^\dagger \right\}$$

$\Phi_t =$ **completely positive map**

Quantum process: **One-parameter family of maps:**

$$\{\Phi_t \,|\, \Phi_0 = I,\ 0 \leq t \leq T\}$$

Examples of quantum Markov processes

Quantum dynamical semigroup:

$$\Phi_{t_1+t_2} = \Phi_{t_2}\Phi_{t_1} \Longrightarrow \Phi_t = e^{\mathcal{L}t}$$

with Lindblad generator:

$$\mathcal{L}\rho_S = -i\,[H_S, \rho_S] + \sum_i \gamma_i \left[A_i \rho_S A_i^\dagger - \frac{1}{2}\left\{A_i^\dagger A_i, \rho_S\right\}\right] \qquad \gamma_i \geq 0$$

$\Longrightarrow$ **Master equation in Lindblad form:**

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

Microscopic derivation: Separation of time scales:

$$\tau_E \ll \tau_R$$

Non-Markovian quantum dynamics

- Standard Markov condition $\tau_E \ll \tau_R$ violated, no rapid decay of environmental correlations
- Correlation functions of higher order play important role, strong memory effects
- Finite revival times (finite reservoir)
- Correlations and entanglement in the initial state

Methods:

- Projection operator techniques
- Memory kernel master equations: Nakajima, Zwanzig, Mori,...
- Time-local master equations: Shibata, van Kampen,...
- Stochastic wave function techniques
- Influence functional/Quantum Monte Carlo
- HEOM
- Multiconfiguration wave function methods
- Exact simulation techniques
- ...

Non-Markovian quantum dynamics

- What is the **key feature** of non-Markovian dynamics?

- How can one **define** non-Markovianity without reference to specific representation, master equation, approximation etc.?

- **Memory and information flow?**

- Construction of a **measure** for non-Markovianity?

- Experimentally **measurable** quantity?

Distance between quantum states

Trace norm of an operator A:

$$||A|| = \mathrm{tr}|A| \qquad |A| = \sqrt{A^\dagger A}$$

For selfadjoint operators:

$$A = \sum_i a_i |i\rangle\langle i|$$

$$||A|| = \sum_i |a_i|$$

Trace distance between quantum states ρ_1 and ρ_2:

$$D(\rho_1, \rho_2) = \frac{1}{2}||\rho_1 - \rho_2|| = \frac{1}{2}\mathrm{tr}|\rho_1 - \rho_2|$$

Properties of the trace distance

- **Metric on state space with $0 \leq D(\rho_1, \rho_2) \leq 1$**

$$\rho_1 = \rho_2 \Longleftrightarrow D = 0$$
$$\rho_1 \perp \rho_2 \Longleftrightarrow D = 1$$
$$\rho_i = |\psi_i\rangle\langle\psi_i| \Longrightarrow D = \sqrt{1 - |\langle\psi_1|\psi_2\rangle|^2}$$

- **Unitary invariance, triangular inequality, subadditivity**

- **Representation through maximum over all projections or positive operators $\Pi \leq I$:**

$$D(\rho_1, \rho_2) = \max_{\Pi} \mathrm{tr}\left\{\Pi(\rho_1 - \rho_2)\right\}$$

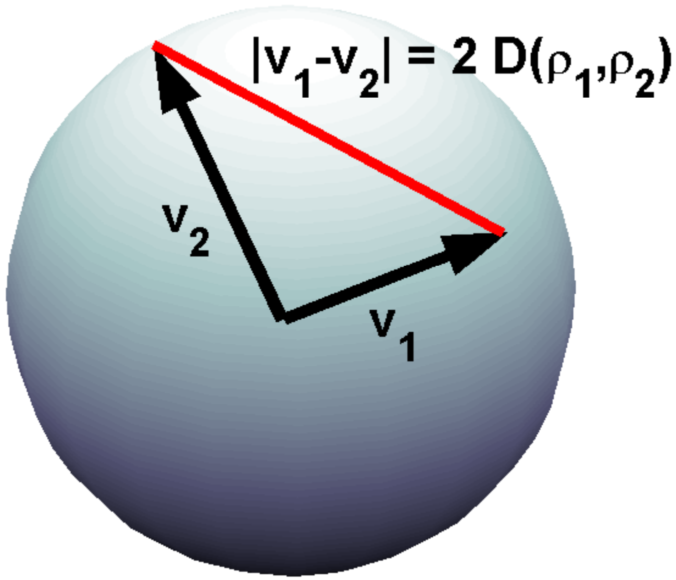
Example: Qubit

Bloch sphere:

$$\rho_{1,2} = \frac{1}{2}\left(I + \vec{v}_{1,2} \cdot \vec{\sigma}\right)$$

Bloch vectors:

$$|\vec{v}_{1,2}| \leq 1$$



Euclidean distance $= 2 \cdot$ (trace distance)

Physical interpretation

Alice

Bob

Preparation:

ρ_1 or ρ_2

with $p_1 = p_2 = 1/2$

Measurement:

ρ_1 or ρ_2 ?

success with

prob = $(1+D(\rho_1,\rho_2))/2$

$\Rightarrow D(\rho_1, \rho_2) =$ **Measure for distinguishability of** ρ_1 **and** ρ_2

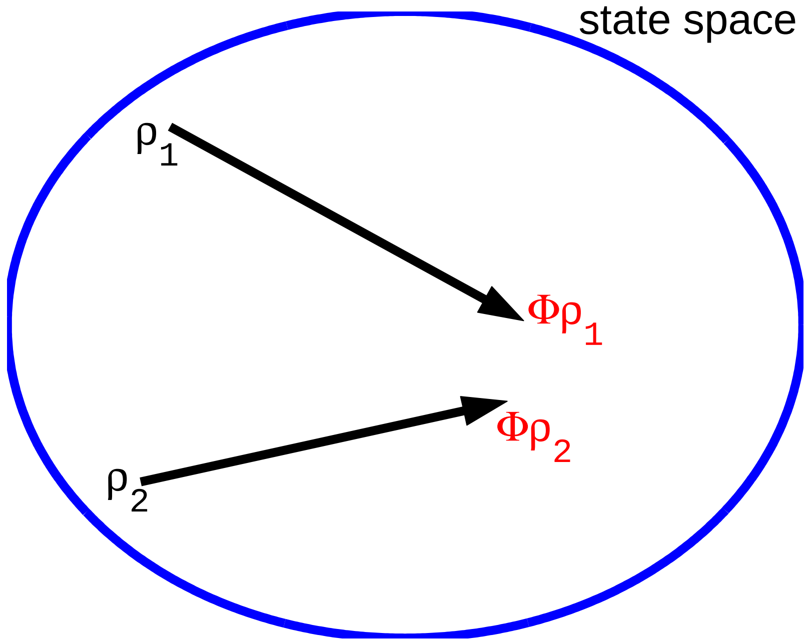
Example: $\rho_1 \perp \rho_2 \Rightarrow$ **prob** $= 1$

Contraction property

Dynamical maps are contractions for the trace distance:

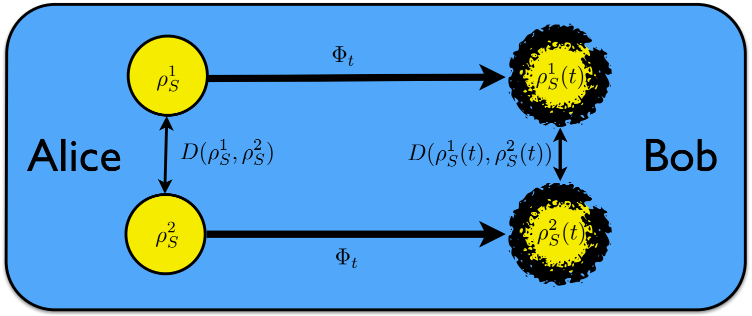
$$D(\Phi\rho_1, \Phi\rho_2) \leq D(\rho_1, \rho_2)$$

⇒ no trace preserving quantum operation can increase the distinguishability of two states



Dynamics of initial state pairs

$$\rho_S^{1,2}(0) \longrightarrow \rho_S^{1,2}(t) = \Phi_t\, \rho_S^{1,2}(0)$$



Trace distance evolution:

$$D(t) = D(\rho_S^1(t), \rho_S^2(t)) \leq D(\rho_S^1(0), \rho_S^2(0))$$

Monotonic decrease of $D(t)$: Decrease of distinguishability:

Flow of information from system to environment

$D(t)$ temporarily increases: Increase of distinguishability:

Flow of information from environment back to system

Definition of quantum non-Markovianity

Definition: A quantum process Φ_t is **non-Markovian** iff

$$\sigma(t) = \frac{d}{dt} D(\rho_S^1(t), \rho_S^2(t)) > 0$$

for some initial state pair $\rho_S^{1,2}(0)$ and some time $t > 0$

- Increase of the distinguishability of the states $\rho_S^{1,2}$
- Flow of information from environment back to system
- Environment acts as memory

Example: Non-Markovian decay

Spectral density:

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

Spectral width:

$$\lambda = \tau_E^{-1}$$

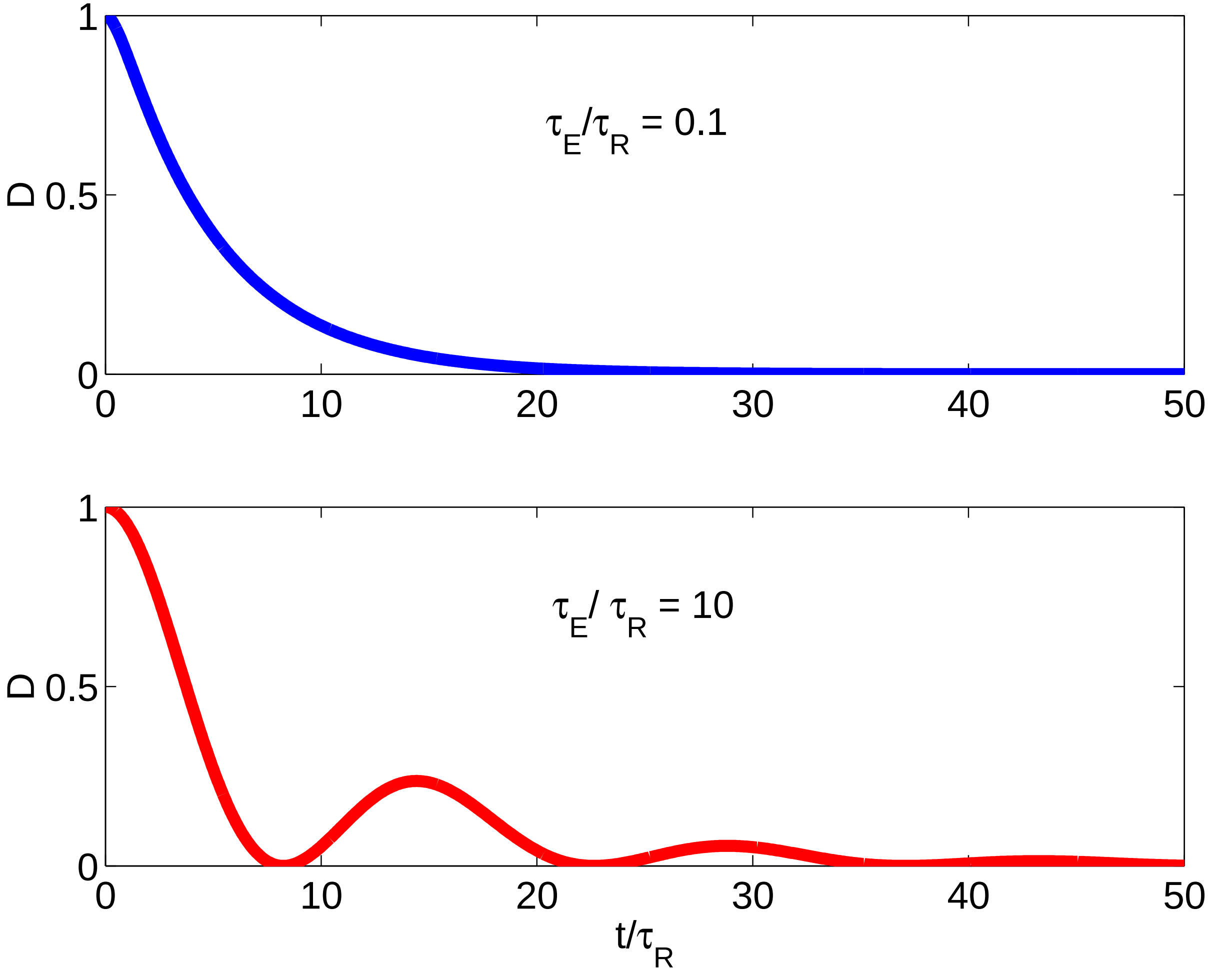
Relaxation rate:

$$\gamma_0 = \tau_R^{-1}$$

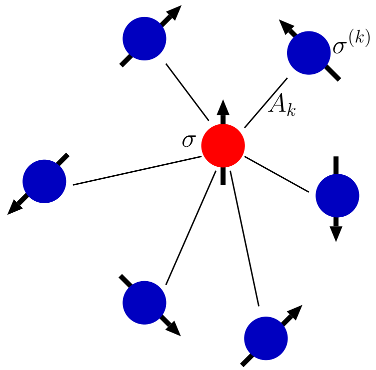
Initial states:

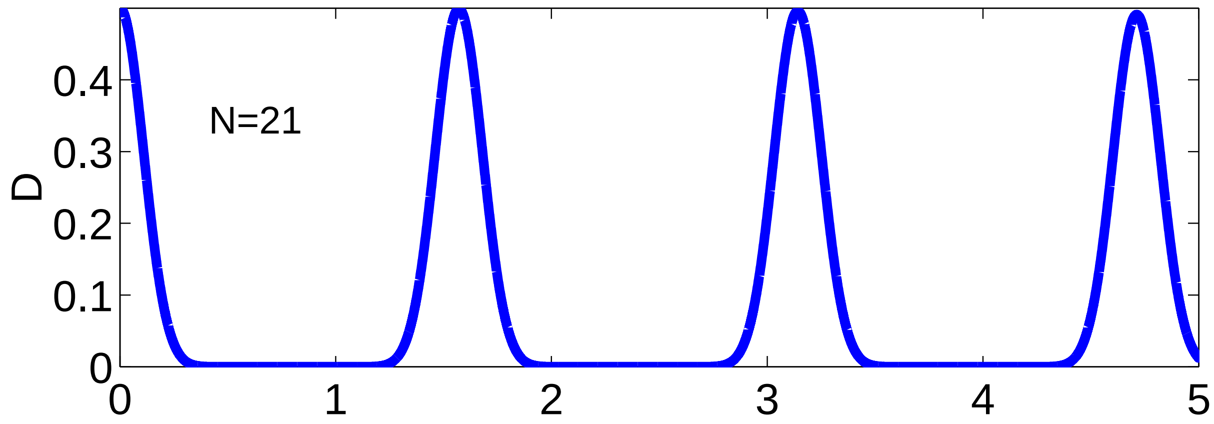
$$\rho_1(0) = |1\rangle\langle 1|$$

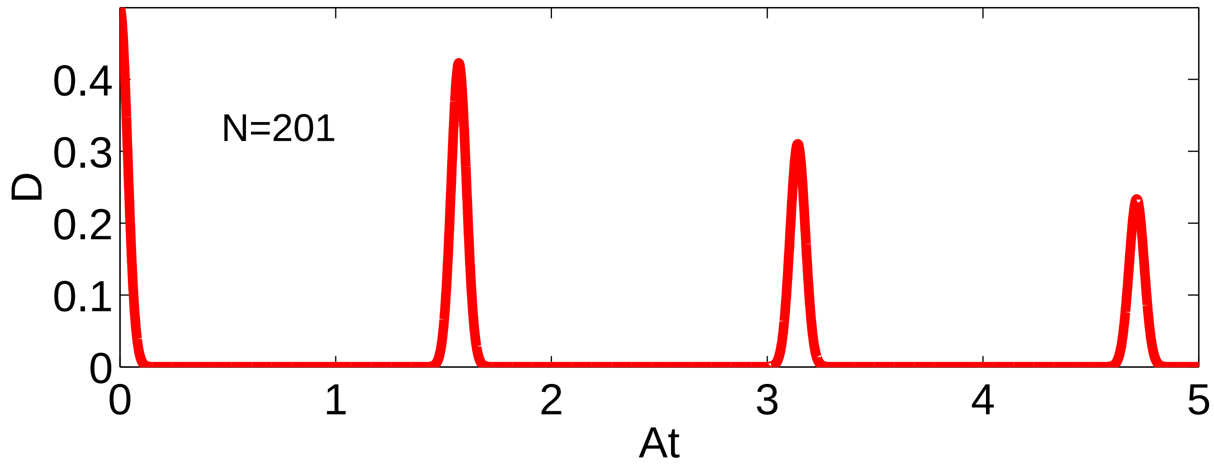
$$\rho_2(0) = |0\rangle\langle 0|$$



Example: Spin bath







Hamiltonian:

$$H = \frac{\omega_0}{2}\sigma_3 + \sum_{k=1}^{N} A_k \, \vec{\sigma} \cdot \vec{\sigma}^{(k)}$$

Initial states:

$$\begin{aligned} \rho_1(0) &= |\psi\rangle\langle\psi| \\ |\psi\rangle &= \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle) \\ \rho_2(0) &= \frac{1}{2}I \end{aligned}$$

Measure for non-Markovianity

$$\mathcal{N}(\Phi) = \max_{\rho_S^{1,2}(0)} \int_{\sigma>0} dt\, \sigma(t) \qquad \sigma(t) = \frac{d}{dt} D(\rho_S^1(t), \rho_S^2(t))$$

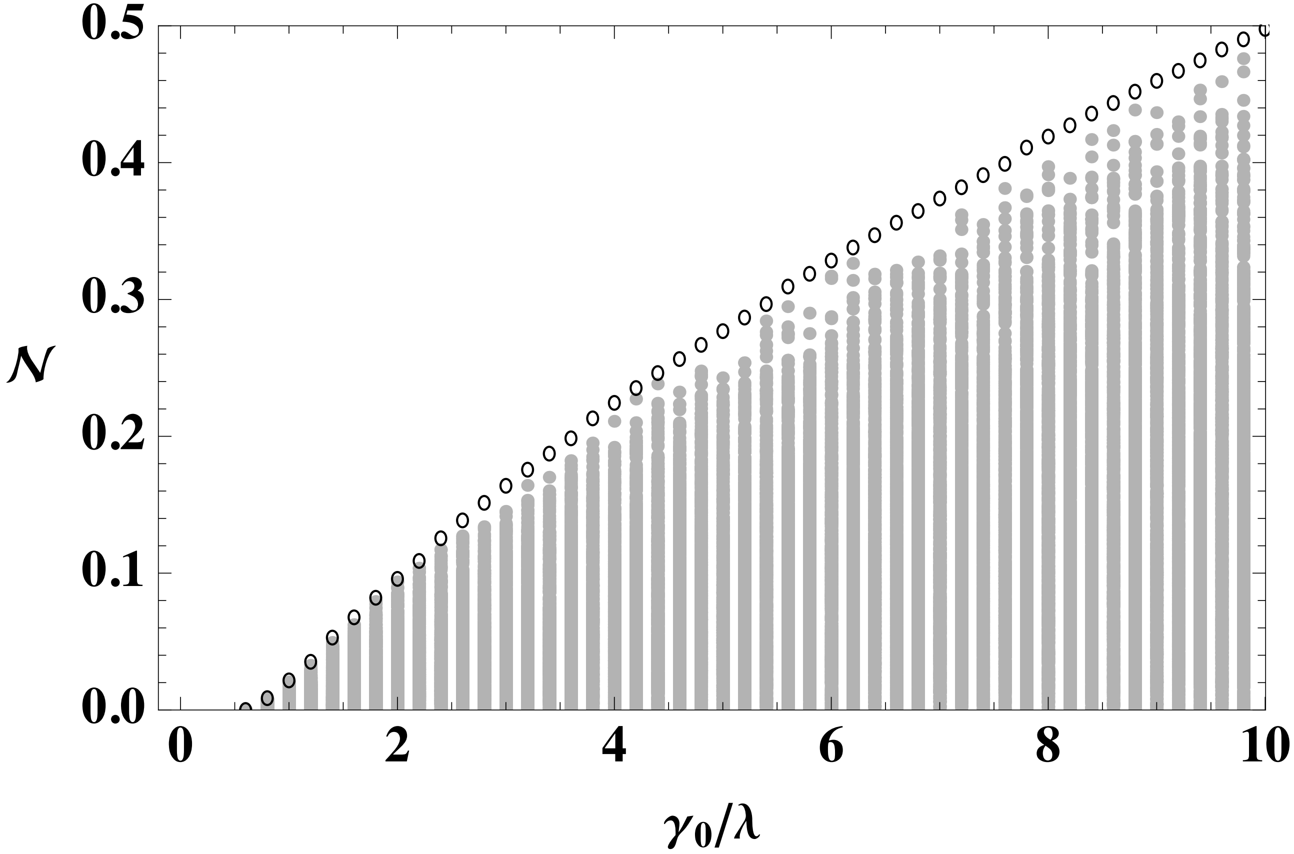
- Measures total backflow of information
- Summation over all time intervals in which $\sigma > 0$
- Maximum over all pairs of initial states $\rho_S^{1,2}(0)$
- $\mathcal{N}(\Phi) > 0 \Longleftrightarrow$ process non-Markovian
- Possible values: $0 \leq \mathcal{N}(\Phi) \leq +\infty$

HPB, E.-M. Laine, J. Piilo, Phys. Rev. Lett. 103, 210401 (2009)

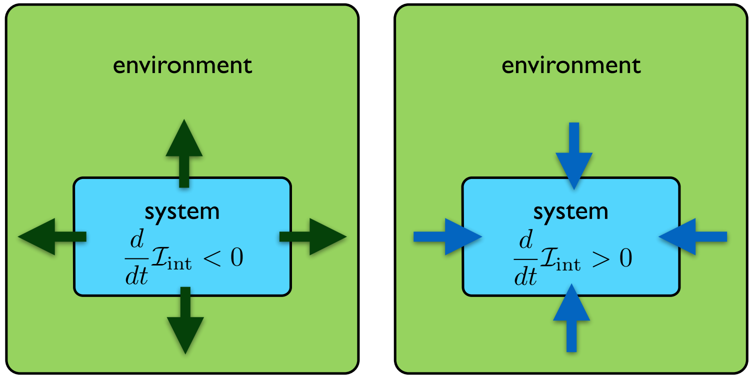
Example: Non-Markovian decay

Gray dots: Random pairs of initial states

Circles: Optimal pure initial state pair: $\left(|1\rangle \pm |0\rangle\right)/\sqrt{2}$



Information flow



Information inside open system:

$$\mathcal{I}_{\rm int}(t) = D(\rho_S^1(t), \rho_S^2(t))$$

Information outside open system:

$$\mathcal{I}_{\rm ext}(t) = D(\rho^1(t), \rho^2(t)) - D(\rho_S^1(t), \rho_S^2(t)) \geq 0$$

Information flow:

$\frac{d}{dt}\mathcal{I}_{\rm int}(t) < 0$ **open system looses information (Markovian)**

$\frac{d}{dt}\mathcal{I}_{\rm int}(t) > 0$ **open system gains information (non-Markovian)**

Information flow

Conservation of information:

$$\mathcal{I}_{\rm int}(t) + \mathcal{I}_{\rm ext}(t) = \mathcal{I}_{\rm int}(0) = \textbf{const}$$

General inequality based on properties of the trace distance:

$$\mathcal{I}_{\rm ext}(t) \leq D(\rho^1(t), \rho_S^1(t) \otimes \rho_E^1(t)) + D(\rho^2(t), \rho_S^2(t) \otimes \rho_E^2(t)) + D(\rho_E^1(t), \rho_E^2(t))$$

Interpretation: Information outside the open system implies

system-environment correlations

or different environmental states

Generalizing the trace distance measure

- Alice prepares two quantum states $\rho_S^{1,2}$ with probabilities $p_{1,2}$ which **need not be equal** (biased preparation of states)

- The maximal probability for a successful state discrimination Bob can achieve by an **optimal strategy** is given by

$$P_{\max} = \frac{1}{2}\{1 + ||\Delta||\}$$

where **Δ is the Helstrom matrix:**

$$\Delta = p_1\rho_S^1 - p_2\rho_S^2$$

D. Chruscinski, A. Kossakowski, A. Rivas, Phys. Rev. A 83, 052128 (2011)

Generalized definition of non-Markovianity

Replacing the trace distance by the norm of the Helstrom matrix leads to generalized non-Markovianity measure:

$$\mathcal{N}(\Phi) = \max_{||\Delta||=1} \int_{\sigma>0} dt\, \sigma(t) \qquad \sigma(t) = \frac{d}{dt}||\Phi_t \Delta||$$

where the maximum is taken over all Helstrom matrices with unit trace norm:

$$\Delta = p_1 \rho_S^1 - p_2 \rho_S^2 \qquad ||\Delta|| = 1$$

S. Wißmann, B. Vacchini, HPB, Phys. Rev. A 92, 042108 (2015)

Generalized definition of non-Markovianity

Advantages of this approach:

- **Markovianity is equivalent to P-divisibility** of dynamical maps
- **Orthogonality of optimal state pairs** and **local representation**
- It leads to a **general classification** of quantum processes in open systems
- It yields direct connection to notion of a **classical Markov process**

Divisibility of quantum processes

If inverse of dynamical maps exists we define for all $t \geq s \geq 0$:

$$\Phi_{t,s} = \Phi_t \, \Phi_s^{-1} \implies \Phi_{t,0} = \Phi_{t,s} \, \Phi_{s,0}$$

Definition:

$\Phi_{t,s}$ **completely positive** $\iff$ **process is CP-divisible**

$\Phi_{t,s}$ **positive** $\iff$ **process is P-divisible**

Definition of non-Markovianity based on CP-divisibility:

A. Rivas, S. F. Huelga, M. B. Plenio, Phys. Rev. Lett. 105, 050403 (2010)

M.M. Wolf, J. Eisert, T. S. Cubitt, J. I. Cirac, Phys. Rev. Lett. 101, 150402 (2008)

For generalized definition based on Helstrom matrix:

Markovianity is equivalent to P-divisibility

Proof: By use of Kossakowski theorem (Rep. Math. Phys. 3, 247 (1972))

Relation to time-local master equation

Most general structure of time-local master equation:

$$\frac{d}{dt}\rho_S = \mathcal{K}_t \, \rho_S$$
$$= -i\left[H_S(t), \rho_S\right] + \sum_i \gamma_i(t)\left[A_i(t)\rho_S A_i^\dagger(t) - \frac{1}{2}\left\{A_i^\dagger(t)A_i(t), \rho_S\right\}\right]$$

- **Dynamics is CP-divisible if and only if**

$$\gamma_i(t) \geq 0$$

- **Dynamics is P-divisible if and only if**

$$W_{nm}(t) \equiv \sum_i \gamma_i(t) |\langle n|A_i(t)|m\rangle|^2 \geq 0$$

Relation to time-local master equation

Pauli master equation in instantaneous eigenbasis of $\rho_S(t)$:

$$\frac{d}{dt}P_n(t) = \sum_m \left[W_{nm}(t)P_m(t) - W_{mn}(t)P_n(t) \right]$$

where

$$W_{nm}(t) = \sum_i \gamma_i(t) |\langle n(t)|A_i(t)|m(t)\rangle|^2$$

$\Longrightarrow$ can be interpreted as **Chapman-Kolmogorov equation of a classical Markov process if and only if**

$$W_{nm}(t) \geq 0$$

Conclusion:

quantum Markovian $\Longleftrightarrow$ P-divisible $\Longrightarrow$ classical Markovian

Local representation and classification of dynamics

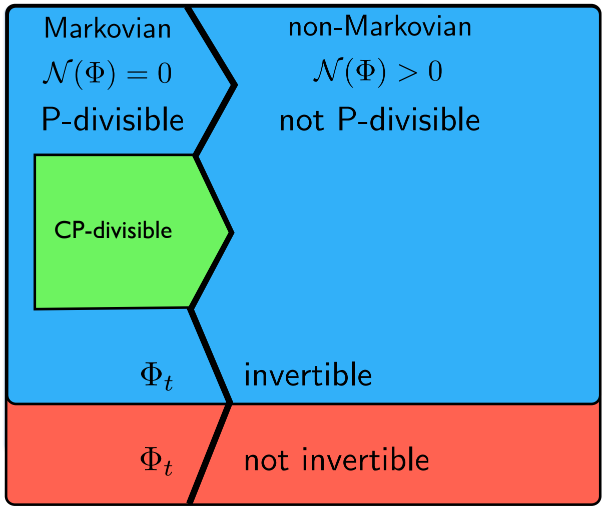
- **Orthogonality of optimal state pairs:**

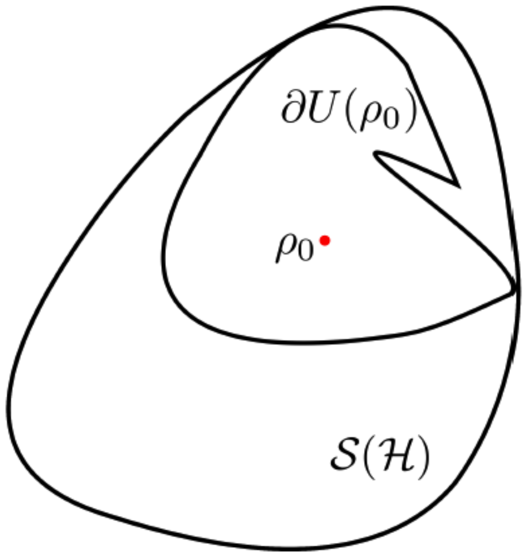
$$\mathcal{N}(\Phi) = \max_{p_{1,2},\, \rho_S^1 \perp \rho_S^2} \int_{\sigma>0} dt\, \sigma(t) \qquad \sigma(t) = \frac{d}{dt}||\Phi_t \Delta||$$

- **Local representation:**

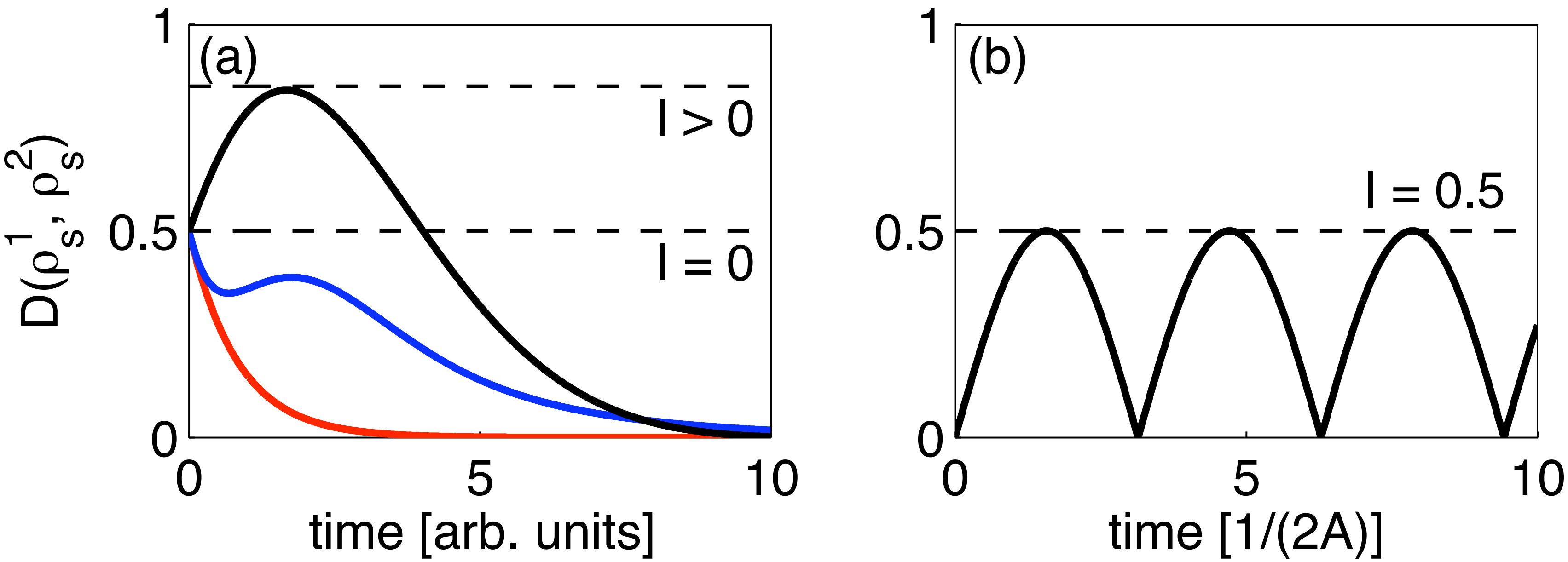
$$\mathcal{N}(\Phi) = \max_{p_{1,2},\, \rho \in \partial U(\rho_0)} \int_{\sigma>0} dt\, \sigma(t) \qquad \sigma(t) = \frac{d}{dt}||\Phi_t \Delta||/||\Delta||$$

- **Classification of quantum processes:**





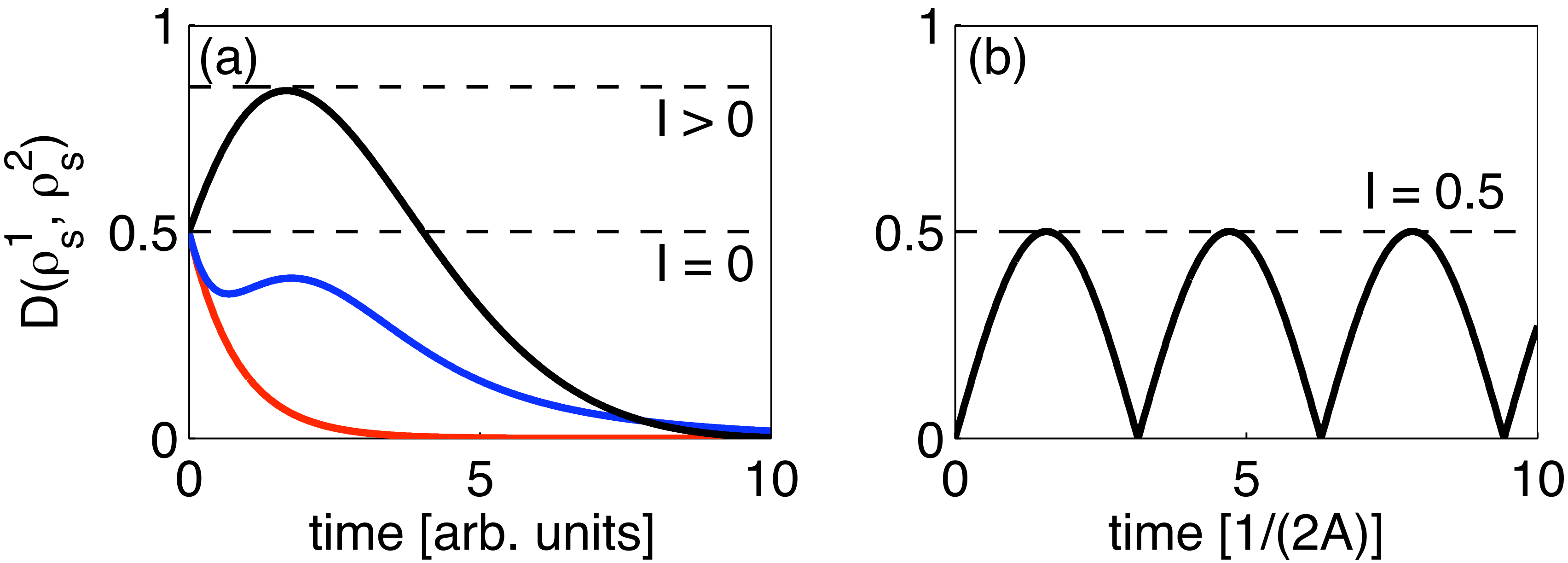
Initial correlations



- **Increase of the trace distance over initial value implies initial system-environment correlations**

- **local detection of correlations**

Initial correlations



Measure for correlations in total state ρ:

$D(\rho, \rho_S \otimes \rho_E)$ = **distinguishability of ρ and $\rho_S \otimes \rho_E$**

Dynamics with initial correlations:

$$D\left(\rho_S^1(t), \rho_S^2(t)\right) - D(\rho_S^1, \rho_S^2)$$
$$\leq D(\rho_{SE}^1, \rho_S^1 \otimes \rho_E^1) + D(\rho_{SE}^2, \rho_S^2 \otimes \rho_E^2) + D(\rho_E^1, \rho_E^2)$$

Dynamical detection of initial correlations

Given state: ρ

Generate second state ρ' **by local operation** Φ**:**

$$\rho' = (\Phi \otimes I)\rho$$

Implications:

- **Environmental states are identical:**

$$\rho_E = \rho'_E$$

- **No correlations are created:**

$$\rho \text{ uncorrelated} \Longrightarrow \rho' \text{ uncorrelated}$$

Dynamical detection of initial correlations

Change of local trace distance:

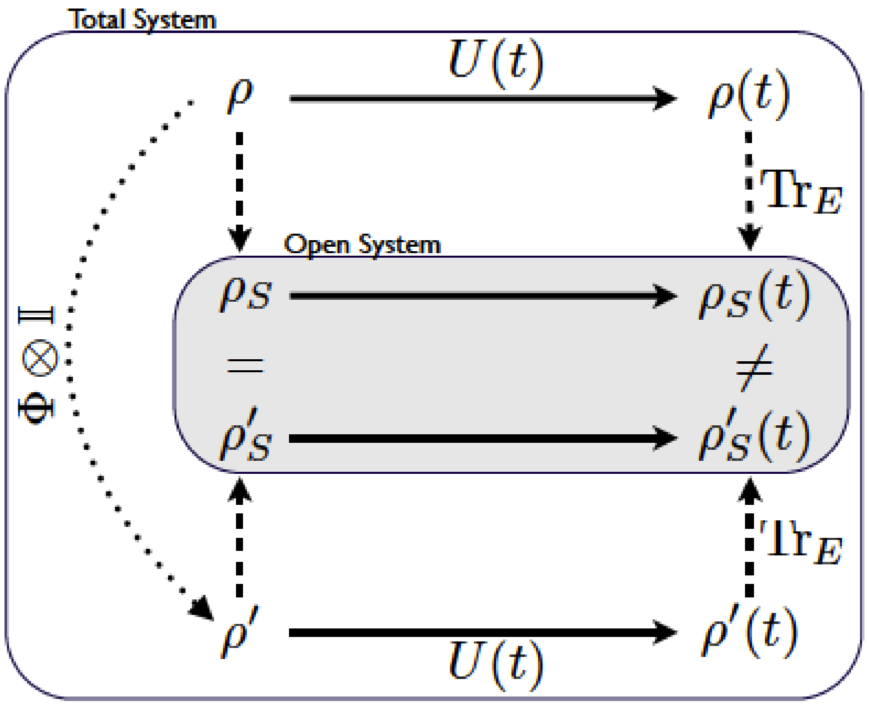
$$D(\rho_S(t), \rho'_S(t)) - D(\rho_S(0), \rho'_S(0)) \leq D(\rho, \rho_S \otimes \rho_E) + D(\rho', \rho'_S \otimes \rho_E)$$

Consequences:

- **Any increase of the trace distance over initial value implies that ρ was correlated**
- **Initial correlations in ρ become dynamically perceivable in the open system at later times**
- **General scheme does not require knowledge of total state, environment, interaction Hamiltonian...**

E. M. Laine, J. Piilo, H. P. B, EPL 92, 60010 (2010)

Local detection of quantum correlations



Φ = local dephasing map

$$D(\rho_S(t), \rho'_S(t)) \leq D(\rho(0), \rho'(0))$$

$\Longrightarrow$ lower bound for quantum correlations (quantum discord)

M. Gessner, H. P. B., Phys. Rev. Lett. 107, 180402 (2011)

M. Gessner, M. Ramm, T. Pruttivarasin, A. Buchleitner, H. P. B. Breuer, H. Häffner, Nature Physics 10, 105 (2014)

Summary

- **Non-Markovian processes:**

$$\sigma(t, \rho_{1,2}(0)) = \frac{d}{dt} D(\rho_1(t), \rho_2(t)) > 0$$

$\Longrightarrow$ **Reversed flow of information from environment to system**

- **Measure for non-Markovianity:**

$$\mathcal{N}(\Phi) = \max_{\rho_{1,2}(0)} \int_{\sigma>0} dt\, \sigma(t, \rho_{1,2}(0))$$

$\Longrightarrow$ **Measure for total backflow of information**

- **Increase of trace distance over initial value:**

$$D(\rho_S(t), \rho'_S(t)) - D(\rho_S(0), \rho'_S(0)) \leq D(\rho, \rho_S \otimes \rho_E) + D(\rho', \rho'_S \otimes \rho_E)$$

$\Longrightarrow$ **local witness for initial quantum correlations**

Further applications

- **Brownian motion/Optomechanical systems:**
  S. Gröblacher, A. Trubarov, N. Prigge, G. D. Cole, M. Aspelmeyer, J. Eisert, Nat. Commun. 6, 7606 (2015)
- **Chaotic systems:**
  C. Pineda, T. Gorin, D. Davalos, D. A. Wisniacki, I. Garcia-Mata, Phys. Rev. A 93, 022117 (2016)
- **Energy transfer in photosynthetic complexes:**
  P. Rebentrost, A. Aspuru-Guzik, J. Chem. Phys. 134, 101103 (2011)
- **Quantum metrology:**
  A.W. Chin, S. F. Huelga, M. B. Plenio, Phys. Rev. Lett. 109, 233601 (2012)
- **Quantum phase transitions:**
  M. Gessner, M. Ramm, H. Häffner, A. Buchleitner, HPB, EPL 107, 40005 (2014)
- **Anderson localization:**
  S. Lorenzo, F. Lombardo, F. Ciccarello, G. M. Palma, arXiv:1609.04158
- ...

Experiments

- **Photonic systems:**

  B.-H. Liu, L. Li, Y.-F. Huang, C.-F. Li, G.-C. Guo, E.-M. Laine, HPB, J. Piilo, Nat. Phys. 7, 931 (2011)

  A. Smirne, D. Brivio, S. Cialdi, B. Vacchini, M.G.A. Paris, Phys. Rev. A 84, 032112 (2011)

  J.-S. Tang, Y.-T.Wang, G. Chen, Y. Zou, C.-F. Li, G.-C. Guo, Y. Yu, M.-F. Li, G.-W. Zha, H.-Q. Ni, Z.-C. Niu, M. Gessner, HPB, Optica 2, 1014 (2015)

- **NMR:**

  N.K. Bernardes, J.P.S. Peterson, R.S. Sarthour, A.M. Souza, C.H. Monken, I. Roditi, I.S. Oliveira, M.F. Santos, Sci. Rep. 6, 33945 (2016)

- **Trapped ions:**

  M. Gessner, M. Ramm, T. Pruttivarasin, A. Buchleitner, HPB, H. Häffner, Nat. Phys. 10, 105 (2014)

  M. Wittemer, G. Clos, HPB, U. Warring, T. Schaetz, arXiv:1702.07518 [quant-ph]