Quantum Non-Markovianity: A Physicist's Perspective

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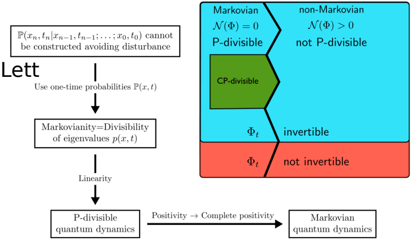
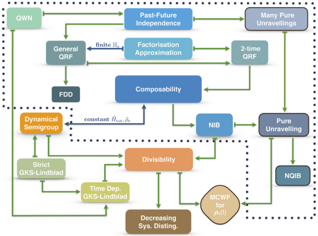
Brief historical perspective

- 2008 Wolf, Eisert, Cubitt, & Cirac, Phys Rev Lett
- 2009 Breuer, Laine, & Piilo, Phys Rev Lett
- 2010 Rivas, Huelga, & Plenio, Phys Rev Lett
- 2014 Rivas, Huelga, & Plenio, Rep Prog Phys
- 2016 Breuer, Laine, Piilo, & Vacchini, Rev Mod Phys
- 2018 Li, Hall, & Wiseman, Phys Rep





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Answers

1. Yes! Use linear response theory. Strasberg, Esposito, PRL **121**, 040601 (2018) A single absorption/emission spectrum suffices to quantify non-Markovianity. Cerrillo, Strasberg, in preparation
2. During the irreversible relaxation of an open system to equilibrium (temporal) negativities of the entropy production rate imply non-Markovianity Strasberg, Esposito, PRE **99**, 012120 (2019); Strasberg, arXiv 1907.01804

Open quantum systems and non-Markovianity: The standard approach

- dynamical map assuming that $\rho_{SB}(t_0) = \rho_S(t_0) \otimes \rho_B(t_0)$

$$\rho_S(t) = \Lambda(t, t_0)\rho_S(t_0),$$
$$\Lambda(t, t_0) = \mathrm{tr}_B \left\{ e^{\mathcal{L}(t-t_0)} \rho_B(t_0) \right\}$$

  with $\mathcal{L}\rho_{SB}(t) \equiv -i[H_{SB}, \rho_{SB}(t)]$
- $\Lambda(t, t_0)$ is completely positive and trace-preserving (cptp)
- quantum Chapman-Kolmogorov equation ('divisibility'): there exists a set of cptp maps $\{\tilde{\Lambda}(t, s) | t > s > t_0\}$ such that

$$\Lambda(t, t_0) = \tilde{\Lambda}(t, s)\Lambda(s, t_0)$$

Linear response theory in a nutshell

- setup:

$$H_S - \delta(t - t_0) \sum_i a_i A_i + H_I + H_B \quad (A_i - \text{system operator})$$

$$\rho_{SB}(t < t_0) = \rho_{SB}^{\text{eq}} \sim e^{-\beta(H_S + H_I + H_B)}$$

- initial kick disturbs the equilibrium state:

$$\rho_{SB}(t < t_0) \mapsto \rho_{SB}(t_0) = U_S \rho_{SB}^{\text{eq}} U_S^\dagger, \quad U_S = e^{\frac{i}{\hbar} \sum_i a_i A_i}$$

- system response within linear order of the a_i (Kubo formula)

$$\langle A_i \rangle(t) = \sum_j \chi_{ij}(t - t_0) a_j, \quad \chi_{ij}(t) \equiv \frac{i}{\hbar} \Theta(t) \langle [A_i(t), A_j] \rangle_\beta$$

- initial nonequilibrium value of the observables

$$\langle A_i \rangle(t_0) = \sum_j \chi_{ij}(0) a_j \quad (\text{assuming } \langle A_i \rangle_\beta = 0)$$

Non-Markovianity in the linear response regime

Strasberg, Esposito, PRL 2018

- $\langle \mathbf{A} \rangle(t_0) = \chi(0)\mathbf{a} \Rightarrow$ if $\chi(0)$ is invertible: $\mathbf{a} = \chi^{-1}(0)\langle \mathbf{A} \rangle(t_0)$
- closed dynamical description of the system observables

$$\begin{aligned}\langle \mathbf{A} \rangle(t) = \chi(t-t_0)\mathbf{a} &= \chi(t-t_0)\chi^{-1}(0)\langle \mathbf{A} \rangle(t_0) \\ &\equiv G(t-t_0)\langle \mathbf{A} \rangle(t_0)\end{aligned}$$

- if the dynamics are Markovian, the propagator $G(t)$ must be divisible:

$$\boxed{G(t) = G(t-s)G(s) \quad \forall s \in (0,t)}$$

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Application: quantum Brownian motion

non-perturbative results indicate complex non-Markovian behaviour

Remark: the quantum regression theorem...

...can be also checked for the equilibrium correlation functions due to the FDT

Non-Markovianity in emission/absorption spectra of multichromophoric systems Cerrillo, Strasberg, in preparation

$$H_{SB} = H_S + \sum_i |e_i\rangle\langle e_i| X_I + H_E, \quad H_E = \sum_i \sum_{k_i} \omega_{k_i} a^\dagger_{k_i} a_{k_i}$$

$$H_S = \sum_i \epsilon_i |e_i\rangle\langle e_i| + \sum_{i<j} v_{ij} |e_i\rangle\langle e_j| + H.c., \quad X_i = \sum_{k_i} \gamma_{k_i}(a_{k_i} + a^\dagger_{k_i})$$

- dipole operator $\mu = \sum_i |e_i\rangle\langle g| + H.c.$
- emission/absorption spectrum (Buser, Cerrillo, Schaller, Cao, PRA 2017)

$$E(t) = \text{tr}\{\mu(t)\mu P_e \rho^{\text{eq}}_{SB} P_e\}$$
$$A(t) = \text{tr}\{\mu(t)\mu P_g \rho^{\text{eq}}_{SB} P_g\} = E(t - i\beta)$$

Knowledge of $E(t)$ *or* $A(t)$ suffices to quantify non-Markovianity!

Entropy production in open systems: Phenomenology

- driven system in contact with a single heat reservoir initially at temperature T:

$$H_{SB}(\lambda_t) = H_S(\lambda_t) + H_I + H_B$$

- second law: entropy production in time-interval $[0, t]$:

$$\Sigma(t) = \Delta S_S(t) - \beta Q(t) \geq 0$$

- entropy production *rate*:

$$\dot{\Sigma}(t) = \frac{d}{dt} S_S(t) - \beta \dot{Q}(t)$$

- **questions:** $\dot{\Sigma}(t) < 0$ possible? What does it mean?

The standard Born-Markov secular (BMS) approach of quantum thermodynamics (Kosloff, Entropy 2013)

$$\dot{\Sigma}_{\mathrm{BMS}}(t) = - \left.\frac{\partial}{\partial t}\right|_{\lambda_t} D\left[\rho_S(t) \middle\| \frac{e^{-\beta H_S(\lambda_t)}}{\mathcal{Z}_S(\lambda_t)}\right] \geq 0$$

$$\text{with } D[\rho\|\sigma] \equiv \mathrm{tr}\{\rho(\ln\rho - \ln\sigma)\}$$

Positivity of $\dot{\Sigma}_{\mathrm{BMS}}(t)$ follows from

1. Gibbs state is "instantaneous fixed point" of the dynamics:

$$\partial_t \rho_S(t) = \mathcal{L}(\lambda_t)\rho_S(t) \;\Rightarrow\; \mathcal{L}(\lambda_t)\frac{e^{-\beta H_S(\lambda_t)}}{\mathcal{Z}_S(\lambda_t)} = 0$$

2. dynamics are Markovian: $\partial_t D[\rho(t)\|\sigma(t)] \leq 0 \;\forall \rho(t), \sigma(t)$

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Beyond BMS: $\dot{\Sigma}_{\mathrm{BMS}}(t)$ no longer valid!

1. $\Sigma_{\mathrm{BMS}}(t) = \int_0^t ds \dot{\Sigma}_{\mathrm{BMS}}(s)$ is not always positive
2. $\dot{\Sigma}_{\mathrm{BMS}}(t) < 0$ even for Markovian dynamics (Strasberg, Esposito, PRE 2019)

A better approach based on the Hamiltonian of mean force

Seifert, PRL 2016; Miller, Anders, PRE 2017; Strasberg, Esposito, PRE 2017

- when left on its own, the system relaxes to the equilibrium state

$$\frac{e^{-\beta H_S^*}}{\mathcal{Z}_S^*} \neq \frac{e^{-\beta H_S}}{\mathcal{Z}_S}, \quad H_S^* \equiv -\frac{1}{\beta} \ln \frac{\mathrm{tr}_B\{e^{-\beta H_{SB}}\}}{\mathcal{Z}_B}$$

H_S^* = Hamiltonian of mean force (Kirkwood, JCP 1935)

- good candidate for entropy production rate in the classical case (Strasberg, Esposito, PRE 2019)

$$\dot{\Sigma}(t) = -\left.\frac{\partial}{\partial t}\right|_{\lambda_t} D\left[\rho_S(t) \left\| \frac{e^{-\beta H_S^*(\lambda_t)}}{\mathcal{Z}_S^*(\lambda_t)}\right.\right]$$

- $\Sigma(t) = \int_0^t ds \dot{\Sigma}(s) \geq 0$ always, but $\dot{\Sigma}(t) < 0$ possible

Results

Strasberg, Esposito, PRE 2019; Strasberg, arXiv 1907.01804

- two sources of non-equilibrium:
  1. driving: $\dot{\lambda}_t \neq 0$
  2. initial out of equilibrium state: irreversible relaxation to equilibrium for $\dot{\lambda}_t = 0$
- main results:
  1. $\dot{\Sigma}(t) < 0 \Rightarrow$ the bath is not in a conditional equilibrium state
  2. $\dot{\Sigma}(t) < 0 \Rightarrow$ non-Markovian dynamics in a rigorous sense!

For quantum systems (Strasberg, arXiv 1907.01804)

The same story, but more subtleties in the details (e.g., how to prepare a non-equilibrium state in a thermodynamically consistent way?)

Summary

- Simple way to detect non-Markovianity:
  - use linear response theory Strasberg, Esposito, PRL **121**, 040601 (2018)
  - single emission/absorption spectrum suffices Cerrillo, Strasberg, in preparation
- connection to non-equilibrium thermodynamics at strong coupling: $\dot{\Sigma}(t) < 0 \Rightarrow$ non-Markovianity for $\dot{\lambda}_t = 0$
  - for classical systems Strasberg, Esposito, PRE **99**, 012120 (2019)
  - for quantum systems Strasberg, arXiv 1907.01804

Quantum thermodynamics for young scientists
(Workshop Bad Honnef, Feb. 3 – 6 2020)

+ tutorial lectures by:
  - **Géraldine Haack** (*mesoscopic physics & quantum transport*)
  - **Javier Cerrillo** (*open quantum systems*)
  - **Nicole Yunger-Halpern** (*quantum info & resource theories*)
  - **Markus Müller** (*many-body physics & equilibration*)
+ many contributed talks
+ special non-physics lecture
  - **Ben Martin** (*What's happening to our universities?*)

Marti
Perarnau-Llobet