Entropy production under non-Markovian dynamical maps

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Introduction

Consider an open quantum system undergoing a **non-Markovian** time-evolution such that the unique asymptotic state is a Gibbs state ϱ_β.
Let us construct the internal **entropy production** as in the Markovian case [1, 2]

$$\boldsymbol{\sigma_t} := \partial_t S_t - \beta \partial_t Q_t, \tag{1}$$

where the heat flux and the entropy variation are defined as follows

$$\partial_t S_t := -\mathrm{Tr}\left[\partial_t \varrho_t \log \varrho_t\right], \tag{2}$$
$$\partial_t Q_t := \mathrm{Tr}\left[\partial_t \varrho_t H\right]. \tag{3}$$

QUESTIONS:

1. **Is the inequality $\boldsymbol{\sigma_t} \geq 0$ true under non-Markovian dynamics?**
2. **Is $\boldsymbol{\sigma_t} \geq 0$ a proper statement of the second law of thermodynamics in a non-Markovian scenario?**

Non-Markovian dynamics

There are many different approaches to non-Markovianity in the quantum domain. In the following we adopt that one based on divisibility of the dynamical map.
A one-parameter family of dynamical maps Λ_t,

$$\Lambda_t = V_{t,s}\Lambda_s, \qquad t \geq s \geq 0, \tag{4}$$

is called

(i) **CP-divisible** if $V_{t,s}$ is completely positive (CP) for all t, s,

(ii) **P-divisible** if $V_{t,s}$ is positive (P) for all t, s.

Following the classification given in Ref. [3] one can say

- Λ_t **non-Markovian** $:=$ Λ_t non CP-divisible
- Λ_t **essentially non-Markovian** $:=$ Λ_t non P-divisible

Qubit in a thermal bath

Consider the following master equation describing the evolution of a qubit interacting with a thermal bath of harmonic oscillators:

$$\partial_t \varrho_t = -i\left[\frac{\omega}{2}\sigma_z, \varrho_t\right] + \frac{\gamma_t}{2}(n+1)\big(2\sigma_-\varrho_t\sigma_+ - \{\sigma_+\sigma_-, \varrho_t\}\big) + \\ + \frac{\gamma_t}{2} n\big(2\sigma_+\varrho_t\sigma_- - \{\sigma_-\sigma_+, \varrho_t\}\big), \tag{5}$$

where $n = (e^{\beta\omega} - 1)^{-1}$, γ_t is a time-dependent damping rate, and σ_a ($a \in \{x, y, z\}$) are the Pauli matrices (with $\sigma_\pm = \sigma_x \pm i\sigma_y$).

1. **This dynamics is both P-divisible and CP-divisible iff $\boldsymbol{\gamma_t \geq 0\ \forall t}$.**
2. **The internal entropy production** (1) **becomes negative when $\boldsymbol{\gamma_t < 0}$.**

One can find $\boldsymbol{\sigma_t} < 0$ with a non-Markovian dynamics.

References

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General form of the second law

TWO POSSIBLE CONCLUSIONS:

(i) The second law of thermodynamics can be violated by physically legitimate dynamical maps,

(ii) A more careful formulation of the second law should be given.

WE CHOOSE (ii): One can prove a very general statement considering explicitly both system S and bath B in the entropy balance [4, 5], namely

$$\Delta S_S(t) + \Delta S_B(t) \geq 0. \tag{6}$$

This inequality is true provided that the **initial state** of the composite system SB is **factorized**, without particular restrictions on the reduced dynamics of both S and B.
Heuristically, one can think of obtaining $\boldsymbol{\sigma_t} \geq 0$ as a particular case of relation (6) under three assumptions [6]

- $\partial_t S_S(t) + \partial_t S_B(t) \geq 0$ (differential form)
- $\partial_t S_B(t) = \beta \partial_t Q_B(t)$
- $\partial_t Q_B(t) = -\partial_t Q_S(t)$

These **assumptions**, though reasonable, can be **violated** if the system and the bath are strongly coupled and correlated.
Thus one should not consider $\sigma_t \geq 0$ as an *a priori* valid formulation of the second law.

Qubit dephasing

The three assumptions in the previous section can be violated, as we show in the following example. Consider a total Hamiltonian given by $H_{\mathrm{tot}} = H_S + H_B + H_{\mathrm{int}}$ with

$$H_S = \frac{\omega_0}{2}\sigma_z, \quad H_B = \sum_{k=1}^{\infty} \omega_k \mathrm{a}_k^\dagger \mathrm{a}_k\ , \quad H_{\mathrm{int}} = \lambda\sigma_z \otimes \sum_{k=1}^{\infty}\left(f_k^* \mathrm{a}_k + f_k \mathrm{a}_k^\dagger\right),$$

where a_k is the bosonic annihilation operator of mode k, satisfying the canonical commutation relations $[\mathrm{a}_k, \mathrm{a}_l^\dagger] = \delta_{kl}$, and the complex parameters f_k are such that $\sum_{k=1}^{\infty} |f_k|^2 < \infty$.

- **Initial state:** $\varrho_{SB}(0) = \varrho_S(0) \otimes \varrho_B^{(\beta)}$, where $\varrho_S(0)$ is the initial state of the qubit and $\varrho_B^{(\beta)}$ is the Gibbs state of the thermal bath at inverse temperature β
- The **dynamics** of the total system can be **analytically solved** (see Ref. [5] for the details) and by partial tracing one can obtain the reduced density matrices of the two subsystems at any time $\varrho_S(t)$ and $\varrho_B(t)$.
- **Thermodynamic quantities computed for both S and B**

RESULTS:

- × $\partial_t S_S(t) + \partial_t S_B(t) \ngeq 0$ depending on the spectral density
- ✓ $\partial_t S_B(t) = \beta \partial_t Q_B(t)$ up to leading order in λ
- × $\partial_t Q_B(t) \neq -\partial_t Q_S(t)$ due to the correlations

Conclusions

- The internal entropy production defined as in the Markovian case can be negative for non-Markovian time-evolutions
- A more general statement of the second law of thermodynamics can be given considering both system and bath explicitly in the entropy balance
- The usual formulation ($\boldsymbol{\sigma_t} \geq 0$) is recovered under three assumptions that can be violated in physically relevant models, as shown with an explicit example