Fundamental constraints of quantum thermodynamics in the Markovian regime

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TEAM-NET

Outline

1. Motivation
2. Statement of the problem
3. Main technical tool
4. Results
5. Applications
6. Outlook

In collaboration with:

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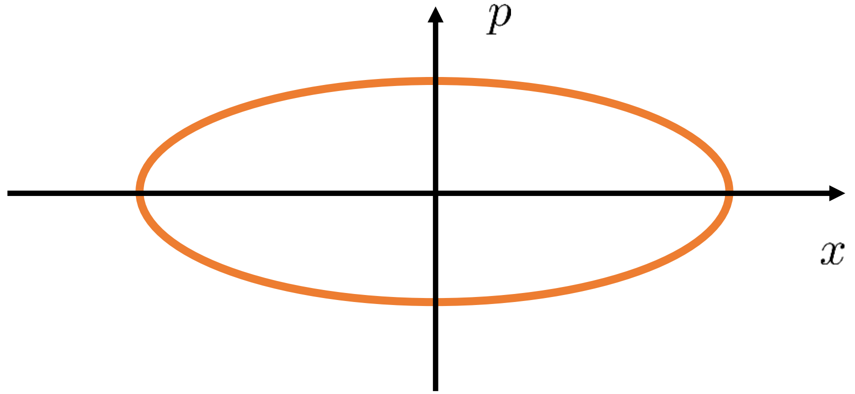
Motivation

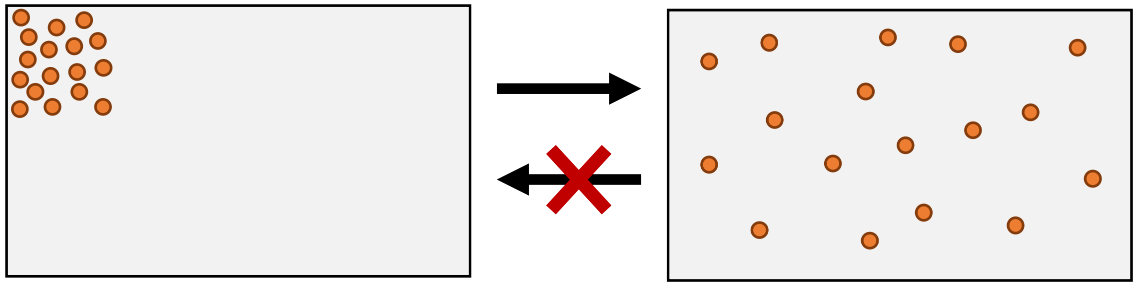
What can we say about the dynamics without solving equations of motion?

Closed systems



Energy conservation

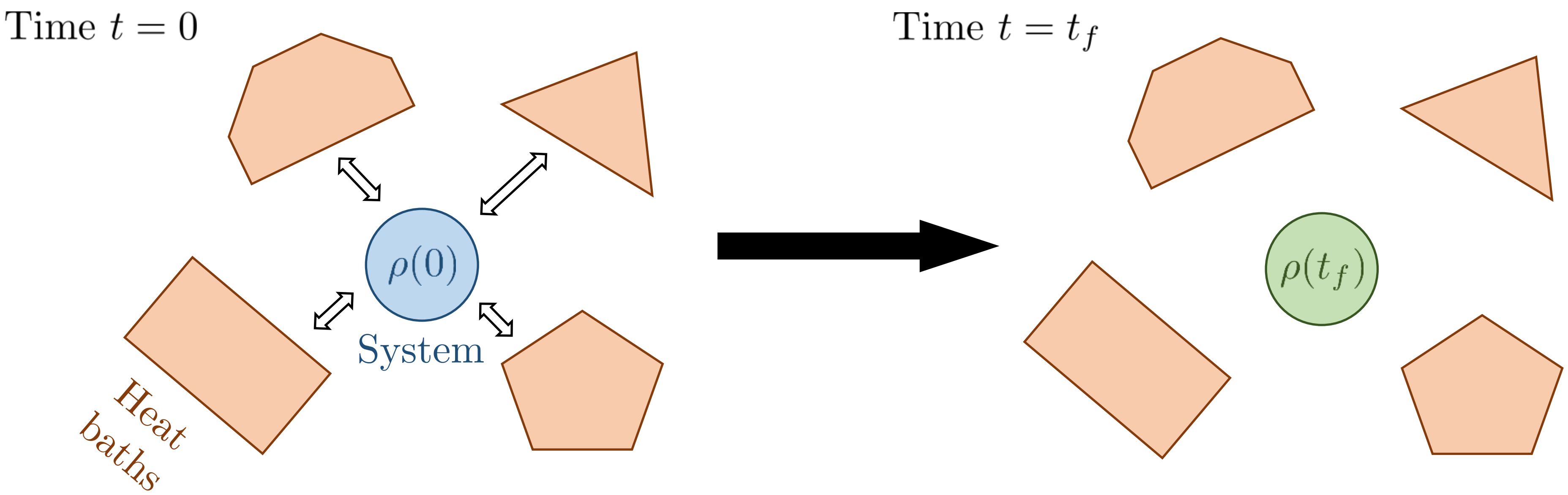
Open systems



Entropy growth

Quantum thermodynamics:
Using minimal assumptions of the quantum theory, find constraints on the evolution of a quantum system interacting with thermal baths.

Statement of the problem



Original question: Given $\rho(0)$ and $\Leftrightarrow$ denoting arbitrary energy-conserving unitary, what can $\rho(t_f)$ be?

M. Horodecki, J. Oppenheim
Nature Commun. **4**, 2059 (2013)

Our question: Given $\rho(0)$ and $\Leftrightarrow$ denoting Markovian energy-conserving interaction, what can $\rho(t_f)$ be?

Formal statement of the problem

General Markovian open quantum dynamics:

$$\frac{d\rho(t)}{dt} = -i[H,\rho(t)] + \mathcal{L}_t(\rho(t)), \quad \text{where} \quad H = \sum_{i=1}^{d} E_i |E_i\rangle\langle E_i| \quad \text{and} \quad \mathcal{L}_t(\rho) = \sum_{i=1}^{d^2-1} r_i(t)\left(L_i \rho L_i^\dagger - \frac{1}{2}\{L_i^\dagger L_i, \rho\}\right)$$

Markovian thermal process (MTP) defined by additional two properties:

- Stationary thermal state: $\forall t: \quad \mathcal{L}_t \gamma = 0, \quad \text{where} \quad \gamma = e^{-\beta H}/\mathrm{Tr}\left(e^{-\beta H}\right)$
- Covariance: $\forall t, \rho: \quad \mathcal{L}_t([H,\rho]) = [H, \mathcal{L}_t(\rho)]$

Solving for possible final states:

$$\rho(0) \xmapsto{\text{MTP}} \rho(t_f)$$

Formal statement of the problem

Covariance encodes total energy conservation at each infinitesimal time and enforces populations and coherences,

$$p_i(t) = \langle E_i|\rho(t)|E_i\rangle, \qquad c_{ij}(t) = \langle E_i|\rho(t)|E_j\rangle$$

to evolve independently.

We can thus analyse a simplified problem:

Solving for possible final energy populations:

$$\boldsymbol{p}(0) \xmapsto{\text{MTP}} \boldsymbol{p}(t_f)$$

Main technical tool

Equation of motion restricted to population reads:

$$\frac{d\boldsymbol{p}(t)}{dt} = L_t \boldsymbol{p}(t), \qquad \text{with} \qquad L_t \boldsymbol{\gamma} = 0 \qquad \left(\text{simplified version of } \frac{d\rho(t)}{dt} = -i[H, \rho(t)] + \mathcal{L}_t(\rho(t))\right)$$

Possible final populations are $T\boldsymbol{p}(0)$ with T being a stochastic matrix satisfying:

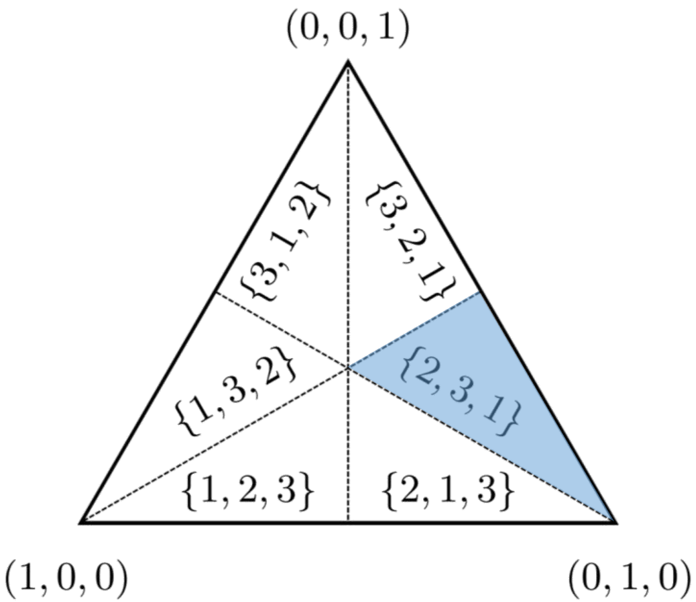
- Stationary thermal state: $T\boldsymbol{\gamma} = \boldsymbol{\gamma}$
- Embeddability: $T = S(t_f)$ with $dS(t)/dt = L_t S(t)$ and $S(0) = \mathbb{1}$

Solution to the first constraint is known as **thermomajorisation**, i.e.,

$$\exists T \text{ such that } T\boldsymbol{\gamma} = \boldsymbol{\gamma} \text{ and } T\boldsymbol{p}(0) = \boldsymbol{p}(t_f) \qquad \Longleftrightarrow \qquad \boldsymbol{p}(0) \succ_{\gamma} \boldsymbol{p}(t_f)$$

Main technical tool

How to verify thermomajorisation condition $\boldsymbol{p} \succ_{\boldsymbol{\gamma}} \boldsymbol{q}$?

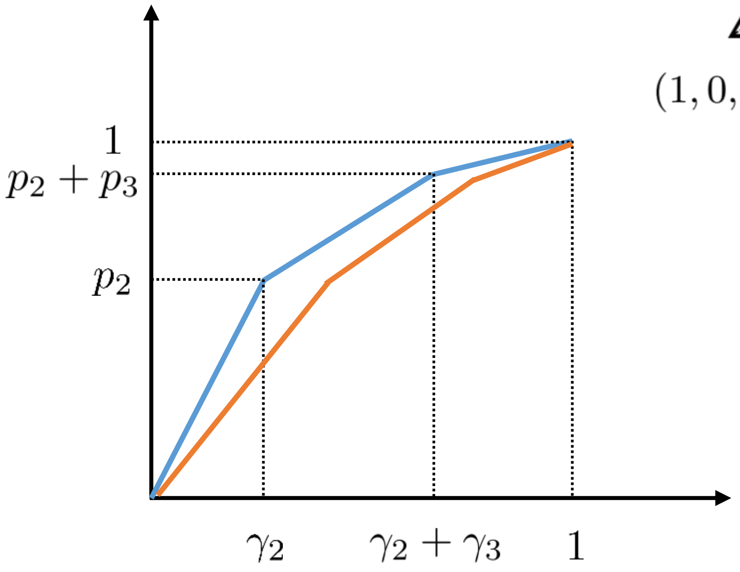


1. Find the γ-ordering of $\boldsymbol{p}$, i.e. arrange p_i/γ_i in a non-increasing order $\downarrow$.

2. Create the Lorenz curve of $\boldsymbol{p}$, i.e. piecewise linear curve with elbow points given by:

$$x_j = \sum_{i=1}^{j} \gamma_i^{\downarrow}, \qquad y_j = \sum_{i=1}^{j} p_i^{\downarrow}$$

3. Do the same for $\boldsymbol{q}$ and check whether the Lorenz curve of $\boldsymbol{q}$ lies below that of $\boldsymbol{p}$.



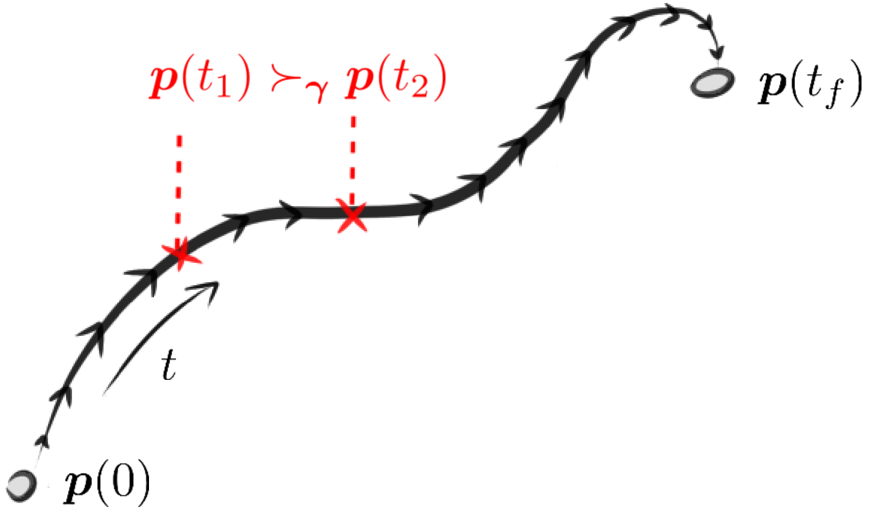
Main technical tool

We introduce **continuous thermomajorisation**:

$$\boldsymbol{p}(0) \ggcurly_\gamma \boldsymbol{p}(t_f)$$

iff there exists a thermomajorising trajectory $\boldsymbol{p}(t)$ such that:

$$\forall t_1, t_2 \in [0, t_f]: \quad t_1 \leq t_2 \Rightarrow \boldsymbol{p}(t_1) \succ_\gamma \boldsymbol{p}(t_2)$$



Why?

Becuase it yields a complete description of population dynamics:

$$\boldsymbol{p}(0) \xmapsto{\text{MTP}} \boldsymbol{p}(t_f) \quad \text{if and only if} \quad \boldsymbol{p}(0) \ggcurly_\gamma \boldsymbol{p}(t_f)$$

Results

Exhaustive H-type theorem:

A dynamical evolution $\boldsymbol{p}(t)$ of populations can be generated by a Markovian thermal process if and only if:

$$\forall a \in [0,1]: \quad \frac{d\Sigma_a(t)}{dt} \geq 0, \qquad \text{where} \qquad \Sigma_a := -\sum_{i=1}^{d} \left| p_i(t) - a\frac{\gamma_i}{\gamma_d} \right|.$$

Universality of elementary thermalisations:

$\boldsymbol{p}(0) \overset{\text{MTP}}{\longmapsto} \boldsymbol{p}(t_f)$ is possible if and only if there exists a sequence of elementary thermalisations such that:

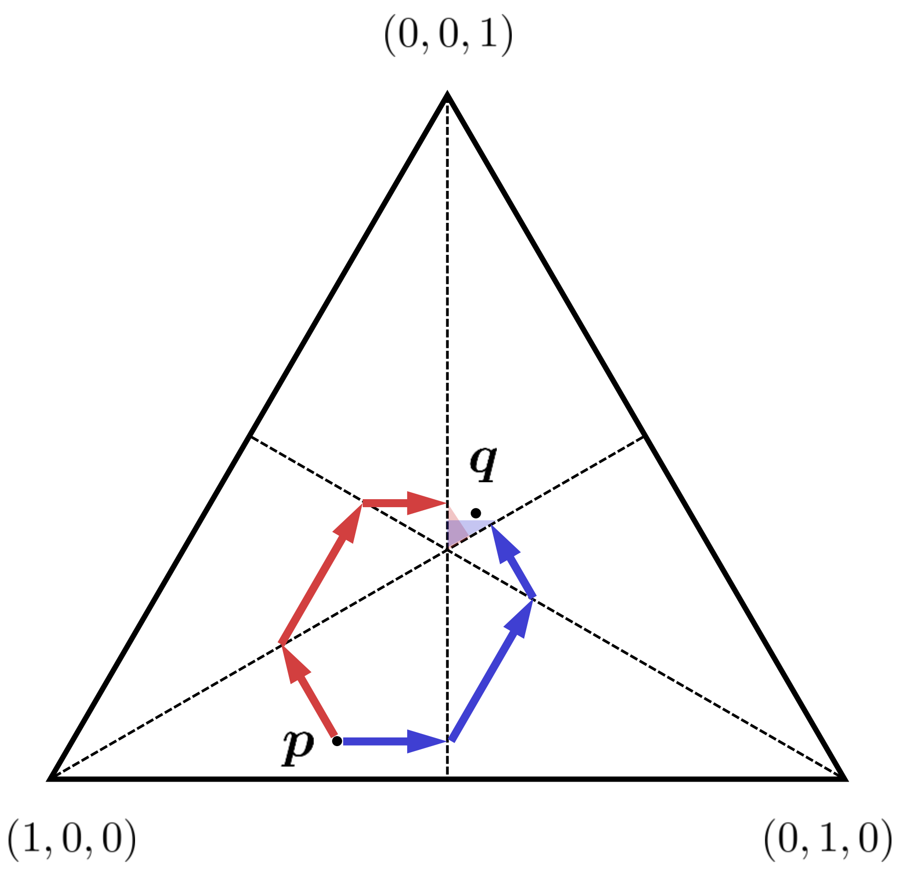
$$\boldsymbol{p}(t_f) = T^{i_f,j_f}(\lambda_f)\ldots T^{i_1,j_1}(\lambda_1)\boldsymbol{p}(0), \quad \text{where} \quad T^{i,j}(\lambda) = \begin{bmatrix} (1-\lambda) + \frac{\lambda\gamma_i}{\gamma_i+\gamma_j} & \lambda\frac{\gamma_i}{\gamma_i+\gamma_j} \\ \lambda\frac{\gamma_j}{\gamma_i+\gamma_j} & (1-\lambda) + \frac{\lambda\gamma_i}{\gamma_i+\gamma_j} \end{bmatrix} \oplus \mathbf{1}_{\setminus(i,j)}$$

Results

Algorithmic verification of $\boldsymbol{p}(0) \overset{\text{MTP}}{\longmapsto} \boldsymbol{p}(t_f)$:

- Only finite set of conditions needs to be verified.
- If the path exists, the algorithm returns the Lindbladian realising it.
- One can also find the full set of states achievable via MTP from given.

github.com/KorzekwaKamil/continuous_thermomajorisation



How is this done?

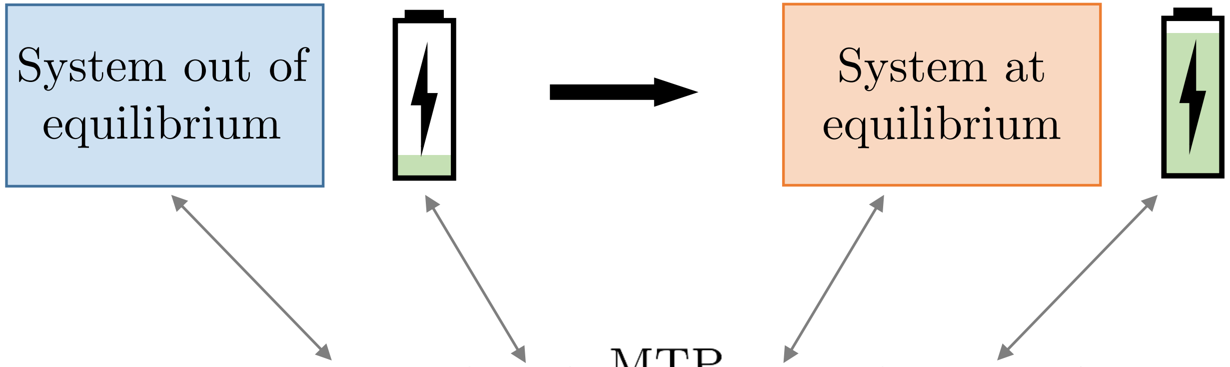
Idea 1: when initial and final state have the same ordering, it's easy.

Idea 2: when changing orderings, there is a unique optimal way to do it.

Idea 3: there are finite number of paths connecting different orderings.

Applications

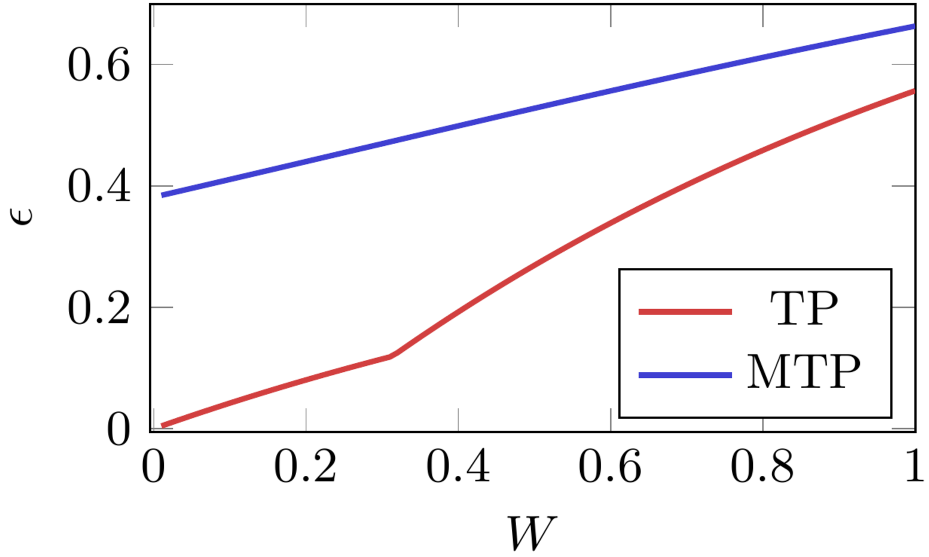
Role of memory in work extraction:



$$\boldsymbol{p} \otimes (1,0) \overset{\text{MTP}}{\longmapsto} \boldsymbol{\gamma} \otimes (\epsilon, 1-\epsilon)$$

versus

$$\boldsymbol{p} \otimes (1,0) \overset{\text{TP}}{\longmapsto} \boldsymbol{\gamma} \otimes (\epsilon, 1-\epsilon)$$



System spectrum $\{0, 1\}$
Battery spectrum $\{0, W\}$
System initially thermal with $\beta_S = 2$
Bath with $\beta_E = 1$

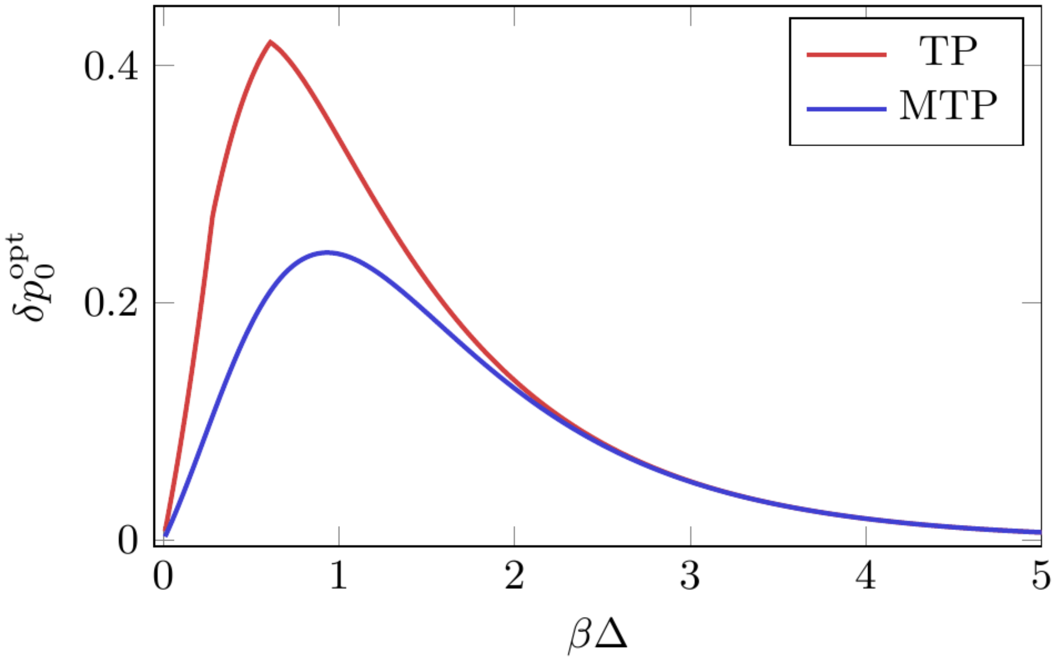
Applications

Role of memory in cooling:

One step of heat-bath algorithmic cooling protocol:

- Take a thermal system and unitarily invert its populations.
- Interact it with the bath and try to maximise ground state population.

Again, we can compare optimal MTP with optimal TP protocols.



System spectrum $\{0, \Delta, 2\Delta, 3\Delta\}$
System initially in equilibrium with bath at β

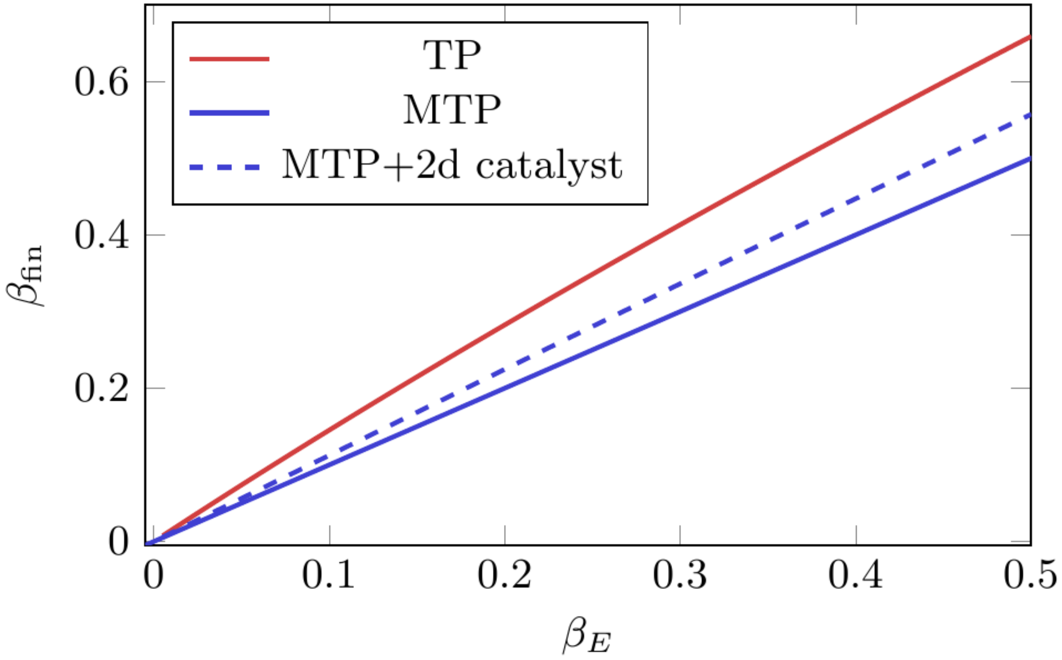
Applications

Catalysts and memory in thermodynamic protocols

Catalyst $\boldsymbol{c}$ is a system that is returned unchanged at the end of the process:

$$\boldsymbol{p} \otimes \boldsymbol{c} \overset{\text{MTP}}{\longmapsto} \boldsymbol{q} \otimes \boldsymbol{c}$$

Thermal catalysts can be used as a memory that enhances or unlocks otherwise impossible tasks to be performed, with catalyst's dimension quantifying the amount of memory.



System and catalyst spectrum $\{0, 1\}$
System initially thermal with $\beta_S = \beta_E/2$
Bath and catalyst thermal with β_E

Outlook

1. Apply to study non-Markovian boosts to relevant processes.

   Non-Markovianity boosts the efficiency of bio-molecular switches
   arXiv:2103.14534 (2021)

2. Understand the asymptotic behaviour of continuous thermomajorisation.

3. Extend the formalism to treat states with coherence.

4. Optimise the runtime of the algorithmic verification procedure.

More soon on arXiv:

Continuous thermomajorisation and a complete set of laws for Markovian thermal processes
M. Lostaglio, K. Korzekwa
arXiv:2110.xxxxx (2021)

Thank you!