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Fluctuation Theorems and Mutual Information

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(3) University of Massachusetts

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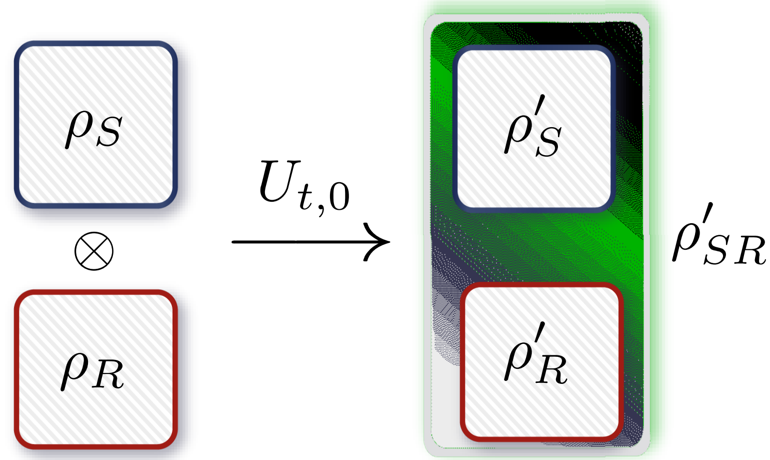
Motivation and model:

- Contribute to the development of a general framework for assessing non equilibrium thermodynamics in fully quantum settings.
- Characterization of the Second Law in open quantum systems for arbitrary systems and reservoirs (not necessarily in equilibrium).



- *Initial state*: $\rho_{SR} = \rho_S \otimes \rho_R$
- *Hamiltonian*: $H_{\text{tot}}(\lambda_t) = H_S + H_R + H_I$
- *Unitary evolution*: $U_{t,0}[\Lambda]$ possibly driven with protocol $\Lambda = \{\lambda_t\}$
- *Final state*: $\rho'_{SR} = U_{t,0}(\rho_S \otimes \rho_R)U^{\dagger}_{t,0}$
- *Local final states*: $\rho'_S = \mathrm{Tr}_R[\rho'_{SR}]$

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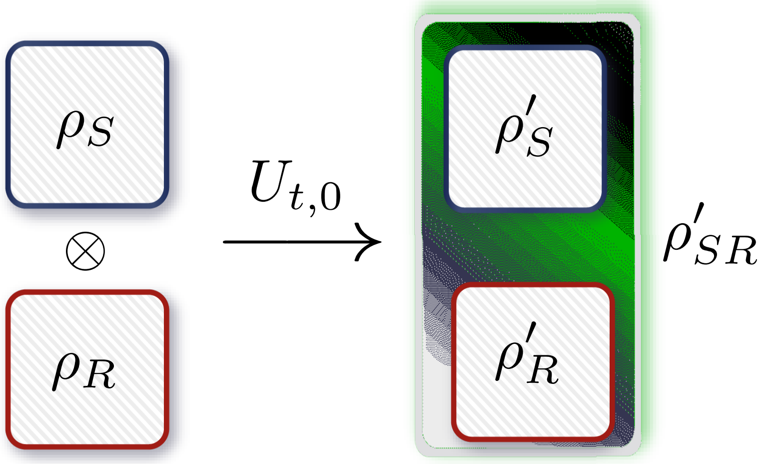

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von Neumman entropy conservation: $\Delta S + \Delta S_R - I(S' : R')_{\rho'_{SR}} = 0$

Quantum Mutual Information (Total amount of correlations) $I(S' : R')_{\rho'_{SR}} = S(\rho'_{SR} || \rho'_S \otimes \rho'_R) \geq 0$

D. Reeb and M. M. Wolf, New J. Phys. **16**, 103011 (2014)
D. Jennyngs and T. Rudolph, Phys. Rev. E **81**, 061130 (2010)
M.H. Partovi, Phys. Lett. A **137**, 440 (1989)
M.H. Partovi, Phys. Rev. E **77**, 021110 (2008)

Outline

I. Mutual Information as the total Entropy Production

II. Fluctuation Theorems

III. Quantum maps and operations

IV. Decomposition of the total Entropy Production

V. Conclusions

Mutual Information as the total Entropy Production:

Entropy production: Positive change in entropy during the evolution of some system due to irreversible processes occurring at their core

Take a local point of view: Partial tracing $\leftrightarrow$ Irreversibility

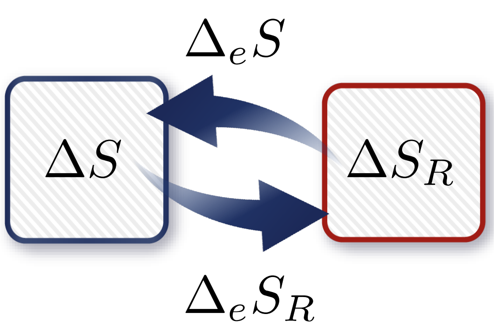
System and reservoir as open quantum systems

Split local entropy changes:

$$\begin{aligned} \Delta S &= \boxed{\Delta_i S} + \boxed{\Delta_e S} \\ \Delta S_R &= \boxed{\Delta_i S_R} + \boxed{\Delta_e S_R} \end{aligned}$$

Positive,
Entropy Production

Positive or Negative,
Entropy Exchange



Total system is closed:

$$\Delta_e S + \Delta_e S_R = 0$$

$$\Delta_i S + \Delta_i S_R = \boxed{\Delta_i S_{\text{tot}} = \Delta S + \Delta S_R = I(S' : R')_{\rho'_{SR}} \geq 0}$$

Mutual Information as the total Entropy Production:

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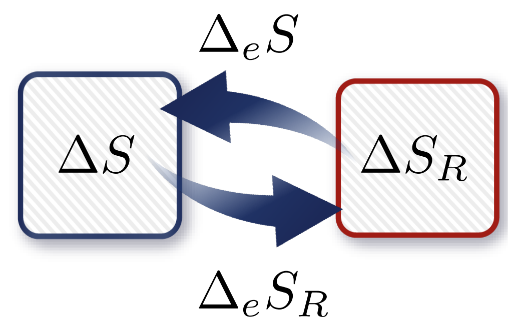
System and reservoir as open quantum systems

If reservoir remains in equilibrium at some β



$$\Delta_i S_R = 0 \qquad \Delta S_R = \Delta_e S_R = -\beta Q$$

$$Q \equiv -\mathrm{Tr}[H_R(\rho'_R - \rho_R)]$$

$$\Delta_i S_{\mathrm{tot}} = \Delta_i S = \Delta S - \beta Q \geq 0$$

Total system is closed:

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Operational interpretation: We have not access to the global state of the system to perform thermodynamic tasks, e.g. isothermal work extraction, but only to the local states of system and reservoir.

Example: isothermal work

Moreover we can relate the mutual information with the isothermal work

- Assume some external relevant temperature T
- Non-equilibrium free energy of the global system:

$$\mathcal{F}(H_{\text{tot}}, \rho_{SR}) = \langle H_{\text{tot}} \rangle_{\rho_{SR}} - kTS(\rho_{SR})$$

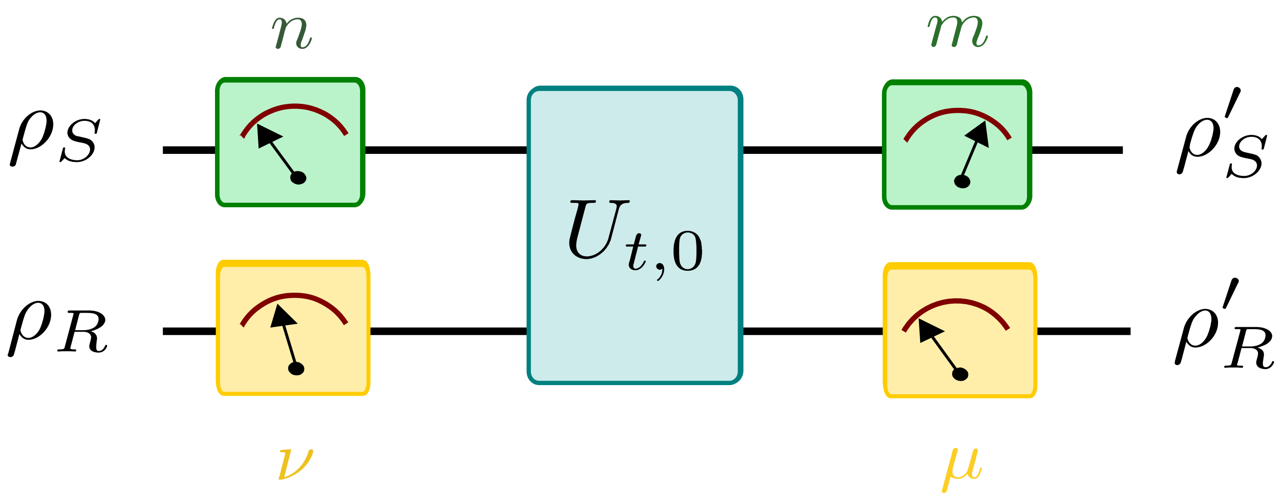
Calculate $\Delta\mathcal{F}$ between initial and final (product) states:

$$\boxed{kTI(S' : R')_{\rho'_{SR}} = W - \Delta\mathcal{F} \geq 0}$$

$W_{\text{diss}} \geq 0$ work lost from the local perspective

where W work from driving (+ work to switch off the interaction)

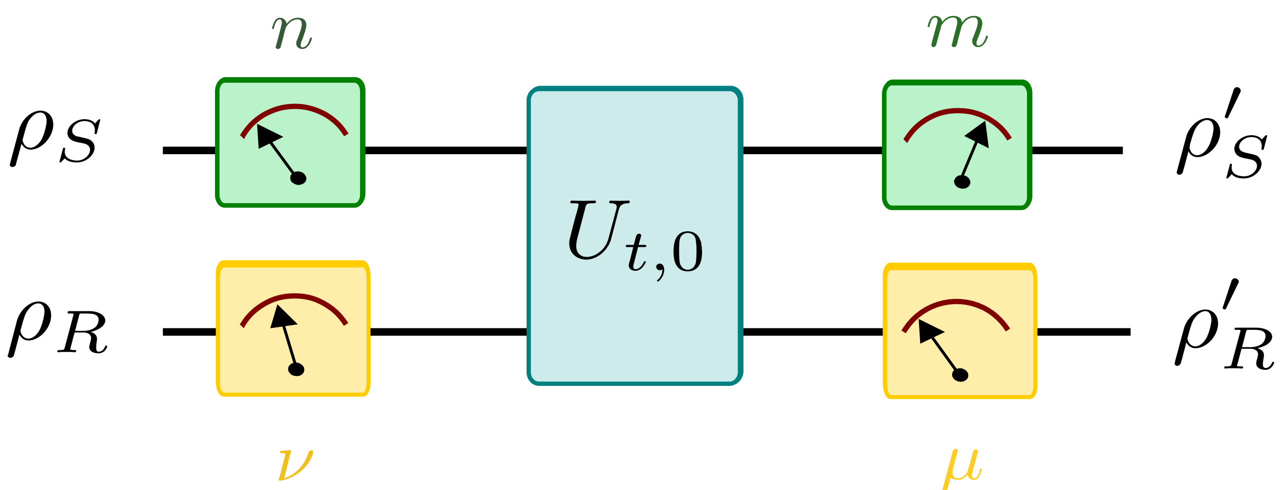
Fluctuation theorems : Two-points measurement scheme



- Initial states: $\rho_S = \sum_n p_n \Pi_n \qquad \rho_R = \sum_\nu q_\nu Q_\nu$
- Final states: $\rho'_S = \sum_m p'_m \Pi'_m \qquad \rho'_R = \sum_\mu q'_\mu Q'_\mu$

Measurements in the diagonal basis of reduced states

Fluctuation theorems : Two-points measurement scheme



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Measurements in the diagonal basis of reduced states

Probability of a "trajectory":

$$P_{m,\mu,n,\nu} = p_n q_\nu \times P_{m,\mu|n,\nu} \qquad P_{m,\mu|n,\nu} = \mathrm{Tr}[(\Pi'_m \otimes Q'_\mu) U_{t,0} (\Pi_n \otimes Q_\nu) U^\dagger_{t,0}]$$

Stochastic entropy changes:

$$\Delta s_{m,n} = -\ln p'_m + \ln p_n \quad \textbf{(system)}$$

$$\Delta s^R_{\mu,\nu} = -\ln q'_\mu + \ln q_\nu \quad \textbf{(reservoir)}$$

Stochastic entropy production:

$$I_{m,\mu,n,\nu} = \Delta s_{m,n} + \Delta s^R_{\mu,\nu}$$

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PDF entropy production: $\mathcal{P}(I) = \sum_{\mu,\nu} \sum_{m,n} P_{m,\mu,n,\nu} \times \delta(I - I_{m,\mu,n,\nu})$

Characteristic function:

$$G(u) = \int dI \mathcal{P}(I) e^{iIu} = \langle e^{iIu} \rangle = \mathrm{Tr}[V'(u) U_{t,0} (\rho_S \otimes \rho_R) V(u) U^\dagger_{t,0}]$$

$$V'(u) = e^{-i \ln(\rho'_S \otimes \rho'_R) u} \qquad V(u) = e^{i \ln(\rho_S \otimes \rho_R) u}$$

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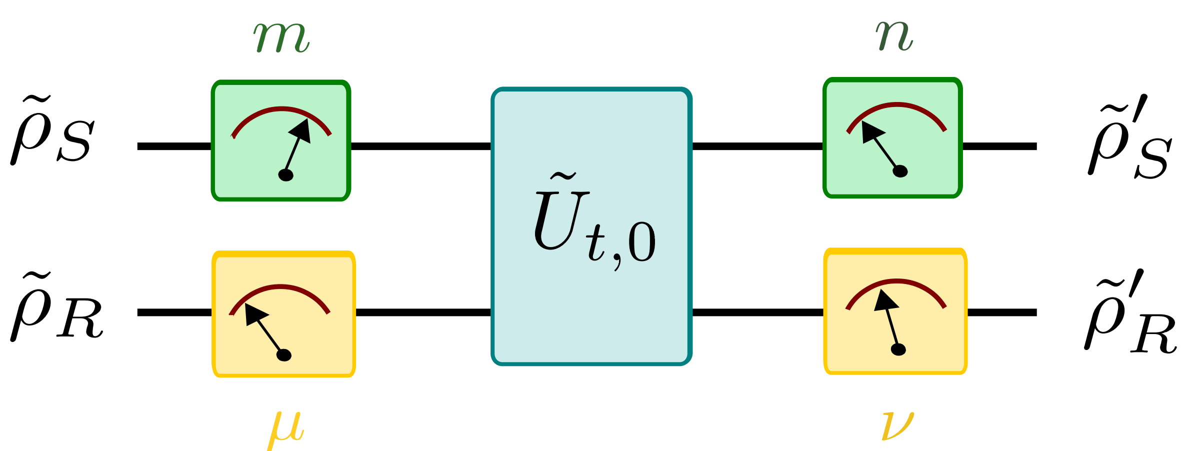
Integral Fluctuation Theorem:

$$\boxed{G(u = i) = 1 \;\Leftrightarrow\; \langle e^{-I} \rangle = 1}$$

Time-reversal anti-unitary operator:

$$\Theta\Theta^\dagger = \Theta^\dagger\Theta = \mathbb{I}$$

Backward (time-reversed) process:



- Initial states: $\tilde{\rho}_S = \Theta\rho'_S\Theta^\dagger$ $\quad \tilde{\rho}_R = \Theta\rho'_R\Theta^\dagger$
- Operational time-reversal evolution: $\tilde{U}_{t,0}$ from: $\Theta H_{\mathrm{tot}}(\tilde{\lambda}_t)\Theta^\dagger \quad \tilde{\Lambda} = \{\tilde{\lambda}_t\}$

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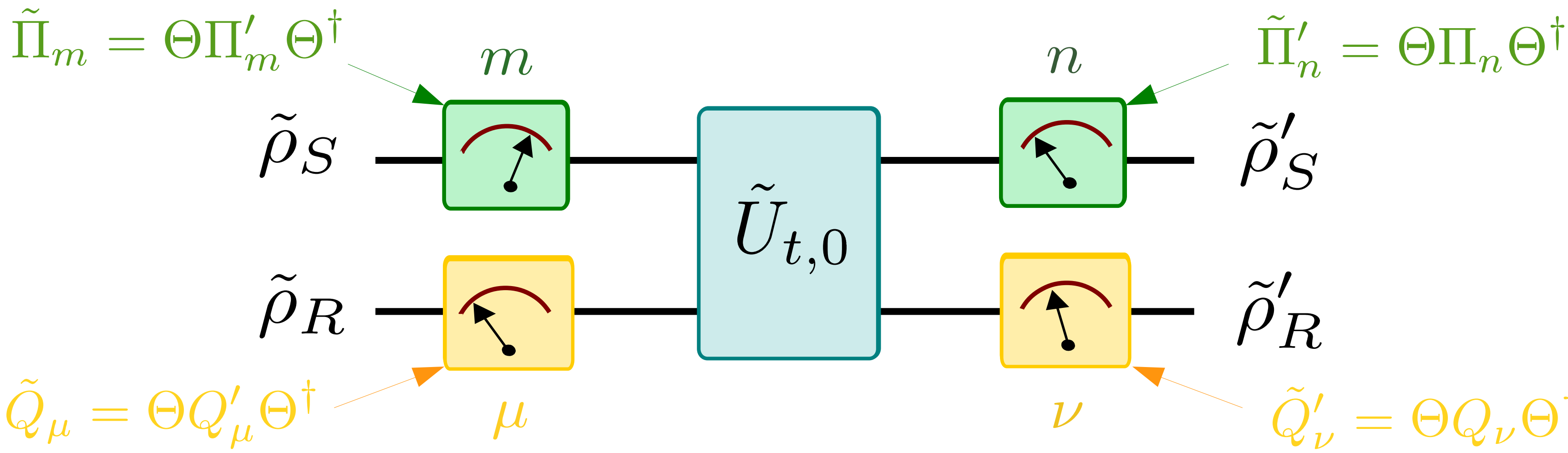

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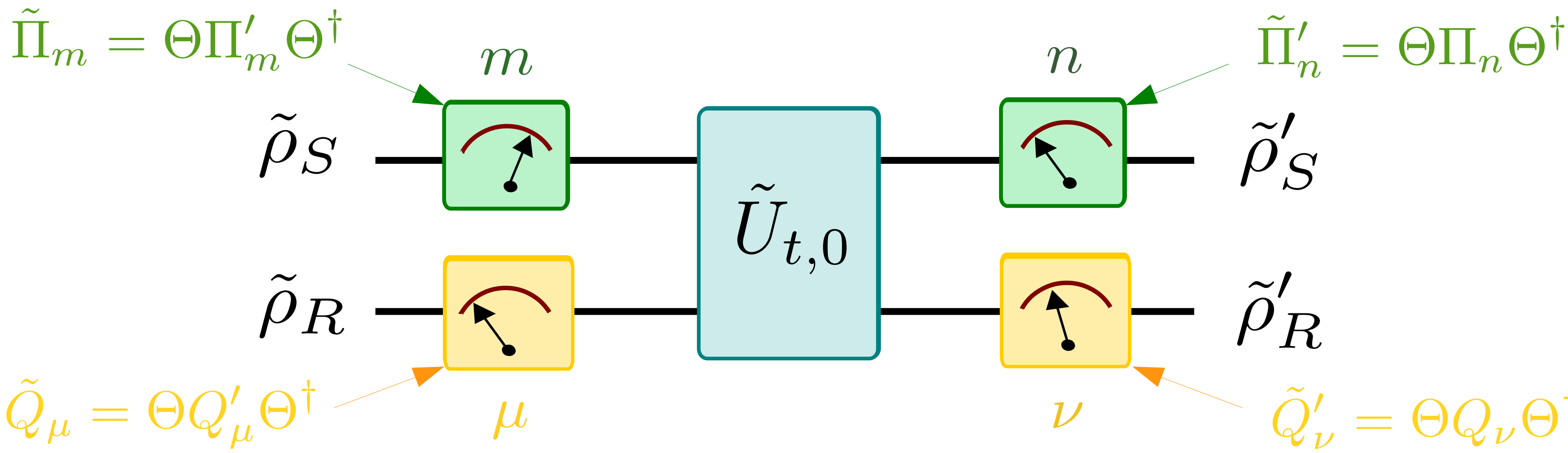

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$$\tilde{P}_{n,\nu,m,\mu} = p'_m q'_\mu \times \tilde{P}_{n,\nu|m,\mu} \qquad \tilde{P}_{n,\nu|m,\mu} = \mathrm{Tr}[(\tilde{\Pi}'_n \otimes \tilde{Q}'_\nu)\tilde{U}_{t,0}(\tilde{\Pi}_m \otimes \tilde{Q}_\mu)\tilde{U}^\dagger_{t,0}]$$

Micro-reversibility for non-autonomous systems:

$$\Theta^\dagger \tilde{U}_{t,0} \Theta = U^\dagger_{t,0}$$

D. Andrieux and P. Gaspard, Phys. Rev. Lett. **100**, 230404 (2008).
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Detailed Fluctuation Theorem:

$$\boxed{\ln \frac{P_{m,\mu,n,\nu}}{\tilde{P}_{n,\nu,m,\mu}} = \ln \frac{p_n}{p'_m} + \ln \frac{q_n}{q'_m} = \Delta s_{m,n} + \Delta s^R_{\mu,\nu} = I_{m,\mu,n,\nu}}$$

$P_{m,\mu,n,\nu}$ probability of jump:

$$|n\rangle \otimes |\nu\rangle \xrightarrow{\Lambda} |m\rangle' \otimes |\mu\rangle'$$

$\tilde{P}_{n,\nu,m,\mu}$ probability of inverse jump:

$$\Theta|m\rangle' \otimes \Theta|\mu\rangle' \xrightarrow{\tilde{\Lambda}} \Theta|n\rangle \otimes \Theta|\nu\rangle$$

$$\boxed{\tilde{P}_{n,\nu,m,\mu} = P_{m,\mu,n,\nu} \times e^{-I_{m,\mu,n,\nu}}}$$

Quantum maps and operations:

We can rewrite previous results in terms of quantum operations:

$$\rho'_S = \mathcal{E}(\rho_S) = \sum_k M_k \rho_S M_k^\dagger \qquad \text{with} \quad \sum_k M_k^\dagger M_k = \mathbb{I}$$

$$M_k = \sqrt{q_\nu}\langle\mu|'U_{t,0}|\nu\rangle \qquad k = \{\mu, \nu\}$$ transition between reservoir eigenstates

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Backward map:

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Trajectories:

$$I_{m,k,n} = \Delta s_{m,n} + \Delta s_k^R$$

$$P_{m,k,n} = p_n \times p_{m,k|n}$$

$$\tilde{P}_{m,k,n} = p'_m \times \tilde{p}_{n,k|m}$$

Micro-reversibility $\Rightarrow$ $\boxed{\tilde{M}_k = e^{-\Delta s_k^R} \Theta^\dagger M_k^\dagger \Theta}$

Extensions:

- Multiples reservoirs:

$$\Delta_i S_{\text{tot}} = \Delta S + \sum_{R=1}^{N_R} \Delta S_R = I(S' : R'_1 : ... : R'_{N_R})_{\rho'_{\text{tot}}} \geq 0$$

$$I_\gamma = \Delta s_{m,n} + \sum_{R=1}^{N_R} \Delta s^R_{\mu_R,\nu_R} \qquad \gamma = \{m, \mu_1, ..., \mu_{N_R}, n, \nu_1, ..., \nu_{N_R}\}$$

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- Concatenation of maps:

$$\rho'_S = \mathcal{E}^{(Z)} \cdot \ldots \cdot \mathcal{E}^{(1)}(\rho_S) \qquad \mathcal{E}^{(z)}(\rho) = \sum_{k_z} M^{(z)}_{k_z} \rho M^{(z)\dagger}_{k_z} \qquad z = 1, \ldots, Z$$

$$I_\gamma = \Delta s_{m,n} + \sum_{z=1}^{Z} \Delta s^R_{k_z} \qquad \gamma = \{m, k_Z, \ldots, k_1, n\}$$

equivalent to the reservoir being measured many times

applications to Markovian Master Equations: $\dot{S}_i^{\rm tot} = \dot{S} + \dot{S}_R \geq 0$

Decomposition of the total Entropy Production:

$$\Delta_i S_{\text{tot}} = \Delta_i S_{\text{ad}} + \Delta_i S_{\text{na}} \geq 0$$

M. Esposito and C. Van der Broeck, Phys. Rev. Lett. 104, 090601 (2010)

irreversibility from non-eq. external constrains

irreversible changes in ρ_S

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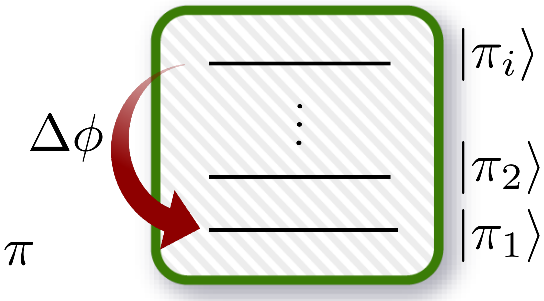

- Positive-definite invariant state: $\mathcal{E}(\pi) = \pi$

Non-eq thermodynamic potential: $\phi_i = -\ln \pi_i \quad \hat{\Phi} = -\ln \pi$

- Kraus operators associated to only one thermodynamic potential change:

$$M_k = \sum_{ij} m_{ij}^k |\pi_j\rangle\langle\pi_i|$$

with $m_{ij}^k = 0$ whenever $\Delta\phi_k \neq \phi_j - \phi_i$

$$\boxed{\pi M_k \pi^{-1} = e^{-\Delta\phi_k} M_k}$$

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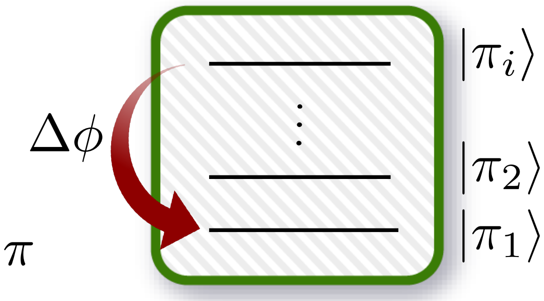

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Under the above conditions FTs follow:

$$\Delta_i s_{\text{na}} = \Delta s_{m,n} + \Delta\phi_k \qquad \langle e^{-\Delta_i s_{\text{na}}} \rangle = 1$$

$$\Delta_i s_{\text{ad}} = \Delta s_k^R - \Delta\phi_k \qquad \langle e^{-\Delta_i s_{\text{ad}}} \rangle = 1$$

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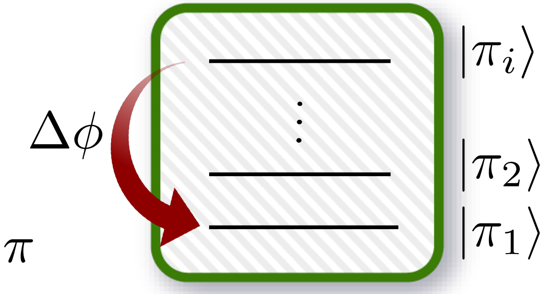

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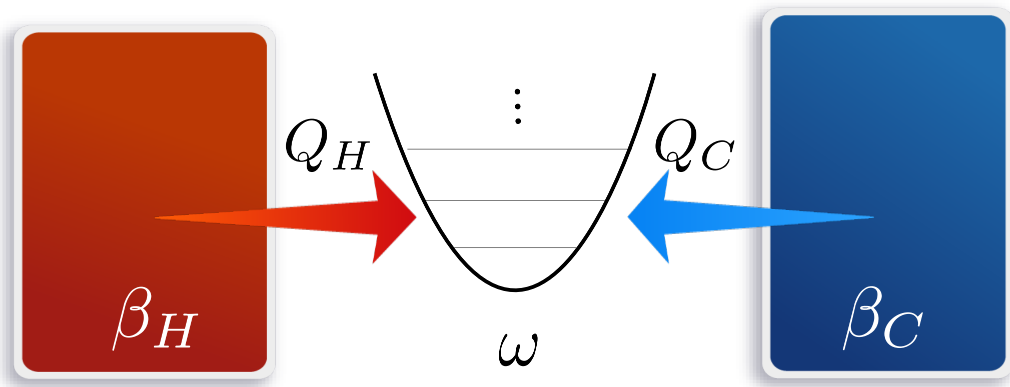
$$\Delta_i s_{\text{na}} = \Delta s_{m,n} + \Delta\phi_k \qquad \langle e^{-\Delta_i s_{\text{na}}}\rangle = 1 \qquad \Delta_i S_{\text{na}} = \Delta S + \Delta\Phi \geq 0$$

$$\Delta_i s_{\text{ad}} = \Delta s_k^R - \Delta\phi_k \qquad \langle e^{-\Delta_i s_{\text{ad}}}\rangle = 1 \qquad \Delta_i S_{\text{ad}} = \Delta S_R - \Delta\Phi \geq 0$$

Simple example:



$$\Delta S_{R_H} = -\beta_H Q_H \qquad \Delta S_{R_C} = -\beta_C Q_C$$

- Two reservoirs in equilibrium at hot and cold temperatures
- Weak coupling and no driving:

$$H_{\text{tot}} = H_S + H_R + H_I = \text{cte}$$

- System with single energy level spacing, e.g. harmonic oscillator, relaxes to a steady state:

$$\pi = e^{-\beta_{\text{eff}} H_S} / Z_{\text{eff}}$$

First law: $\Delta U = Q_H + Q_C$

Second law: $\Delta_i S_{\text{tot}} = I(S' : R')_{\rho'_{SR}} = \Delta S - \beta_H Q_H - \beta_C Q_C \geq 0$

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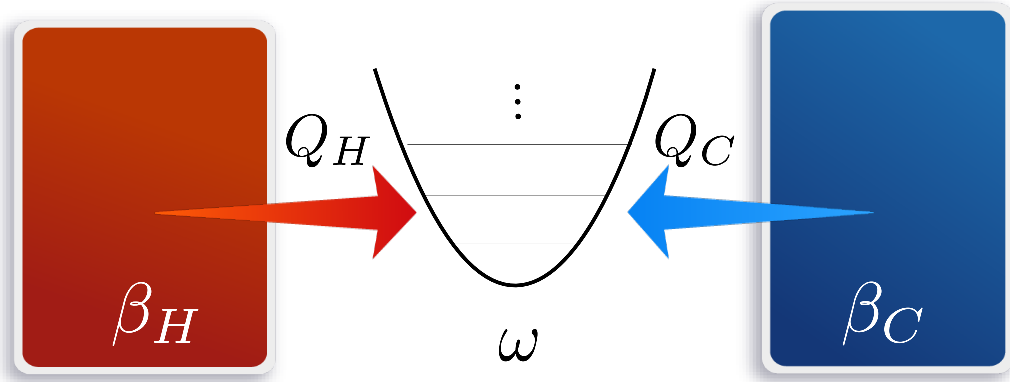

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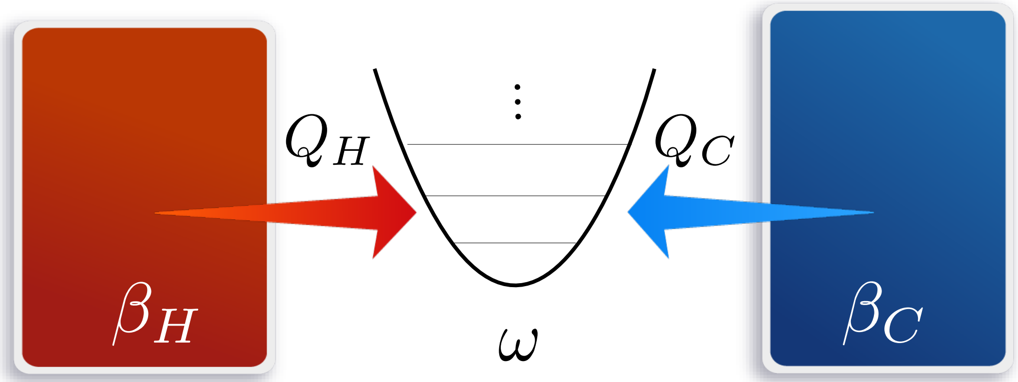
Decomposition: $\quad \Delta_i S_{\text{na}} = \Delta S - \beta_{\text{eff}}(Q_H + Q_C) \geq 0$

$\Delta \Phi = \beta_{\text{eff}} \Delta U \qquad \Delta_i S_{\text{ad}} = (\beta_{\text{eff}} - \beta_H) Q_H + (\beta_{\text{eff}} - \beta_C) Q_C \geq 0$

Simple example:



$\Delta S_{R_H} = -\beta_H Q_H$ $\quad\quad$ $\Delta S_{R_C} = -\beta_C Q_C$

- Two reservoirs in equilibrium at hot and cold temperatures
- Weak coupling and no driving:

$$H_{\text{tot}} = H_S + H_R + H_I = \text{cte}$$

- System with single energy level spacing, e.g. harmonic oscillator, relaxes to a steady state:

$$\pi = e^{-\beta_{\text{eff}} H_S}/Z_{\text{eff}}$$

First law: $\Delta U = Q_H + Q_C$

Second law: $\Delta_i S_{\text{tot}} = I(S' : R')_{\rho'_{SR}} = \Delta S - \beta_H Q_H - \beta_C Q_C \geq 0$

Decomposition: $\Delta_i S_{\text{na}} = \Delta S - \beta_{\text{eff}}(Q_H + Q_C) \geq 0$

$\Delta\Phi = \beta_{\text{eff}} \Delta U$ $\quad\quad$ $\Delta_i S_{\text{ad}} = (\beta_{\text{eff}} - \beta_H) Q_H + (\beta_{\text{eff}} - \beta_C) Q_C \geq 0$

Starting in the steady state: $\Delta S = 0$, $\Delta U = 0$ $\quad\quad$ $\Delta_i S_{\text{na}} = 0$ $\quad\quad$ $\Delta_i S_{\text{tot}} = \Delta_i S_{\text{ad}} = (\beta_C - \beta_H) Q \geq 0$

Main conclusions:

- Irreversibility in open quantum systems, measured by the total entropy production is given by the mutual information developed between system and reservoir during evolution.
- A Fluctuation theorem for the total entropy production in quantum systems holds for arbitrary out of equilibrium conditions in system and reservoir.
- The total entropy production can be split into two positive terms (adiabatic and non-adiabatic contributions) for a broad class of quantum maps. What happens with the others?

G. Manzano, J. M. Horowitz and J.M.R. Parrondo, in preparation.

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Thanks for your attention!

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