Nonequilibrium potential and fluctuation theorems for quantum maps

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More information: Physical Review E, **92**, 032129 (2015)

IFISC

QuProCS II 6-7/4/2017 | IFISC (Mallorca)

Outline of the talk:

- **Introduction**
  a. Classical Fluctuation Theorems
  b. Quantum generalizations
  c. Quantum CPTP maps and operations

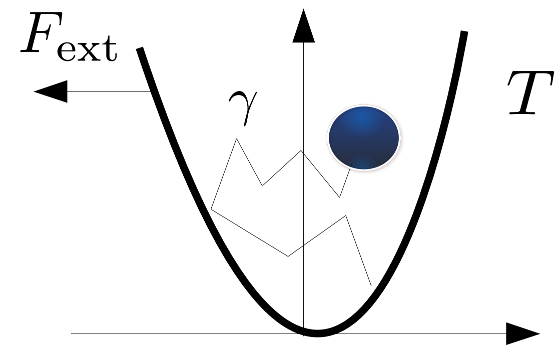
- **Fluctuation theorem for quantum maps**
  a. Nonequilibrium potential
  b. Dual-reverse process
  c. Main results

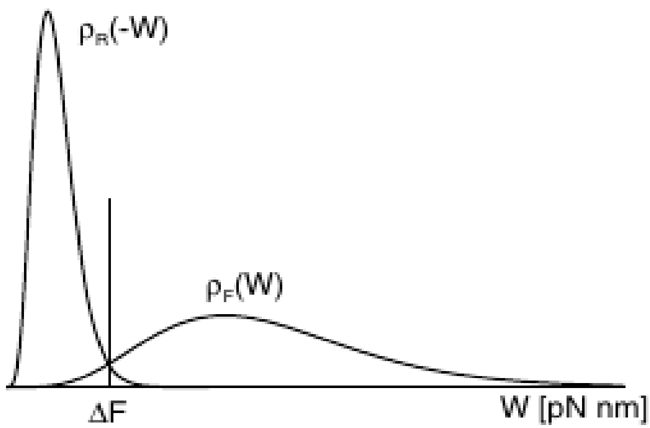
- **Basic applications: maps concatenations**
  a. Unital dynamics
  b. Thermalization and heat

- **Discussion**

Fluctuation Theorems (FT's)

Exact and universal statements for the probability of thermodynamic events (performing work, dissipating heat, producing entropy) in driven systems subjected to **fluctuations** and **arbitrary out of equilibrium**.





Energy balance: $\Delta E[\gamma] = W[\gamma] + Q[\gamma]$

Jarzynski equality: $\langle e^{-W/T} \rangle_\gamma = e^{-\Delta F/T}$

Crooks work FT: $p_F(W) = p_R(-W) e^{(W - \Delta F)/T}$

[equilibrium initial states]

Entropy production FT's: [general initial states for the system]

$$\langle e^{-\Delta_{\mathrm{i}} s} \rangle_\gamma = 1$$

$$p_R(-\Delta_{\mathrm{i}} s) = p_F(\Delta_{\mathrm{i}} s) e^{-\Delta_{\mathrm{i}} s}$$

Entropy production: $\Delta_{\mathrm{i}} s[\gamma] = \Delta s[\gamma] - Q[\gamma]/T$

System entropy per trajectory: $s = -\ln p(x,t)\big|_\gamma$

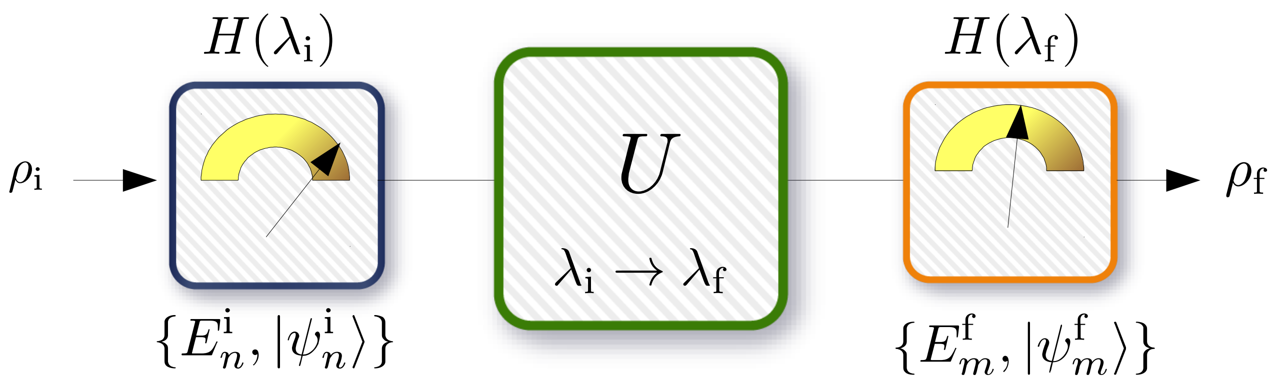
Second law: events decreasing the total entropy are much less probable than those increasing it !

[C. Jarzynski, Annu. Rev. Condens. Matter Phys. (2011) ; U. Seifert, Rep. Prog. Phys. (2012)]

Quantum generalizations

- Thermal fluctuations + Quantum fluctuations
- Thermodynamic quantities are defined through (projective) quantum measurements

Inclusive Hamiltonian approach:



$$\gamma : \; |\psi^{\rm i}_n\rangle \to |\psi^{\rm f}_m\rangle$$

$$W_{m,n} = E^{\rm f}_m - E^{\rm i}_n$$

- Work FT's for isolated driven quantum systems
- Work and entropy production FT's for composite systems [system + ideal thermal reservoir]

[M. Campisi *et. al.* Rev. Mod. Phys. (2011) ; S. Deffner and E. Lutz, PRL (2011) ; T. Sagawa (2012)]

Complications:

- Projective measurements on the whole environment are needed
- Extensions to more general environments without knowing all its properties

Quantum CPTP maps: $\rho_{\mathrm{f}} = \mathcal{E}(\rho_{\mathrm{i}})$

- Kraus operator-sum representation:

$$\mathcal{E}(\rho) = \sum_k M_k \rho M_k^\dagger \quad \text{where} \quad \sum_k M_k^\dagger M_k = \mathbb{I}$$

Different random operations $\mathcal{E}_k(\rho) = M_k \rho M_k^\dagger$ occurring with probability $p_k = \mathrm{tr}[M_k \rho M_k^\dagger]$

Previous results:

- Restricted to unital maps or need a correction term:

Unital maps: $\langle e^{-\sigma} \rangle = 1$ iff $\mathcal{E}(\mathbb{I}) = \mathbb{I}$

Otherwise: $\langle e^{-\sigma} \rangle = c$ $\quad 0 \leq c < 1$

Our result:

- New general FT beyond the unital case:

$$\langle e^{-\Sigma} \rangle = 1 \qquad \Sigma = \sigma - \Delta\phi_k$$

where:

σ system boundary term

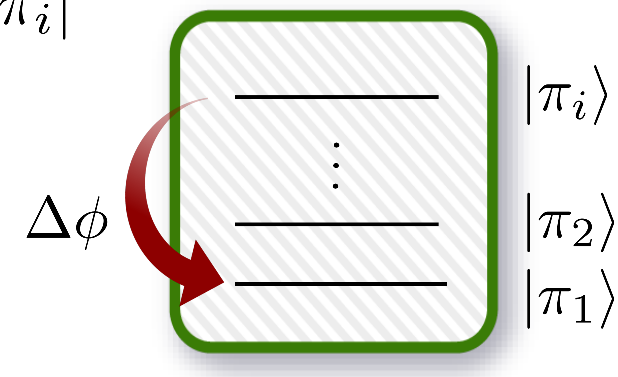
$\Delta\phi_k$ fluctuations induced by the map operations in a very particular observable of the system

[G. Manzano *et. al.* PRE, **92**, 032129 (2015)]

Sufficient conditions on the map:

- I. The map has at least one positive-definite invariant state: $\mathcal{E}(\pi) = \pi$

Nonequilibrium potential: $\Phi = -\ln\pi = \sum_i \phi_i |\pi_i\rangle\langle\pi_i|$



Examples: $\pi = \mathbb{I} \quad \Rightarrow \quad \Delta\phi = 0$

$$\pi = \frac{e^{-\beta H}}{Z} \quad \Rightarrow \quad \Delta\phi = \beta Q$$

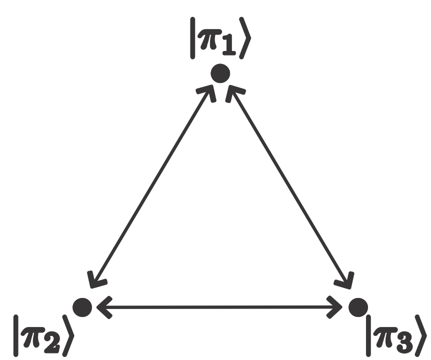
- II. Kraus operators are associated with only one change in the nonequilibrium potential:

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

with $m_{ij}^k = 0$

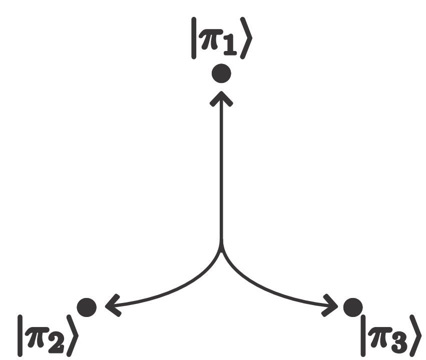
whenever $\Delta\phi_k \neq \phi_j - \phi_i$

$$M_{ij} = m_{ij}|\pi_j\rangle\langle\pi_i|$$



Classical Markov Chain

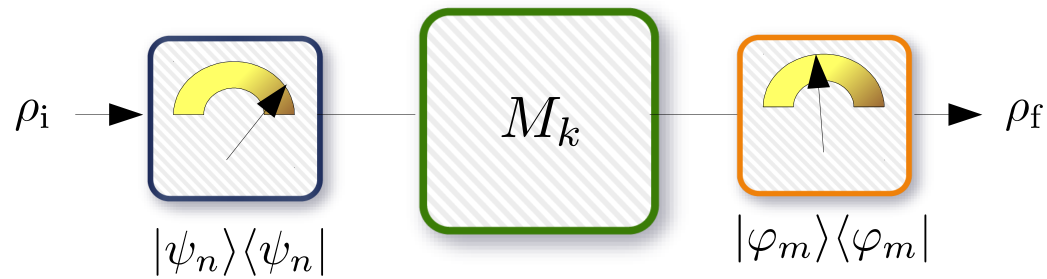
$$M_k = \sum_{ij} m_{ij}^k |\pi_j\rangle\langle\pi_i|$$



Coherent Markov Chain

Forward process:

$$\rho_{\rm i} = \sum_n p_n |\psi_n\rangle\langle\psi_n|$$



$$\gamma = \{n, k, m\}$$

Dual-reverse process:

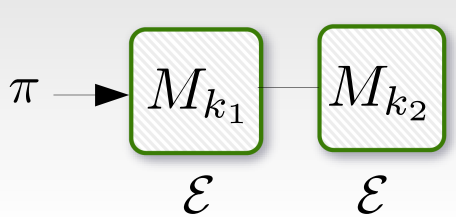
$$\tilde{\rho}_{\rm f} = \sum_m \tilde{p}'_m \Theta |\varphi_m\rangle\langle\varphi_m| \Theta^\dagger$$

$$\tilde{\gamma} = \{m, k, n\}$$

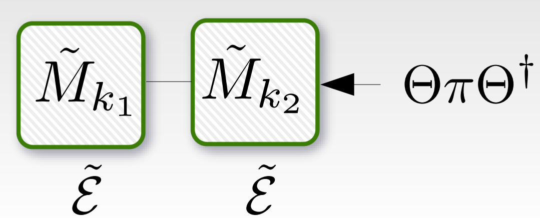
Anti-unitary time-reversal operator: $\Theta\Theta^\dagger = \Theta^\dagger\Theta = \mathbb{I}, \quad \Theta i = -i\Theta$

Dual-reverse map: $\tilde{\mathcal{E}}(\rho) = \sum_k \tilde{M}_k \rho \tilde{M}_k^\dagger$ [G.E. Crooks, PRA **77**, 034101 (2008)]

The map generating same probabilities for consecutive operations over the invariant state when dynamics are time-reversed



$$p(k_1, k_2) = \tilde{p}(k_2, k_1)$$



Combining condition II + Dual-reverse map properties:

Generalized detailed balance relation: $$\tilde{M}_k = e^{-\Delta\phi_k/2}\,\Theta M_k^\dagger \Theta^\dagger$$

Detailed fluctuation theorem:

$$\boxed{\ln \frac{P[\gamma]}{\tilde{P}[\tilde{\gamma}]} = \ln \frac{p_n}{\tilde{p}'_m} + \ln \frac{|\langle \phi_m | M_k | \psi_n \rangle|^2}{|\langle \tilde{\psi}_n | \tilde{M}_k | \tilde{\phi}_m \rangle|^2} = \sigma_{m,n} - \Delta\phi_k \;\equiv\; \Sigma_{m,k,n}}$$

Corollaries:

$\Rightarrow\ \langle e^{-\Sigma_{mkn}} \rangle = 1$ (Integral FT / Jarzynski-like equality)

$\Rightarrow \langle \sigma_{m,n} \rangle \geq \langle \Delta\phi \rangle$ (Second-law-like inequality)

Boundary term: $\sigma_{m,n} := -\ln \tilde{p}'_m + \ln p_n$

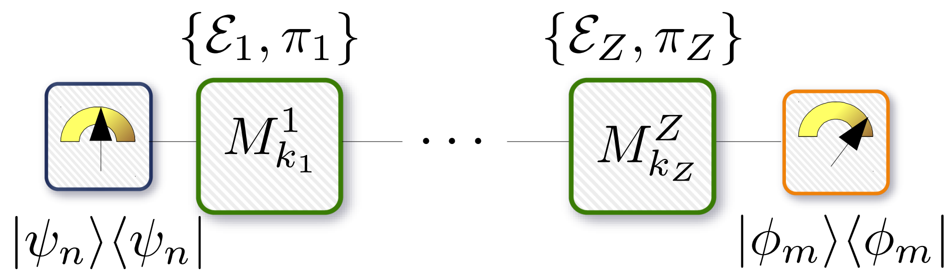
a. Equilibrium boundaries $(\tilde{\rho}_\mathrm{f} = \Theta e^{-\beta H_\mathrm{f}} \Theta^\dagger / Z)$ $\quad \sigma_{m,n} = \beta(E'_m - E_n - \Delta F)$

b. Reversible boundaries $(\tilde{\rho}_\mathrm{f} = \Theta \rho_\mathrm{f} \Theta^\dagger)$ $\quad \sigma_{m,n} = -\ln p'_m + \ln p_n = \Delta s_{m,n}$

Concatenation of CPTP maps

$$\Sigma_{m,k,n} = \ln \frac{P[\gamma]}{\tilde{P}[\tilde{\gamma}]} = \sigma_{m,n} - \sum_{z=1}^{Z} \Delta\phi_{k_z}^{\pi_z}$$

$$\gamma = \{n, k_1, ..., k_Z, m\}$$

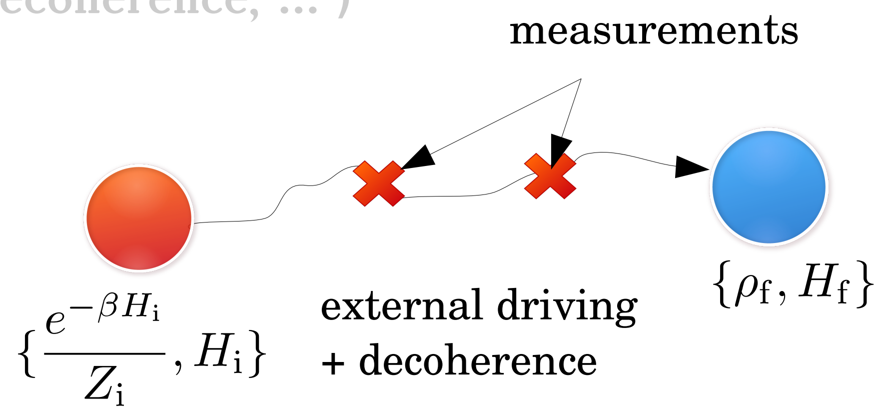


- **Unital dynamics** (driving, measurements, decoherence, ...)

$$\pi = \mathbb{I} \quad \Rightarrow \quad \Delta\phi_k = 0 \;\; \forall\; k$$

a. $\Sigma_{m,k,n} = \beta(W_{m,n} - \Delta F)$

b. $\Sigma_{m,k,n} = \Delta s_{m,n}$



- **Thermalization** (Gibbs-Preserving maps)

$$\pi = e^{-\beta(H-F)} \quad \Rightarrow \quad \Delta\phi_k = \beta Q_k$$

M_k describes energy jumps

Combining thermalization steps with unital dynamics:

a. $\Sigma_{m,k,n} = \beta(\Delta E_{m,n} - Q_\gamma - \Delta F_i) = \beta(W_{m,n} - \Delta F)$

b. $\Sigma_{m,k,n} = \Delta s_{m,n} - \beta Q_\gamma$

Discussion

- Our theorem can be applied to more general situations, e.g. to dynamics leading to nonequilibrium steady states, or also to generalized Gibbs ensembles.

$$\pi = e^{-\sum_a \beta_a C_a}/\Omega \qquad \Rightarrow \qquad \langle \Delta\phi_k \rangle = \sum_a \beta_a \langle \Delta C_a \rangle$$

- The quantity fulfilling our theorem has the properties of a non-adiabatic entropy production: it accounts for the irreversibility generated from being far from the invariant state of the map.

$$\Sigma[\gamma] = 0 \;\; \forall\gamma \;\; \text{if} \;\; \rho_{\mathrm{i}} = \pi \qquad \text{and} \qquad \langle \Sigma \rangle = S(\rho_{\mathrm{i}}||\pi) - S(\rho_{\mathrm{f}}||\pi) \geq 0$$

THANK YOU

for your attention

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