Quantum Martingale Theory for Entropy Production

GONZALO MANZANO[1,2] ROSARIO FAZIO[1,2] ÉDGAR ROLDÁN[1]

SCUOLA NORMALE SUPERIORE

[1] Abdus Salam ICTP, Trieste (Italy). [2] Scuola Normale Superiore, Pisa (Italy).

ICTP

Workshop on Martingales in Finance and Physics
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Outline:

- **Introduction**
  - **From stochastic to quantum thermodynamics**
  - **Superposition and coherence**
- **Thermodynamics and fluctuations for quantum systems**
  - **Quantum trajectories**
  - **Entropy production and fluctuation theorems**
- **Quantum Martingale Theory**
  - **Classical-Quantum split of entropy production**
  - **Stopping-times and finite-time infimum**
- **Main conclusions**

Thermal fluctuations

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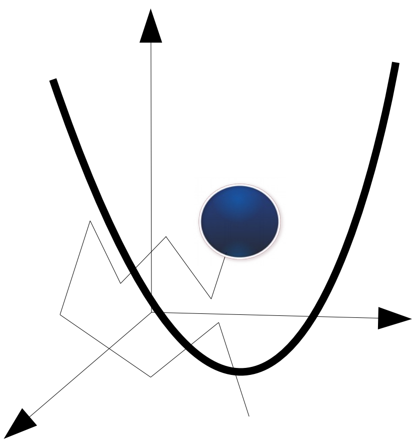

Quantum fluctuations, coherence, entanglement ...

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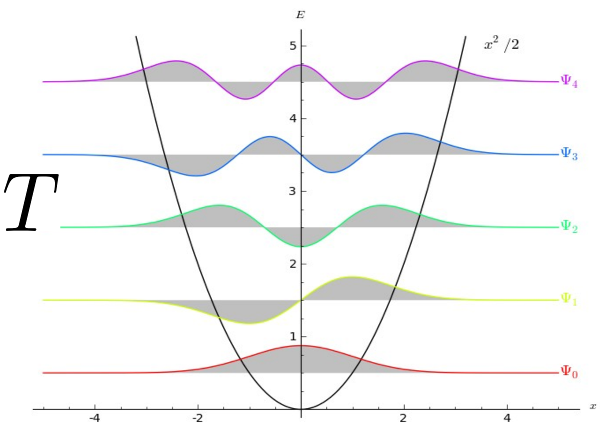
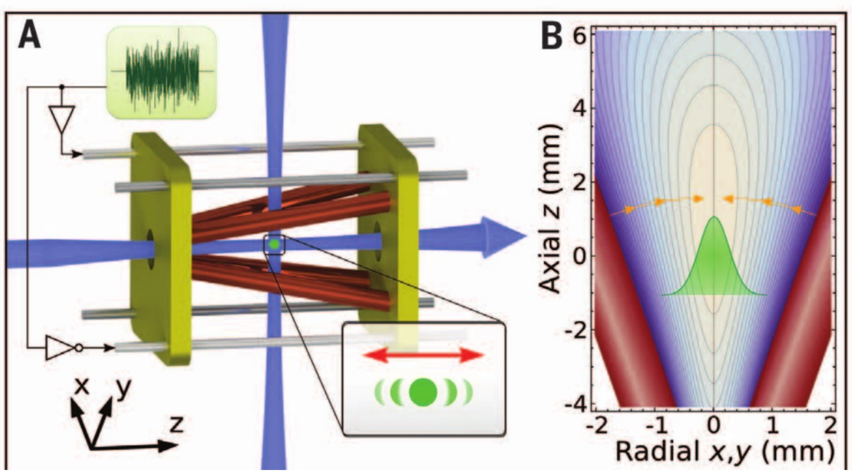


Stochastic Thermodynamics

Quantum Thermodynamics

Fundamental and practical questions:

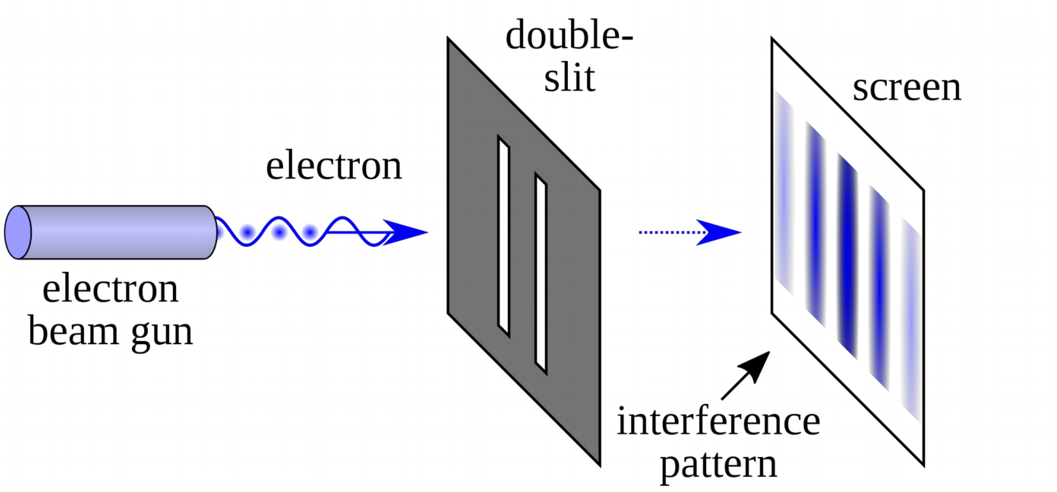
- How heat, work and entropy are defined ?
- How to define effective "trajectories" ?
- Can quantum effects modify thermodynamic behavior?
- Influence of quantum measurements?
- How small can thermal machines be?

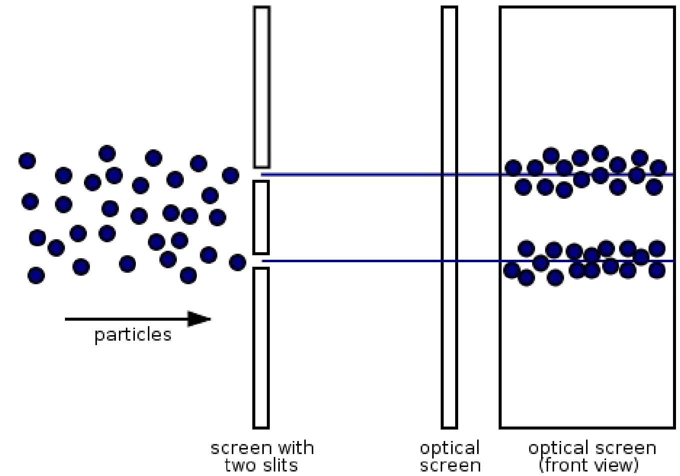


[J. Roßnagel, *et al.* Science (2016)]

Superposition principle:

If $|a\rangle$ and $|b\rangle$ are possible states of a quantum system $\Longrightarrow$ $|\psi\rangle = c_a|a\rangle + c_b|b\rangle$ too



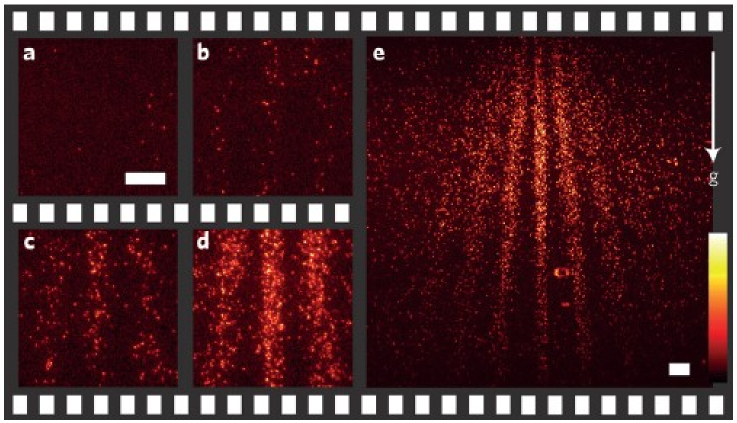


Quantum superposition:

both “left” and “right” slits

Classical particles:

either “left” or “right” slits

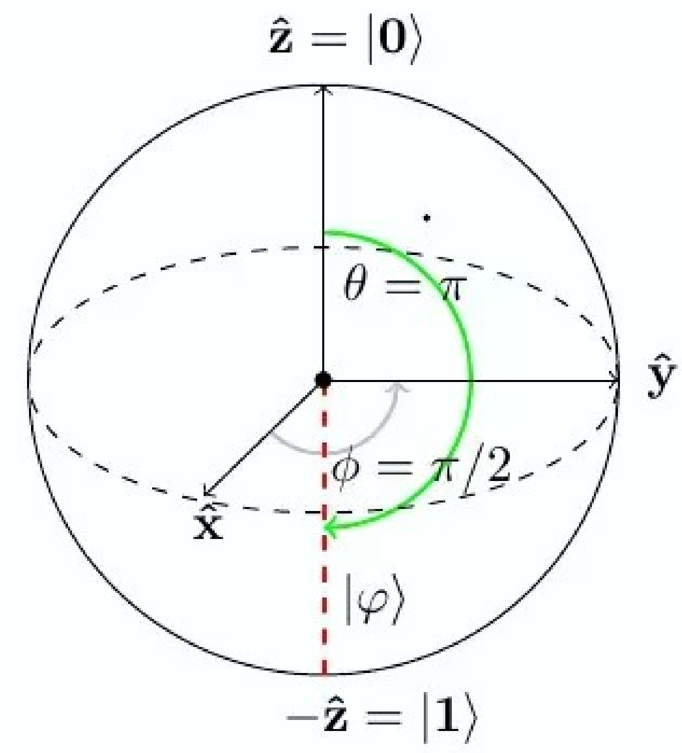


Modern *which-path* experiment with stochastically arriving phthalocyanine (PcH2) molecules (one at a time)

[T. Juffmann *et al.* Nat. Nano (2012)]

Classical mixtures vs. superposition states:

Example: **Two-level system (qubit):** $\{|0\rangle, |1\rangle\}$



$$|\psi\rangle = \cos(\theta/2)|0\rangle + e^{i\phi}\sin(\theta/2)|1\rangle$$

ρ density operator (matrix)

- Compare the following two states:

$$\rho_{\text{class}} = p_0|0\rangle\langle 0| + p_1|1\rangle\langle 1| \longrightarrow \rho_{\text{class}} = \begin{bmatrix} p_0 & 0 \\ 0 & p_1 \end{bmatrix}$$

state of the system is either $\{|0\rangle, |1\rangle\}$ with probs. $\{p_0, p_1\}$

$$\rho_{\text{sup}} = |\psi\rangle\langle\psi| \quad \text{with} \quad |\psi\rangle = \sqrt{p_0}|0\rangle + \sqrt{p_1}|1\rangle \longrightarrow \rho_{\text{class}} = \begin{bmatrix} p_0 & \sqrt{p_0 p_1} \\ \sqrt{p_0 p_1} & p_1 \end{bmatrix}$$

state of the system is $|\psi\rangle$ i.e. both $\{|0\rangle, |1\rangle\}$

COHERENCES

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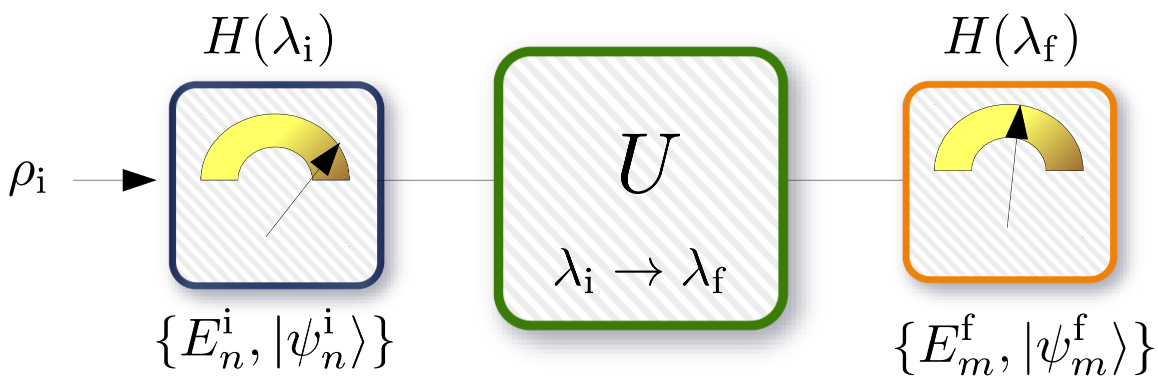
Fluctuation Theorems in quantum systems

- Thermal fluctuations + Quantum fluctuations
- Thermodynamic quantities are defined through (projective) quantum measurements which allow us to define "trajectories" using the measurement outcomes.



$$\gamma : \ |\psi_n^{\rm i}\rangle \to |\psi_m^{\rm f}\rangle$$

$$W_{m,n} = E_m^{\rm f} - E_n^{\rm i}$$

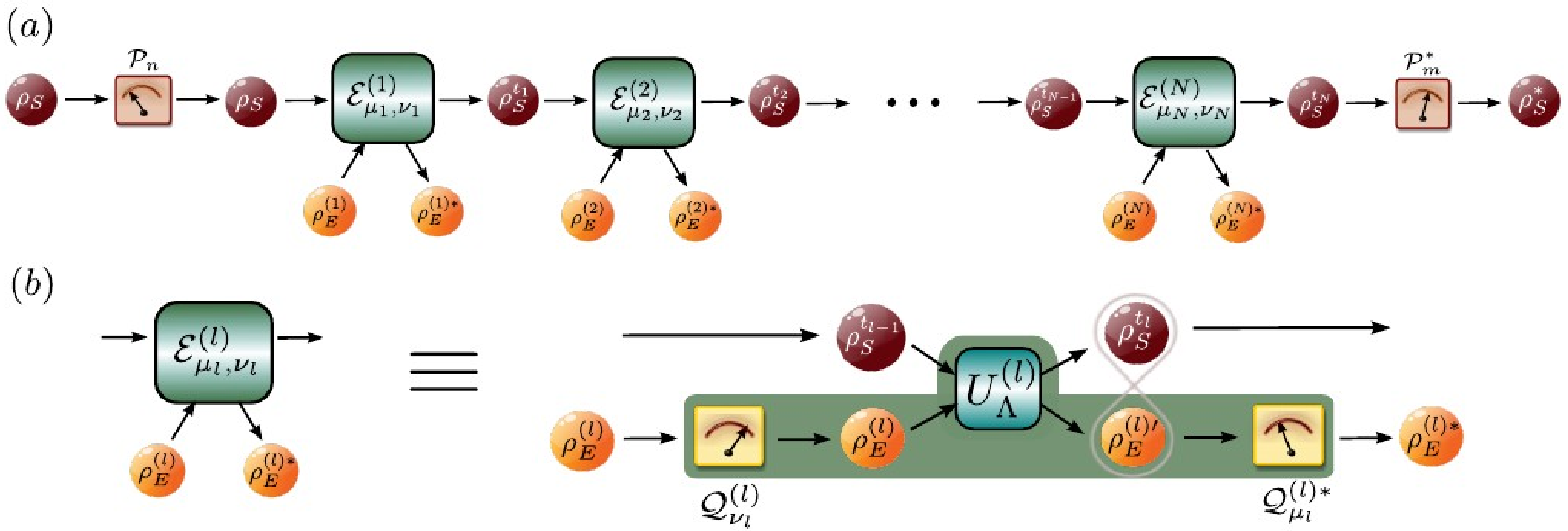
- Useful for work Fluctuation Theorems for isolated driven quantum systems

Open quantum systems?

- Scheme needs to be extended to the environment → Environmental monitoring
- Usually the environment is assumed to be a thermal reservoir
- More general environments such as finite-size and/or engineered quantum reservoirs ?

Reviews: M. Campisi *et al.* Rev. Mod. Phys. (2011) ; M. Esposito *et al.* Rev. Mod. Phys. (2009)

System interacts "sequentially" with the environment:



- Trajectories now comprise all the measurements in system and environmental ancillas:

$$\gamma = \{n, (\mu_1, \nu_1), (\mu_2, \nu_2), ..., (\mu_N, \nu_N), m\}$$

- The continuous limit can be obtained if the following limit exist:

$$N \to \infty \qquad dt \to 0 \qquad \qquad \lim_{dt\to 0} \frac{\mathcal{E}^{(l)}(\rho_S^{(t_l)}) - \rho_S^{(t_l)}}{dt} \to \mathcal{L}_l(\rho_t) \ = \text{ finite}$$

Quantum-jump trajectories:

$$\rho_{t+dt} = \mathcal{E}(\rho_t) = \sum_j M_j \rho_t M_j^\dagger$$

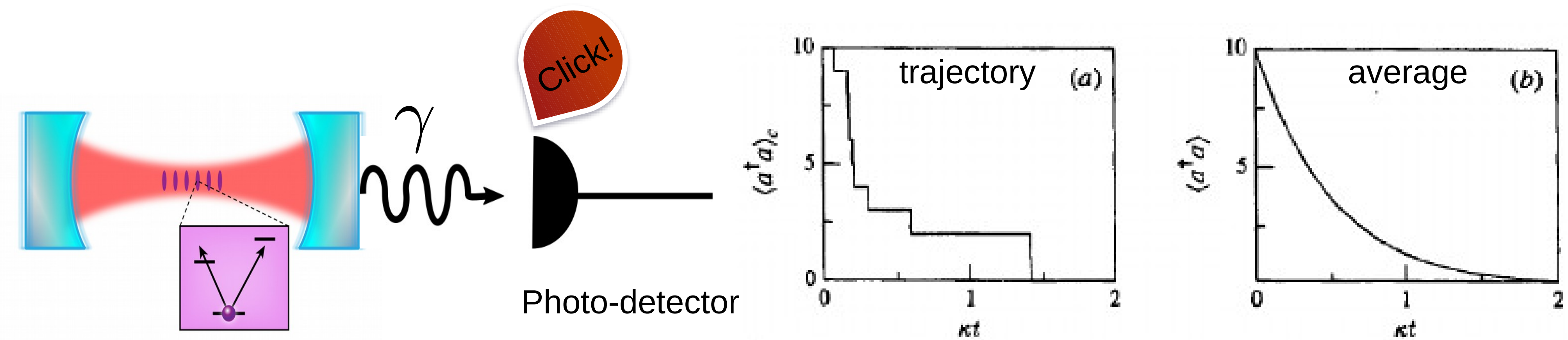
Measurements backaction can be recasted as:

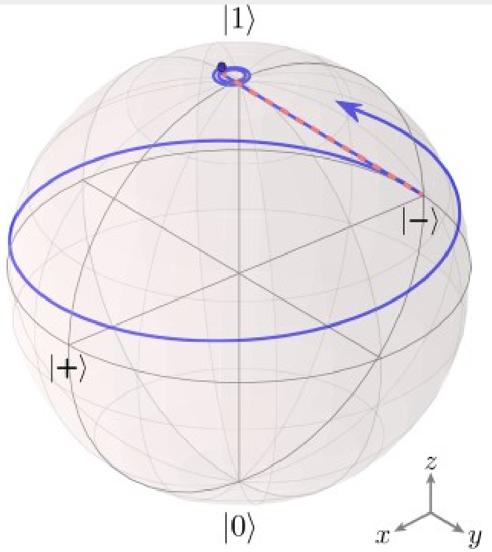
Probability during any dt:

$$M_0(dt) \equiv \mathbb{I} - dt(iH + \sum_k L_k^\dagger L_k/2)$$ smooth evolution → $$P_0(t) = 1 - dt \sum_k \langle L_k^\dagger L_k \rangle_t$$

$$M_k(dt) \equiv \sqrt{dt} L_k$$ quantum jump of type k → $$P_k(t) = dt \langle L_k^\dagger L_k \rangle_t$$

Example: Optical cavity





Evolution under environmental monitoring

Assuming an initial pure state and keeping the record of the outcomes:

Stochastic Schrödinger equation (Langevin-like)

Introducing Poisson increments $dN_k(t)$

$$\mathrm{d}|\psi\rangle_t = \mathrm{d}t\left(-\frac{i}{\hbar}H + \sum_k \frac{\langle L_k^\dagger L_k\rangle_t - L_k^\dagger L_k}{2}\right)|\psi\rangle_t + \sum_k \mathrm{d}N_k(t)\left(\frac{L_k}{\sqrt{\langle L_k^\dagger L_k\rangle_t}} - \mathbb{I}\right)|\psi\rangle_t$$

Smooth evolution (No jump) Jump of type k

The average evolution is a Lindblad master equation (Fokker-Planck-like):

$$\dot{\rho}_t = \mathcal{L}_t(\rho_t) = -\frac{i}{\hbar}[H,\rho_t] + \sum_k \left(L_k \rho L_k^\dagger - \frac{1}{2}\{L_k^\dagger L_k, \rho_t\}\right)$$

STEADY STATE:

$$\mathcal{L}_t(\pi) = 0$$

$$\pi = \sum_l \pi_k |\pi_k\rangle\langle\pi_k|$$

→ micro-states

→ populations/probabilities of micro-states

Entropy production and FT's *

- **Trajectories:** Initial and final measurements (system) + jumps and times (environment):

$$\gamma_{\{0,t\}} \equiv \{n(0), \mathcal{R}_0^t, n(t)\}$$ with environmental record $$\mathcal{R}_0^t = \{(k_1, t_1), (k_2, t_2), ..., (k_J, t_j)\}$$

- **Entropy production:**

system entropy — environment entropy

$$\Delta s_{\rm tot}(t) \equiv \log\left(\frac{P(\gamma_{\{0,t\}})}{\tilde{P}(\tilde{\gamma}_{\{0,t\}})}\right) = \log\left(\frac{\pi_n}{\pi_m}\right) + \sum_{k_j} \Delta s_{k_j}^{\rm env}$$

- **Local detailed-balance**
  - For Lindblad operators coming in pairs: $$L_k = e^{\Delta s_k^{\rm env}} L_{k'}^\dagger$$

    e.g. for a thermal bath: $$\Delta s_{k_j}^{\rm env} = -\beta \Delta E_{k_j}$$
  - For any self-adjoint Lindblad operator $L_k = L_k^\dagger \Rightarrow \Delta s_k^{\rm env} = 0$

- **Fluctuation theorems:** $$\langle e^{-\Delta s_{\rm tot}(t)}\rangle_\gamma = 1 \quad \Rightarrow \quad \langle \Delta s_{\rm tot}(t)\rangle_\gamma \geq 0$$

[G. Manzano, J.M. Horowitz, and J.M.R. Parrondo, PRX (2018);
J.M. Horowitz and J. M. R. Parrondo, NJP (2013); J.M. Horowitz, PRE (2012)]

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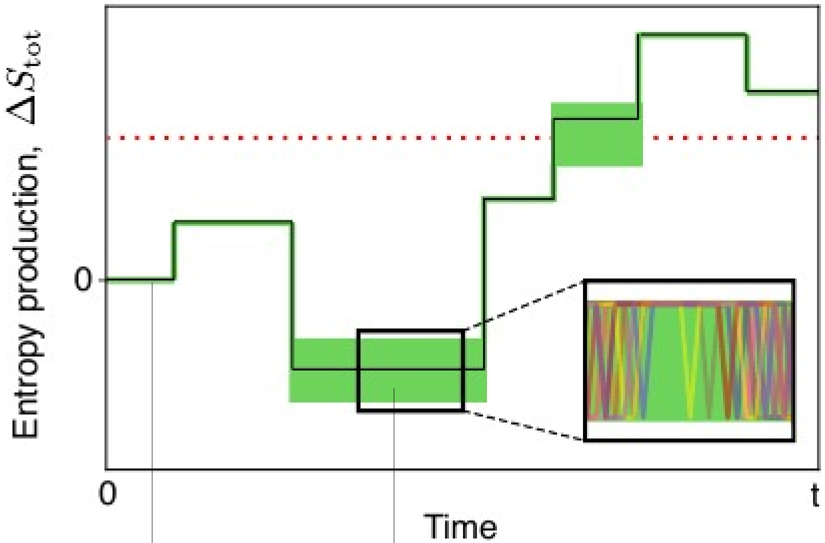
- **Does classical martingale theory for entropy production apply to quantum thermo?**

$$\langle e^{-\Delta s_{\rm tot}(t)}|\gamma_{\{0,\tau\}}\rangle = e^{-\Delta s_{\rm tot}(\tau)} \quad \text{for} \quad 0 \le \tau \le t$$

average conditioned on trajectory at past times [I. Neri, É. Roldán, and F. Jülicher, PRX (2017)]

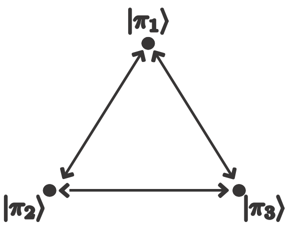
- **Quantum generalization becomes problematic !**



- Entropy production needs measurements on the system.
- Sometimes it is not well defined at intermediate times
- How to make meaningful conditions on past times ?

$|\psi\rangle_t$ in a superposition of eigenstates (of the steady state)
[EP would depend on an eventual measurement]

$|\psi\rangle_t$ in a eigenstate (microstate) of the steady state [well defined without measurements]



Classical Markov

- **Quantum fluctuations spoil the Martingale property!**

$$\langle e^{-\Delta s_{\rm tot}(t)} | \gamma_{[0,\tau]} \rangle = e^{-\Delta s_{\rm tot}(\tau) + \Delta s_{\rm unc}(\tau)} \quad \text{for} \quad 0 \leq \tau \leq t$$

  - The extra term measures the entropic value of the uncertainty in $|\psi\rangle$:

$$\Delta s_{\rm unc}(t) = -\log\left(\frac{\pi_{n(t)}}{\langle \pi \rangle_{\psi(t)}}\right)$$

which fulfills:

$$\langle e^{-\Delta s_{\rm unc}(t)} | \gamma_{[0,\tau]} \rangle = 1$$

$\langle \pi \rangle_{\psi(t)} = \sum_i \pi_i |\langle \psi(t) | \pi_i \rangle|^2$ is the "average probability" when measuring $|\psi(t)\rangle$

- **Decomposition of the stochastic EP:**

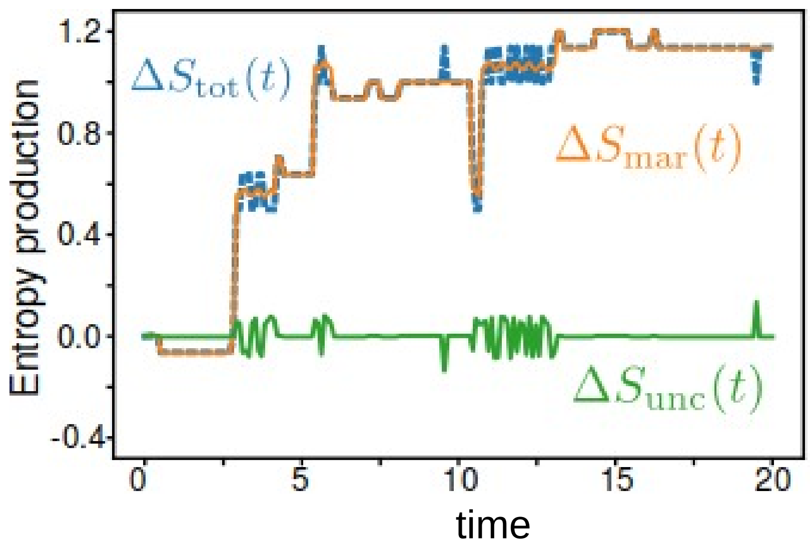
$$\Delta s_{\rm tot}(t) = \Delta s_{\rm unc}(t) + \Delta s_{\rm mar}(t)$$

  - $\Delta s_{\rm mar}(t)$ "classicalization" of EP and is an exponential martingale

$$\langle e^{-\Delta s_{\rm mar}(t)} | \gamma_{\{0,\tau\}} \rangle = e^{-\Delta s_{\rm mar}(\tau)}$$

  - Both terms fulfill fluctuation theorems:

$$\langle e^{-\Delta s_{\rm mar}(t)} \rangle = 1 \qquad \langle e^{-\Delta s_{\rm unc}(t)} \rangle = 1$$



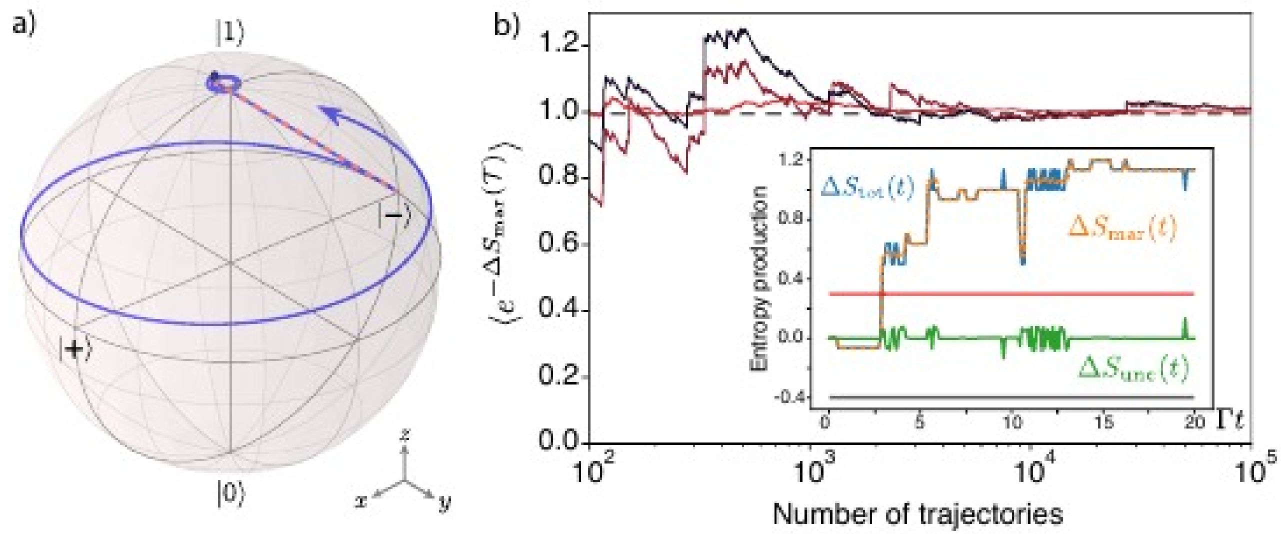
- **Stopping-time fluctuation theorem**

$$\langle e^{-\Delta s_{\mathrm{mar}}(\mathcal{T})}\rangle = 1 \quad \Longrightarrow \quad \langle \Delta s_{\mathrm{tot}}(\mathcal{T})\rangle \geq \langle \Delta s_{\mathrm{unc}}(\mathcal{T})\rangle \longrightarrow$$ either positive or negative

$\mathcal{T}$ stochastic stopping-time

Example: 2-level system with orthogonal jumps

Minimum between first-passage time with 1 or 2 thresholds and a fixed maximum t



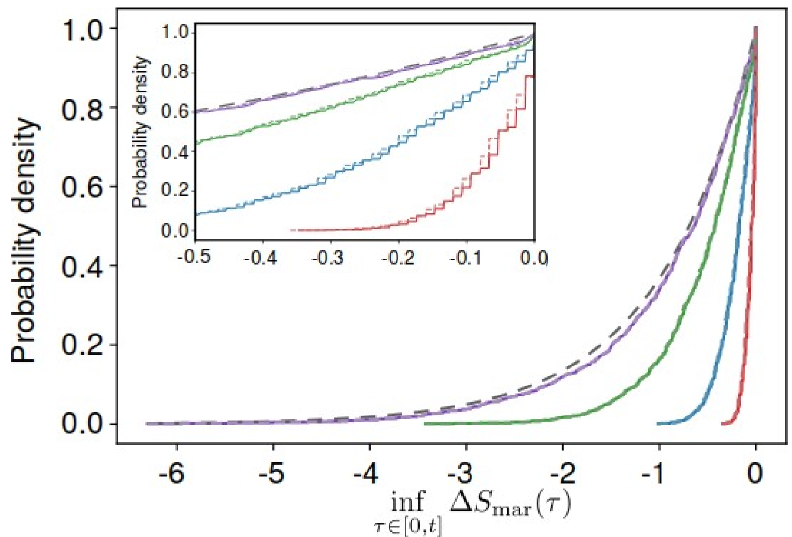
- **Finite-time infimum inequality:**

$$\Pr\left(\inf_{\tau\in[0,t]}\Delta s_{\mathrm{mar}}(\tau) \leq \xi\right) \leq e^{-\xi}$$

Modified infimum law:

$$\langle \inf_{\tau\in[0,t]}\Delta s_{\mathrm{tot}}(\tau)\rangle \geq -1 - \frac{\pi_{\max}}{\pi_{\min}}$$

max and min eigenvalues of the steady state



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Main conclusions

- Stochastic thermodynamics can be extended to the quantum realm by properly defining “trajectories”, trough quantum measurements.
- The quantum jump trajectory formalism can be employed to asses the thermodynamics of open quantum systems beyond thermal reservoirs.
- For nonequilibrium steady states, the entropy production is not always an exponential Martingale due to quantum fluctuations.
- A quantum martingale theory can be however developed by performing a quantum-classical split of the entropy production.
- We obtain quantum corrections in several results for stopping times and finite-time infimum, whose consequences are still to be fully understood.

THANK YOU

for your attention

FOR MORE INFORMATION:

G. Manzano., R. Fazio, and É. Roldán, arXiv: 1903.02925 (2019); [accepted in PRL]