Quantum Martingale Theory and Entropy Production

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Outline:

- **Introduction**
  - **Fluctuation theorems**
  - **Martingales in stochastic thermodynamics**

- **Framework**
  - **Quantum-jump trajectories**
  - **Entropy production and fluctuation theorems**

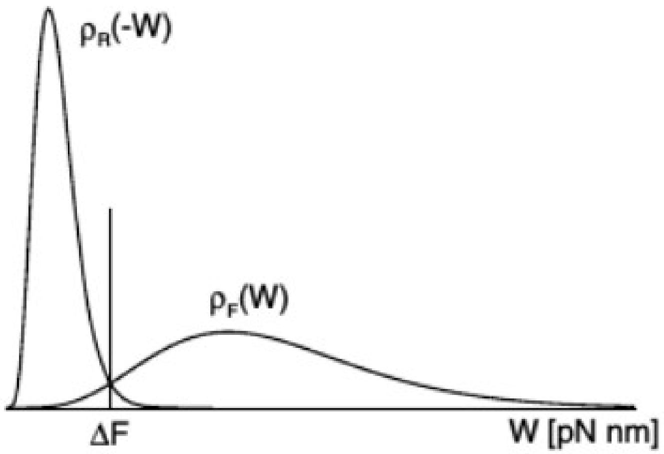
- **Quantum martingale theory**
  - **Classical-Quantum split**
  - **Stopping times and extreme-events statistics**

- **Main conclusions**

Fluctuation Theorems

Refined second law

Extend the second law to small systems subjected to fluctuations, where thermodynamic quantities are random variables



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

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

$\langle W(t)\rangle_\gamma \geq \Delta F$ $\qquad$ $\Pr(W - \Delta F \leq \xi) \leq e^{-\xi/k_B T}$

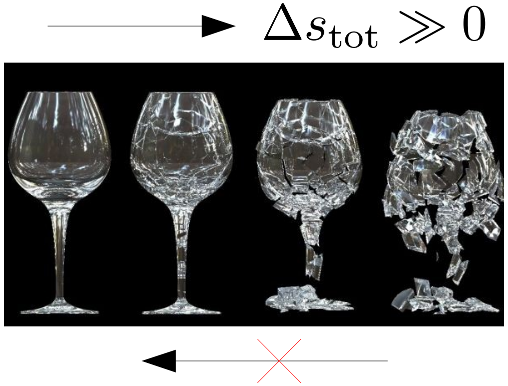
C. Jarzynski, EPJ B (2008); Annu. Rev. Condens. Matter Phys. (2011)

Stochastic entropy production: $\Delta s_{\rm tot}(t) = \Delta s(t) - Q(t)/T$ *(system + environment)*

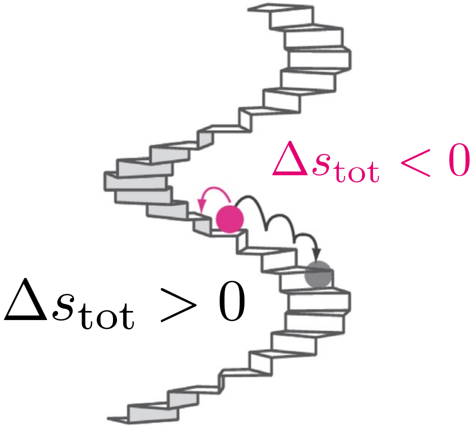
Key: system entropy per trajectory $s(t) \equiv -\log \rho_t(\gamma(t))$ U. Seifert PRL (2005); Rep. Prog. Phys. (2012)

$$\log\left(\frac{P(\gamma_{\{0,t\}})}{\tilde{P}(\tilde{\gamma}_{\{0,t\}})}\right) = \Delta s_{\rm tot}(t)$$

$$\langle e^{-\Delta s_{\rm tot}}\rangle_\gamma = 1 \quad \Rightarrow \quad \langle \Delta s_{\rm tot}\rangle_\gamma \geq 0$$



$\Delta s_{\rm tot} \gg 0$



$\Delta s_{\rm tot} < 0$

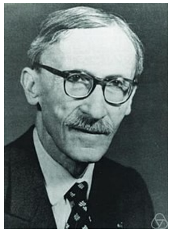
$\Delta s_{\rm tot} > 0$

Martingales

In nonequilibrium steady states, the stochastic process $e^{-\Delta s_{\rm tot}(t)}$ is a MARTINGALE:

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

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

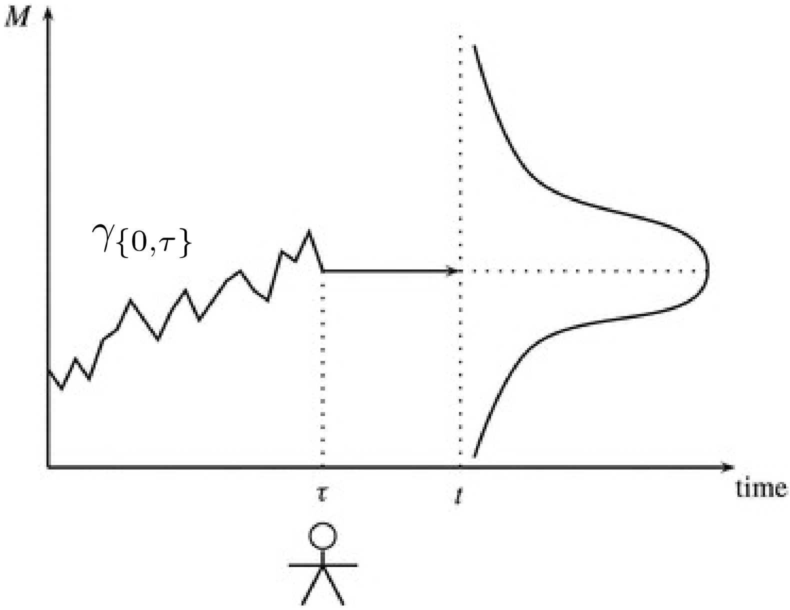


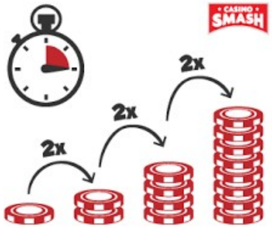
Introduced in probability theory by Paul Lévy in 1934 and named by Ville (1939)

$M(t) < \infty$ is Martingale iff:

$$\langle M(t) | \gamma_{\{0,\tau\}} \rangle = M(\tau)$$

For times $0 \leq \tau \leq t$

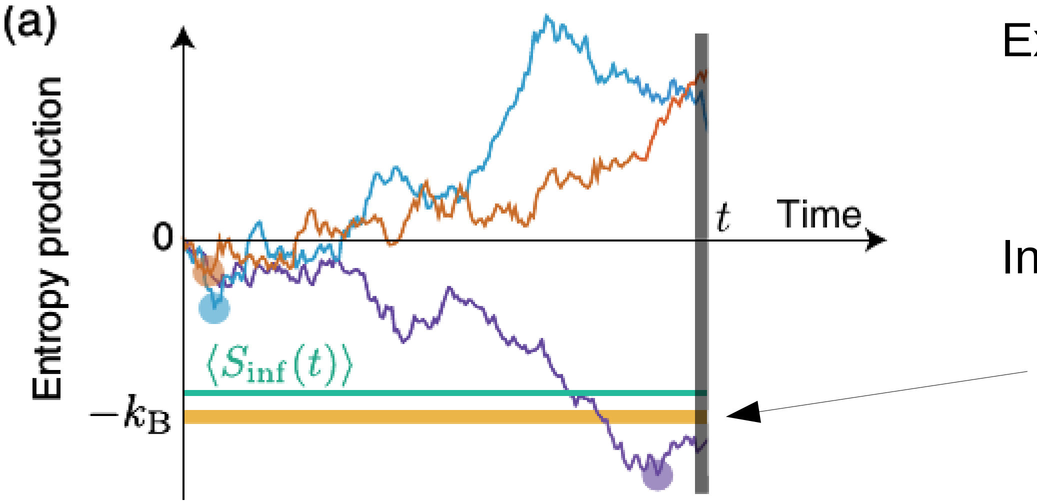




- More general than the Fluctuation Theorem !! $\tau = 0 \;\Rightarrow\; \langle e^{-\Delta s_{\rm tot}(t)} \rangle = 1$
- Martingale processes are well known in mathematics of finance ⟶ No arbitrage opportunities

Implications for entropy production

- **Statistics of EP finite-time infima**: via Doob's maximal inequality



Extreme reductions of entropy:

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

Infimum law:

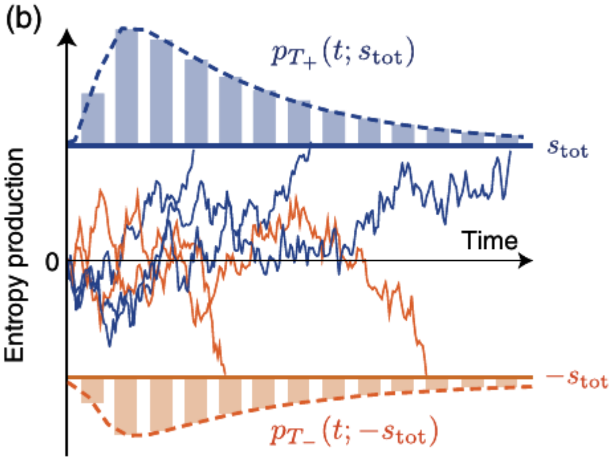
$$\langle S_{\rm inf}(t)\rangle\geq-1$$

- **Statistics of EP at (random) stopping times**: via Doob's optional sampling theorem

Stopping times: times at which some condition of the process is verified for the first time

Fluctuation theorems for stopping times $\mathcal{T}$:

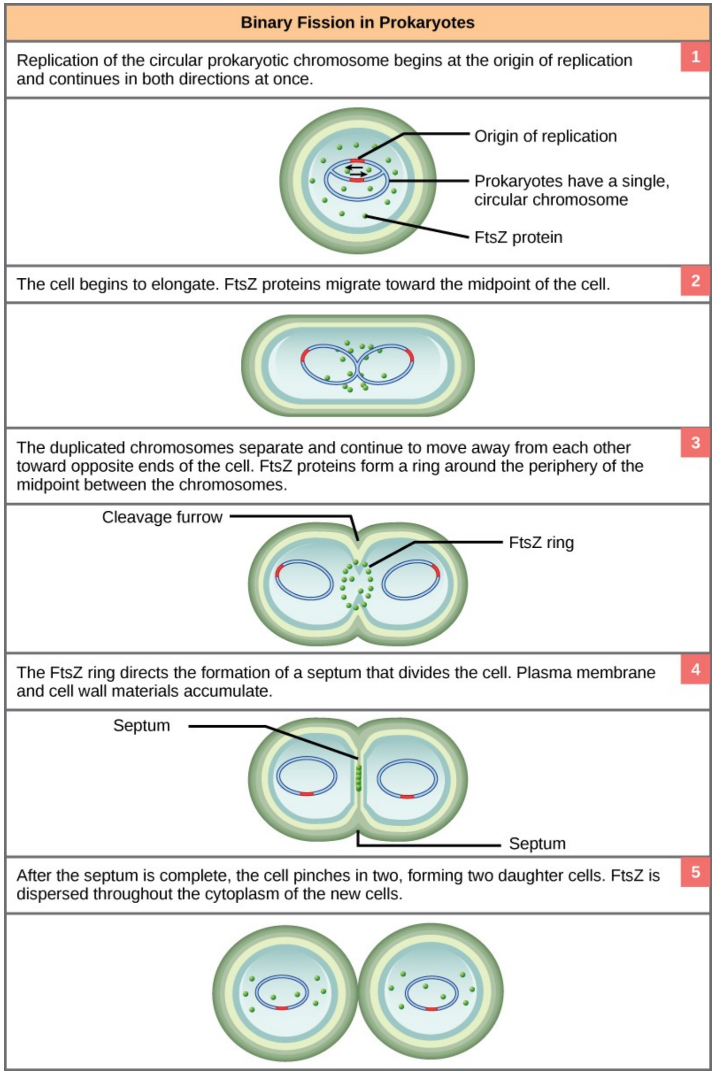
$$\langle e^{-\Delta s_{\rm tot}(\mathcal{T})}\rangle=1$$



[I. Neri, É. Roldán, and F. Jülicher, PRX (2017)]

Stopping times are ubiquitous in many autonomous processes...

Cellular functions: bacterial cell cycle



Binary Fission in Prokaryotes

1 Replication of the circular prokaryotic chromosome begins at the origin of replication and continues in both directions at once.

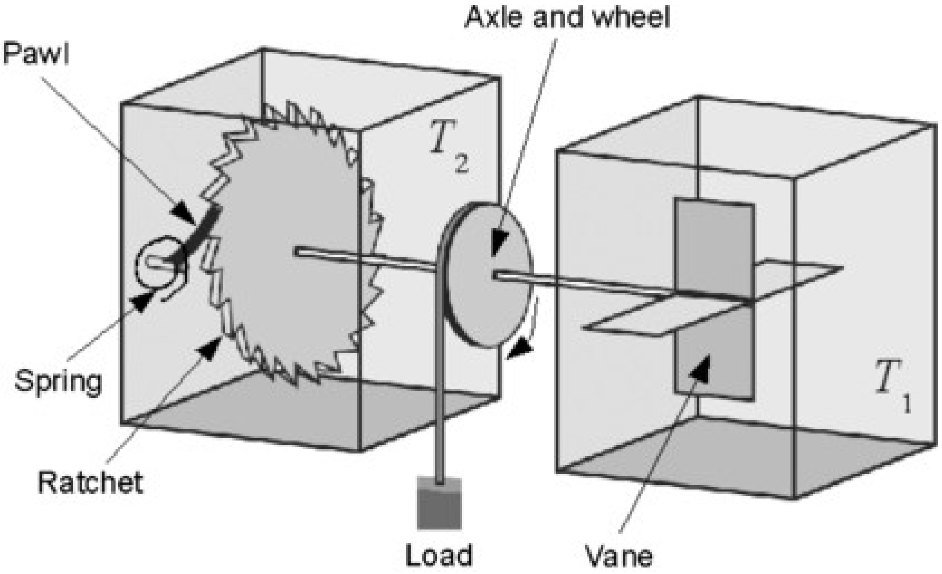
2 The cell begins to elongate. FtsZ proteins migrate toward the midpoint of the cell.

3 The duplicated chromosomes separate and continue to move away from each other toward opposite ends of the cell. FtsZ proteins form a ring around the periphery of the midpoint between the chromosomes.

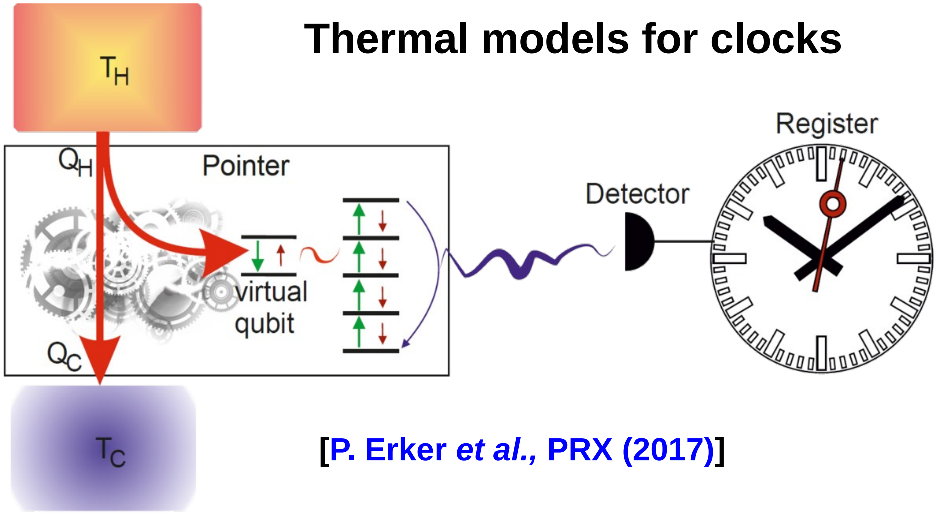
4 The FtsZ ring directs the formation of a septum that divides the cell. Plasma membrane and cell wall materials accumulate.

5 After the septum is complete, the cell pinches in two, forming two daughter cells. FtsZ is dispersed throughout the cytoplasm of the new cells.

Feynman’s ratchet



Thermal models for clocks



[P. Erker *et al.*, PRX (2017)]

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    - Fluctuation theorems
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- **Framework**
    - **Quantum jump trajectories**
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    - Classical-Quantum split of entropy production
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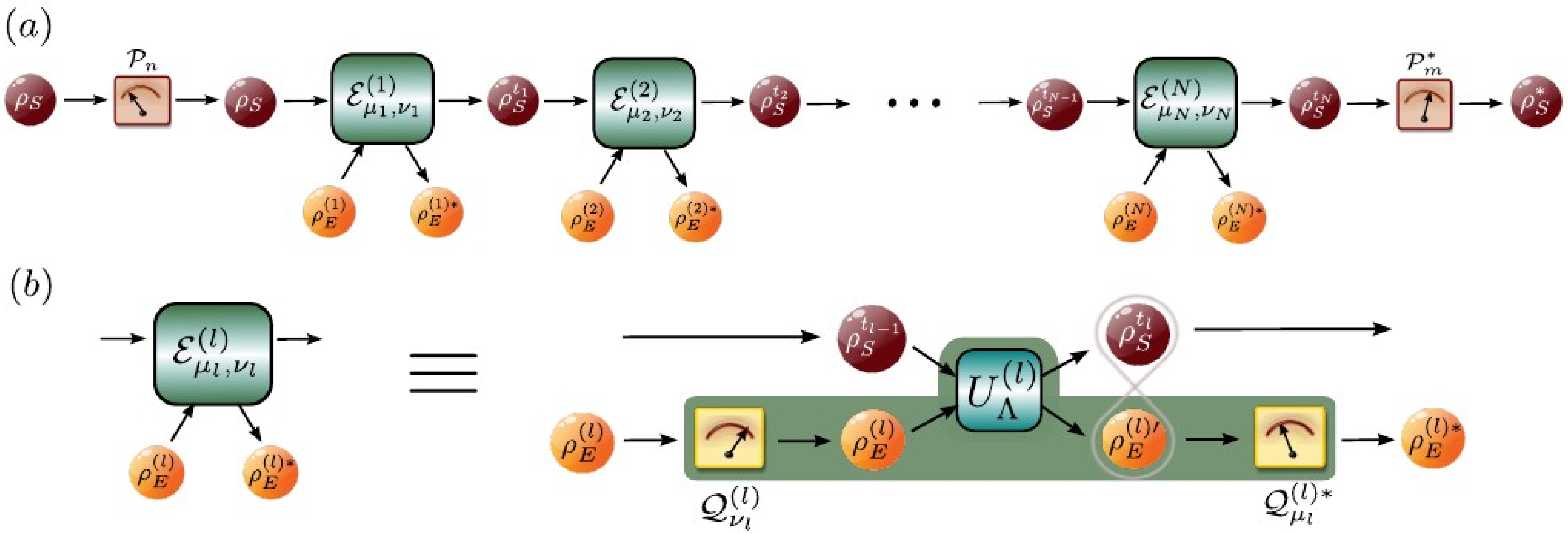
- Main conclusions

Quantum jump trajectories

System interacts “sequentially” with the environment:



- “Trajectories” 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:

$$N \to \infty \qquad dt \to 0$$

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

Quantum jump trajectories:

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

Measurements backaction can be recasted as:

Probability during any dt:

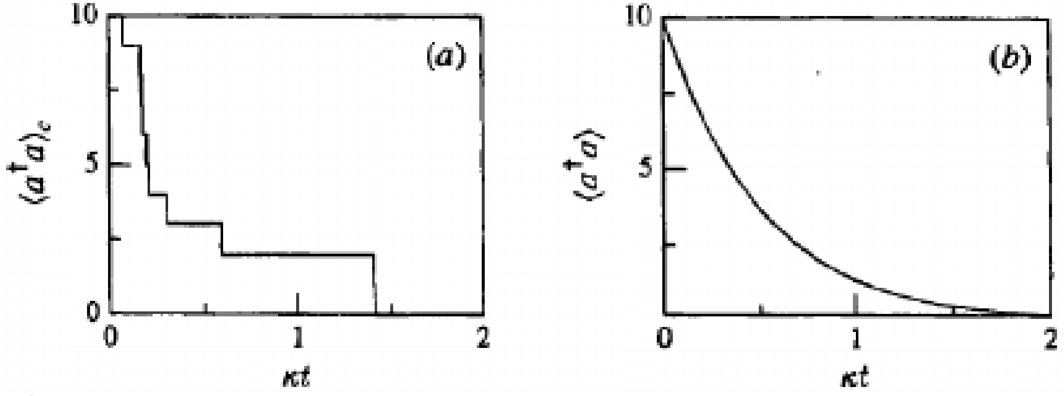
$$M_0(dt) \equiv \mathbb{I} - dt(iH + \sum_k L_k^\dagger L_k/2)$$ smooth evolution $\longrightarrow$ $$P_0(t) = 1 - dt\sum_k \langle L_k^\dagger L_k\rangle_t$$

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

Example: Optical cavity photo-detection

single trajectory

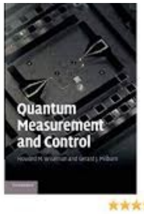
average: exponential decay

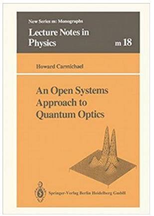


Spontaneous emission

$$M_0(dt) \equiv \mathbb{I} - dt(iH + \gamma a^\dagger a/2)$$

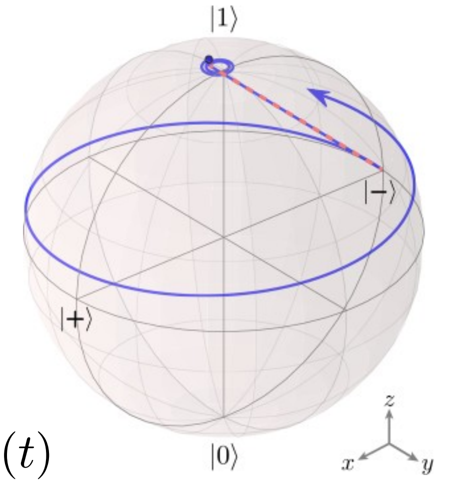
$$M_\downarrow(dt) \equiv \sqrt{dt\gamma}\; a$$





Books: H. M. Wiseman and G. J. Milburn, Quantum measurement and control (2010).
H. Carmichael, An open systems approach to quantum optics (1993).

Quantum jump trajectories



Evolution under environmental monitoring

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

Stochastic Schrödinger equation

Introducing Poisson increments $dN_k(t)$ associated to the number of jumps $N_k(t)$

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

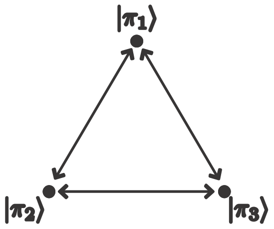
Smooth evolution (No jump)

Jump of type k

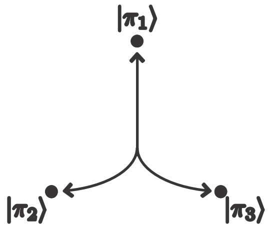
The average evolution verifies a Lindblad master equation:

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

Classical Markov



Quantum



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 $\mathcal{R}_0^t = \{(k_1, t_1), (k_2, t_2), \dots, (k_J, t_J)\}$

- **Entropy production:**

system entropy

environment entropy

$$\Delta s_{\mathrm{tot}}(t) \equiv \log\left(\frac{P(\gamma_{\{0,t\}})}{\tilde{P}(\tilde{\gamma}_{\{0,t\}})}\right) = \log\left(\frac{\pi_{n(0)}}{\pi_{n(t)}}\right) + \sum_{j=1}^{J} \Delta s_{k_j}^{\mathrm{env}}$$

$$\langle \Delta s(t) \rangle_\gamma = \Delta S = 0$$

steady state

$$\sum_j \langle \Delta s_{k_j}^{\mathrm{env}}(t) \rangle_\gamma = -\int_0^t dt' \mathrm{Tr}[\dot{\rho}_{\mathrm{env}} \ln \rho_{\mathrm{env}}]$$

- **Local detailed-balance**
  - For Lindblad operators coming in pairs: $\boxed{L_k = e^{\Delta s_k^{\mathrm{env}}/2} L_{k'}^\dagger}$

e.g. for a thermal bath:
$\Delta s_{k_j}^{\mathrm{env}} = -\beta \Delta E_{k_j}$

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

[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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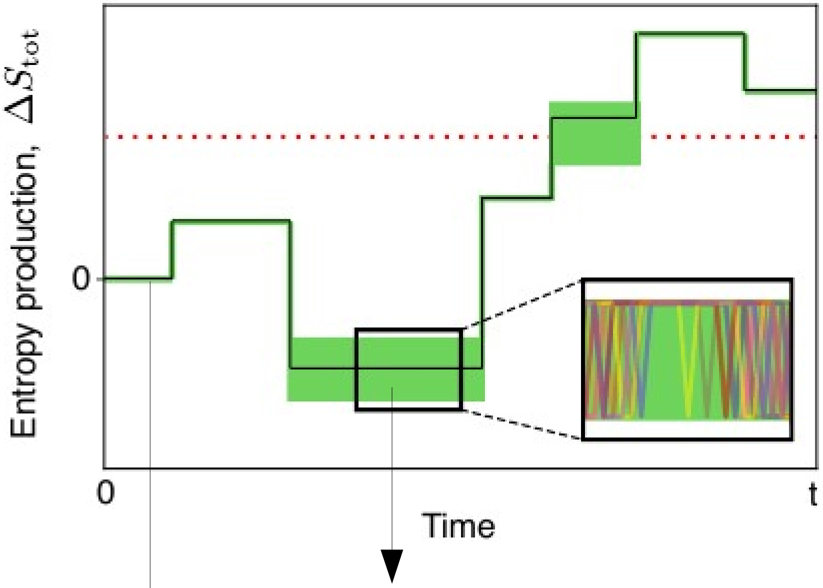
Quantum Martingale Theory

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

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

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

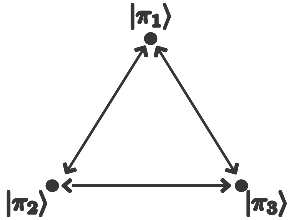
- **Quantum generalization becomes problematic !**



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

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

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



Classical Markov

Uncertainty entropy production

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

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

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

"Uncertainty" entropy production

stochastic entropy of state $|\pi_{n(t)}\rangle$

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

stochastic entropy of $|\psi(t)\rangle$

where:

prob. microstate conditional prob.

$$\langle \pi \rangle_{\psi(t)} = \langle \psi(t) | \pi | \psi(t) \rangle = \sum_i \pi_i |\langle \psi(t) | \pi_i \rangle|^2$$

squared fidelity between
the steady state π and $|\psi(t)\rangle$

In the classical limit: $|\psi(t)\rangle = |\pi_{n(t)}\rangle \quad \forall t \quad \Longrightarrow \quad \Delta s_{\text{unc}}(t) = 0 \quad \forall t$

The uncertainty EP fulfills: $\boxed{\langle e^{-\Delta s_{\text{unc}}(t)} | \gamma_{[0,\tau]} \rangle = 1} \qquad 0 \leq \tau < t$

Classical-Quantum split

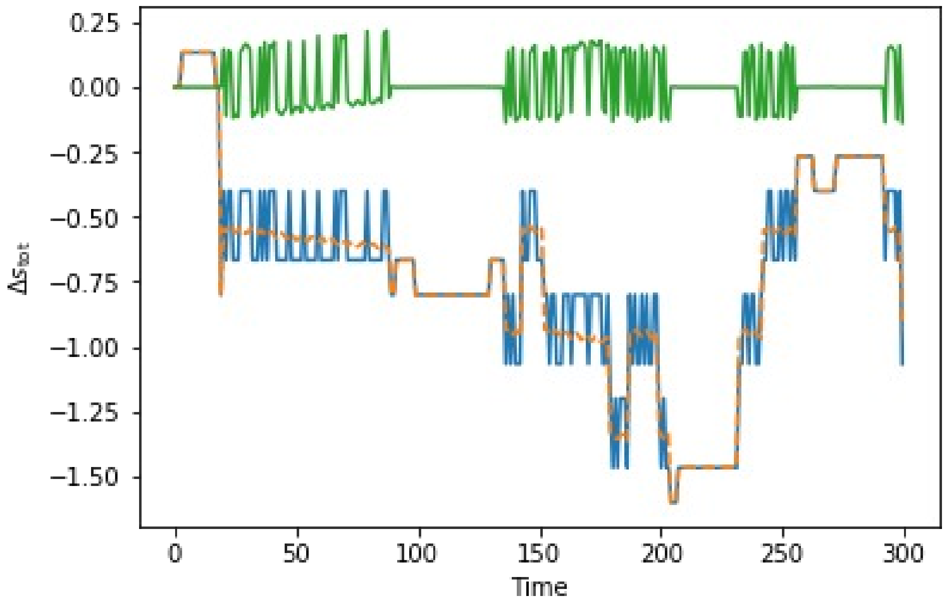
- **Decomposition of the stochastic EP:**

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

$$\Delta s_{\rm mar}(t) \equiv \log\left(\frac{\pi_{n(0)}}{\langle\pi\rangle_{\psi(t)}}\right) + \sum_{k_j} \Delta s^{\rm env}_{k_j}$$

- $\Delta s_{\rm mar}(t)$ is a “classicalization” of the entropy production

Martingale property: $\boxed{\langle e^{-\Delta s_{\rm mar}(t)} | \gamma_{\{0,\tau\}}\rangle = e^{-\Delta s_{\rm mar}(\tau)}}$ for $0 \leq \tau \leq t$



- Both terms fulfill fluctuation theorems:

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

- Both terms are non-negative:

$$\langle \Delta s_{\rm mar}(t)\rangle \geq 0 \qquad \langle \Delta s_{\rm unc}(t)\rangle \geq 0$$

Stopping-time fluctuations and Extreme-value statistics

- **Fluctuation theorem at stopping times**

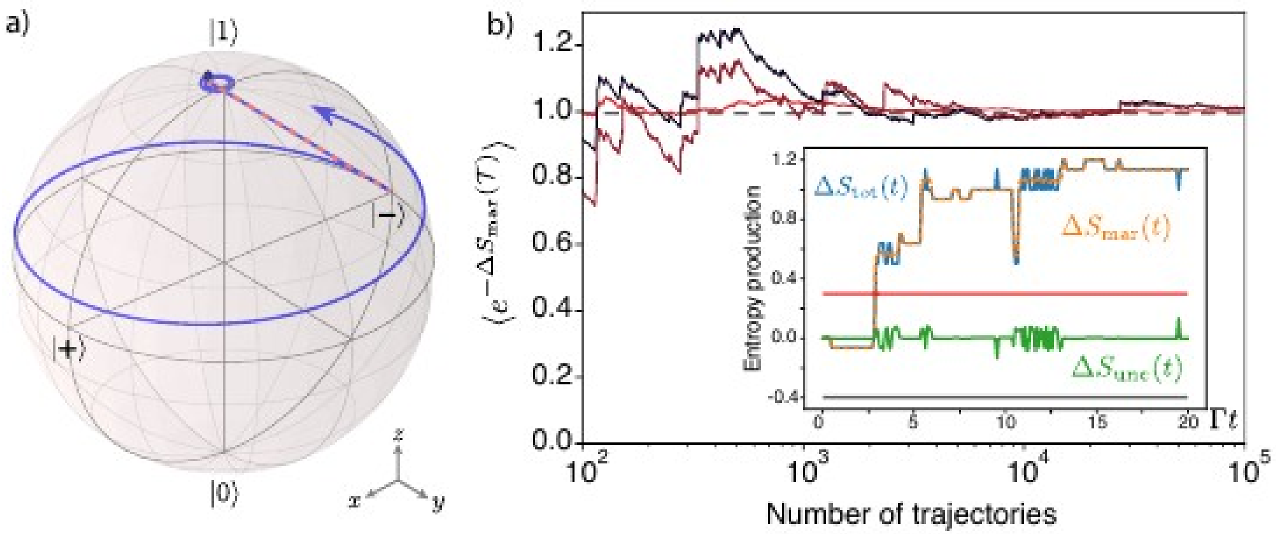
$$\langle e^{-\Delta s_{\mathrm{mar}}(\mathcal{T})}\rangle = 1 \quad \Longrightarrow \quad \langle \Delta s_{\mathrm{tot}}(\mathcal{T})\rangle \geq \langle \Delta s_{\mathrm{unc}}(\mathcal{T})\rangle$$

may be 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



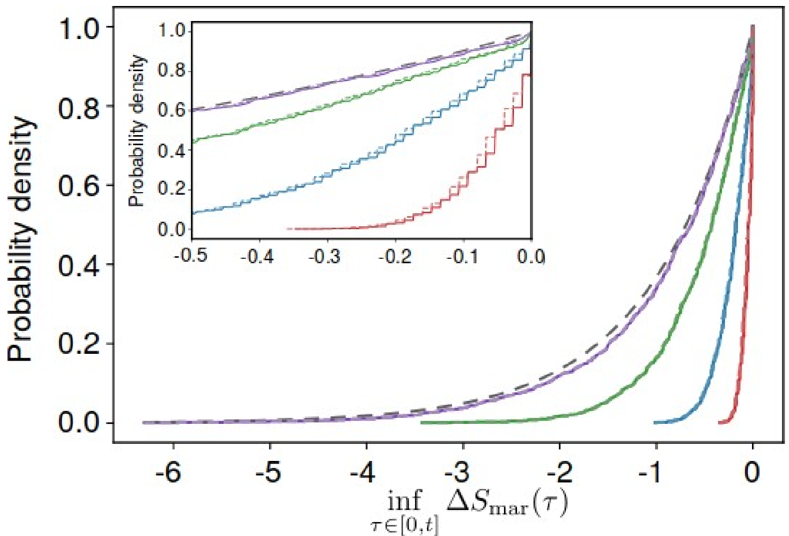
- **Finite-time infimum inequality:**

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

Modified infimum law:

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

max and min eigenvalues of the steady state



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Main conclusions

- For nonequilibrium steady states, the entropy production fulfills stronger constraints than fluctuation theorems (Martingale property).
- The Martingale property may break down due to quantum fluctuations induced by measurements.
- A quantum martingale theory can be however developed by performing a quantum-classical split of the entropy production, where both terms fulfill some generalized form of fluctuation theorem.
- We obtain quantum corrections in several results for stopping times fluctuations and finite-time infimum, whose consequences are still to be fully understood.

Outlook

- Effects of coherence in probability distributions of thermodynamic quantities ?!

Main conclusions

THANK YOU

for your attention

FOR MORE INFORMATION:

G. Manzano, R. Fazio, and É. Roldán, PRL **122**, 220602 (2019)