Quantum fluctuation theorem from modified superoperators

G. De Chiara, A. Imparato, arXiv:2108.05937

A. Hewgill, G. De Chiara, A. Imparato, Phys. Rev. Res. 2021

Alberto Imparato

Institut for Fysik og Astronomi
Aarhus Universitet
Denmark

AARHUS UNIVERSITET

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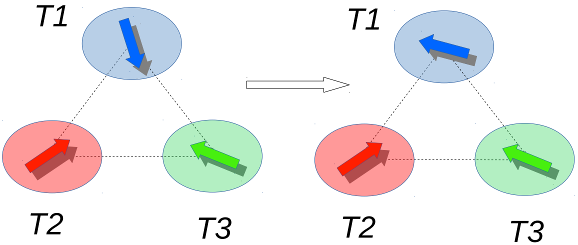
N subsystems with N_b baths (here $N = N_b$)

A given bath drives the transition of the corresponding subsystem



In the classical case

- $\Delta S_B = -\sum_\alpha \beta_\alpha Q_\alpha$
- $\Delta S_S = -\log p(\mathbf{x},t)/p(\mathbf{x},0)$

$$\langle \exp\left(-\Delta S_B - \Delta S_S\right)\rangle = 1$$

the entropy production reads $\dot{\Sigma} = d_t S_S - \sum_\alpha \beta_\alpha \dot{Q}_\alpha > 0$

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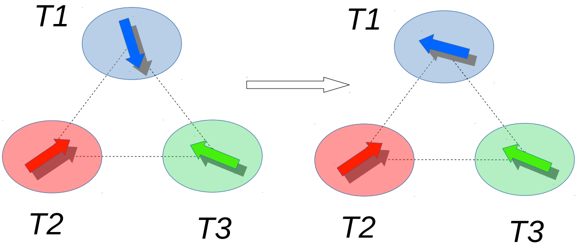

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Today's talk

- Given that the dynamics is described by a quantum (possibly local) master equation in Gorini-Kossakowski-Lindblad-Sudarshan (GKLS) form
- can I write a quantum FT in the form $\langle \exp\left(-\Delta S_B - \Delta S_S\right)\rangle = 1$?

GKLS Master Equation

a system with Hamiltonian H, in contact with N_b baths

$$\frac{d\rho}{dt} = -\mathbb{i}\,[H, \rho] + \sum_{\alpha=1}^{N_b} D_\alpha[\rho]$$

with dissipators

$$D_\alpha[\rho] = \sum_\lambda \gamma_{\lambda,\alpha} \left(L_\lambda \rho L_\lambda^\dagger - \frac{1}{2}\{L_\lambda^\dagger L_\lambda, \rho\} \right)$$

- An arbitrary set of kets $|j\rangle$ that form an orthogonal basis for the system.
- choose the jump operator $L_\lambda = |j'\rangle\langle j|$
- $\lambda(j \to j')$ denotes a transition between two states $|j\rangle$ and $|j'\rangle$ dissipation rates

$$\frac{\gamma_{\lambda,\alpha}(\omega_\lambda)}{\gamma_{\lambda,\alpha}(-\omega_\lambda)} = \mathrm{e}^{-\beta_\alpha \omega_\lambda}, \qquad \omega_\lambda = \langle j'|H|j'\rangle - \langle j|H|j\rangle$$

Connection between the dynamics and the thermodynamics

- Jumps between two states with rates $\gamma_{j'j}$
- the baths absorb/emit quanta of energy:
  $\beta_\alpha^{-1} \log(\gamma_{\alpha,j'j}/\gamma_{\alpha,jj'}) = \omega_{j'j}$
- entropy change in the bath α:
  $\Delta s_{\alpha,j'j} = -\log(\gamma_{\alpha,jj'}/\gamma_{\alpha,j'j})$
- $\omega_{j',j} = \langle j'|H|j'\rangle - \langle j|H|j\rangle$
  $|j\rangle$ can or cannot be the eigenstates of H (global/local ME)
- Our results hold for $H(t)$ too

FT: learn from the classical case

The classical case

- A classical master equation: $\dot{\mathbf{p}}(t) = \mathbf{M} \cdot \mathbf{p}(t)$
- $p_j(t) \Rightarrow \Phi_j(\Delta S_B, t)$: joint probability distribution of finding the system at time t in the state j with a total bath(s) entropy ΔS_B
- An extended master equation: $\dot{\mathbf{\Phi}} = \mathcal{L}_{\mathbf{M}} \mathbf{\Phi}$
- The FT follows from the symmetries of the differential operator $\mathcal{L}_{\mathbf{M}}$

Lebowitz and H. Spohn, J. Stat. Phys. 1999

AI and L. Peliti J. Stat. Mec. 2007

The quantum case

- A quantum master equation for $\rho(t)$
- introduce a modified density matrix $\tilde{\rho}(\Delta S_B, t)$ such that $\tilde{\rho}_{jj}(\Delta S_B, t)$ is the joint probability distribution of finding the system at time t in the state $|j\rangle$ with a total entropy ΔS_B

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Modified density matrix and ME

Entropy change in the bath α:
$\Delta s_{\alpha,j'j} = -\log(\gamma_{\alpha,jj'}/\gamma_{\alpha,j'j})$

$$\star \qquad \partial_t \tilde{\rho}_{j'j'}(\Delta S_B, t) = -\mathbb{i}[H,\tilde{\rho}]_{j'j'} + \sum_{\alpha,j}\left\{\gamma_{\alpha,j'j}\left[\sum_{n=0}^{\infty}\frac{\left(\Delta s_{\alpha,j'j}\right)^n}{n!}\frac{\partial^n \tilde{\rho}_{jj}}{\partial \Delta S_B^n}\right] - \gamma_{\alpha,jj'}\tilde{\rho}_{j'j'}\right\},$$

$$\star\star \qquad \partial_t \tilde{\rho}_{lk}(\Delta S_B, t) = -\mathbb{i}[H,\tilde{\rho}]_{lk} + \sum_{\alpha} D_{ND,\alpha}[\tilde{\rho}_{ND}]_{lk}, \quad l \neq k,$$

- the dissipative term in ★ is identical to the classical case, see *AI and L. Peliti J. Stat. Mec. 2007*
- the RHS of ★★ is identical to the one in the quantum ME $D_{ND,\alpha}[\cdot]$ is a super-operator such that $D_{ND}[\tilde{\rho}_{ND}]$ has vanishing diagonal terms and only couples non-diagonal terms of ρ in the chosen basis

Modified ME, cont.

- Specify the initial condition $\rho^{(0)}$
- Introduce $\Psi(\xi, t)$ akin to the generating function in classical physics

$$\Psi(\xi, t) = \int d\Delta S_B \, \tilde{\rho}(\Delta S_B, t) \mathrm{e}^{-\xi \Delta S_B},$$

$$\left\langle \mathrm{e}^{-\xi \Delta S_B} \right\rangle_{\rho^{(0)}} = \mathrm{tr}[\Psi(\xi, t|\rho^{(0)})]$$

- Let $\Psi^{(1)}(t) = \Psi(\xi = 1, t)$, a straightforward calculation gives

$$\partial_t \Psi^{(1)}(t) = -\mathbb{i}[H, \Psi^{(1)}(t)] + \sum_\alpha D^*_\alpha[\Psi^{(1)}(t)],$$

- dual of the dissipator D_α: $D^*_\alpha[\cdot] = \sum_\lambda \gamma_{\alpha,\lambda} \left(L^\dagger_\lambda \cdot L_\lambda - \frac{1}{2}\{L^\dagger_\lambda L_\lambda, \cdot\} \right)$. time evolution of an operator in the Heisenberg picture

$$\partial_t A = \mathbb{i}[H, A] + \sum_\alpha D^*_\alpha[A],$$

FT for the extended density matrix $\Psi^{(1)}$

The operator $\Psi^{(1)}$

$$\Psi^{(1)}(t) = \int d\Delta S_B \, \tilde{\rho}(\Delta S_B, t) \mathrm{e}^{-\Delta S_B}$$

$$\left\langle \mathrm{e}^{-\Delta S_B} \right\rangle_{\Pi_j, \rho^{(0)}} = \Psi^{(1)}_{jj}(t|\rho^{(0)}), \qquad \text{where } \Pi_j = |j\rangle\langle j|$$

$$\left\langle \mathrm{e}^{-\Delta S_B} \right\rangle_{\rho^{(0)}} = \mathrm{tr}[\Psi^{(1)}(t|\rho^{(0)})]$$

The FT

- Choose an arbitrary initial basis $\{|b_0\rangle\}$

$$\Psi^{(1)}(t|\rho^{(0)}) = \sum_{b_0, b_0'} \rho^{(0)}_{b_0, b_0'} \Psi^{(1)}(t||b_0\rangle\langle b_0'|)$$

-

$$\bar{\Psi}^{(1)}(t) = \sum_{b_0} \Psi^{(1)}(t|\Pi_{b_0}) = \mathbb{I}, \quad \forall t \geq 0.$$

FT for the extended density matrix $\Psi^{(1)}$

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The integral FT

The initial basis $\{|b_0\rangle\}$ is arbitrary
Choose an arbitrary final state $\rho^{(\mathrm{f})}$ (e.g. $\rho^{(\mathrm{f})} \neq \rho(t)$)

$$\mathrm{tr}[\sum_{b_0} \rho^{(0)}_{b_0 b_0} \Psi^{(1)}(t \,|\, \Pi_{b_0}) \mathrm{e}^{-\log \rho^{(0)}_{b_0 b_0}} \mathrm{e}^{\log \rho^{(\mathrm{f})}}] = \mathrm{tr}[\bar{\Psi}^{(1)}(t) \rho^{(\mathrm{f})}] = 1,$$

The final state $\mathbf{p}^{(f)}$ is arbitrary also in the classical case
see *U. Seifert, Rep. Progr. Phys. 2012*

Classical form
$\langle \exp\left(-\Delta S_B - \Delta S_S\right) \rangle = 1$?
Introduce the eigenbasis $\{|r_\mathrm{f}\rangle\}$ of $\rho^{(\mathrm{f})}$

$$\sum_{r_\mathrm{f}, b_0} \int \mathrm{d}\Delta S_B \, \mathrm{e}^{-\Delta S_B + \overbrace{\log \rho^{(\mathrm{f})}_{r_\mathrm{f} r_\mathrm{f}} - \log \rho^{(0)}_{b_0 b_0}}^{-\Delta S_S}} \tilde{\rho}_{r_\mathrm{f}}(\Delta S_B, t | \Pi_{b_0}) \rho^{(0)}_{b_0 b_0} = 1.$$

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A few comments

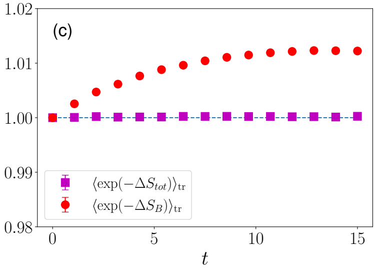
- the initial basis $\{|b_0\rangle\}$ is arbitrary: choosing the initial projection in the eigenbasis of $\rho^{(0)}$ preserves its quantum coherence in other bases
- Our protocol does not require the final system's projection or the continuous measurement of the work

Numerical examples: Quantum Monte Carlo

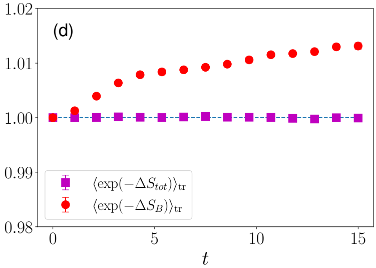
Two spin-1/2 particles at T_a and T_b

$$H = -J\sigma_{x,a}\sigma_{x,b} - h(\sigma_{z,a} + \sigma_{z,b})$$

The jump operators "flip" the individual spins:
$L_\lambda = \sigma_{-,a} \otimes \mathbb{I}_b$ or $L_\lambda = \mathbb{I}_a \otimes \sigma_{-,b}$



(c): non-diagonal $\rho^{(0)}$, $J = 0.1$, $h = 0.2$, $T_a = 1$, $T_b = 1.2$



(d): non-diagonal $\rho^{(0)}$, $J = 0.2$, $T_b = 1.2$, $h(t) = 0.4t/\Delta t$, $\Delta t = 15$

Conclusions

- Quantum FT as conservation of an Hermitian operator
- entirely based on the Lindblad master equation
- valid for arbitrary number of baths and for time-dependent Hamiltonians (Jarzynsky equality)
- requires the continuous monitoring of the baths but neither the final systems projection nor the continuous measurement of the work done
- holds for non-thermal baths as long as microreversibility is preserved