Inferring entropy production from time-dependent moments

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Frontiers in Statistical Physics
RRI, Bangalore (Dec, 2023)

The Niels Bohr International Academy

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Benefiting people and society

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In collaboration with Karel Proesmans
(arXiv:2310.16627)

INTRODUCTION

Classical thermodynamics

Deals with the rules that govern conversion of different forms of energy in macroscopic systems

First law: $dE = dQ + dW$

Second law: $$\Delta S_{\mathrm{tot}} = \Delta S_{\mathrm{sys}} + \Delta S_{\mathrm{env}}$$
$$\geq 0$$

Stochastic thermodynamics

Framework to study thermodynamics of stochastic systems, which can be arbitrarily from the equilibrium.

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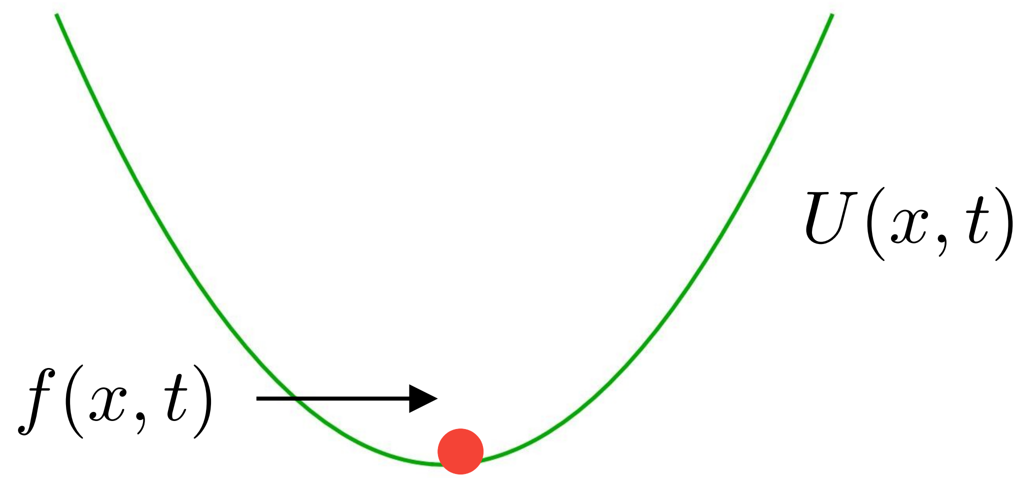


$$\gamma \frac{dx}{dt} = -\frac{\partial U(x,t)}{\partial x} + f(x,t) + \sqrt{2D}\eta(t)$$

Stochastic thermodynamics

$$\gamma \frac{dx}{dt} = -\frac{\partial U(x,t)}{\partial x} + f(x,t) + \sqrt{2D}\eta(t)$$

Heat $$Q(\{x(t)\}) \equiv \int \left[-\gamma \frac{dx}{dt} + \sqrt{2D}\eta(t) \right] \circ dx(t)$$

Work $$W(\{x(t)\}) \equiv \int \left[\frac{\partial U(x,t)}{\partial t} dt + f(x,t) \circ dx(t) \right]$$

First law for a single trajectory $$Q(\{x(t)\}) + W(\{x(t)\}) = \Delta U(x,t)$$

K. Sekimoto, Prog. Th. Phys. (1998)

Stochastic entropy production

U. Seifert, PRL (2005)

$$S_{\rm sys}(t) \equiv -k_B \ln P(x(t),t)$$

$$S_{\rm env}(t) \equiv \frac{Q(t)}{T}$$

$$\Delta S_{\rm tot}(t) = S_{\rm sys}(t) + S_{\rm env}(t)$$

Stochastic entropy production

U. Seifert, PRL (2005)

$$S_{\rm sys}(t) \equiv -k_B \ln P(x(t), t)$$

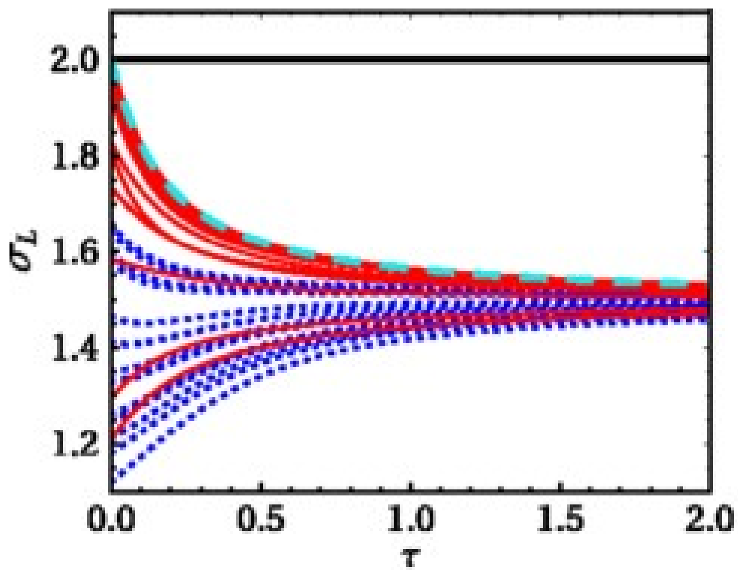
$$S_{\rm env}(t) \equiv \frac{Q(t)}{T}$$

$$\Delta S_{\rm tot}(t) = S_{\rm sys}(t) + S_{\rm env}(t)$$

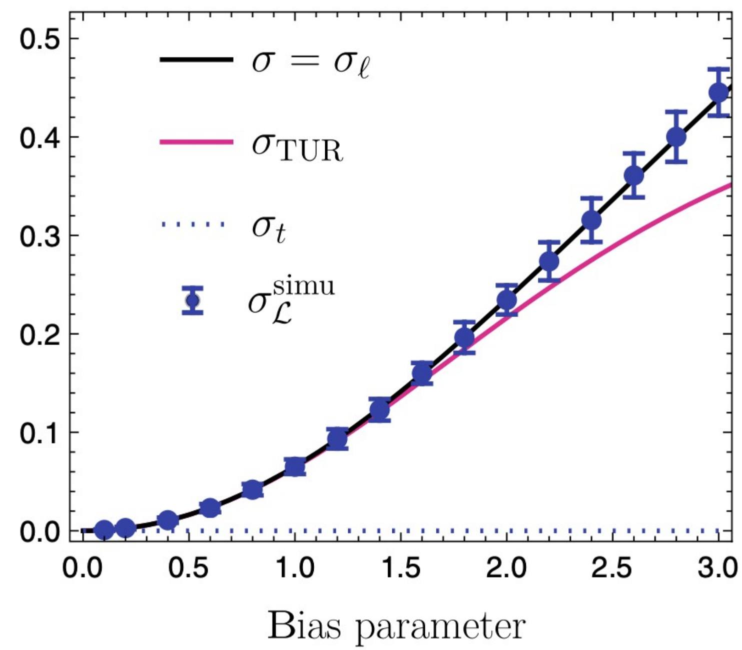
$$\langle \Delta S_{\rm tot}(t_f) \rangle = \frac{k_B}{D} \int_0^{t_f} dt \int dx \; P(x,t) \; v^2(x,t)$$

$$v(x,t) = \frac{D}{k_B T} \left[F(x,t) - k_B T \frac{\partial}{\partial x} \ln P(x,t) \right]$$

Inferring thermodynamic quantities



TUR based

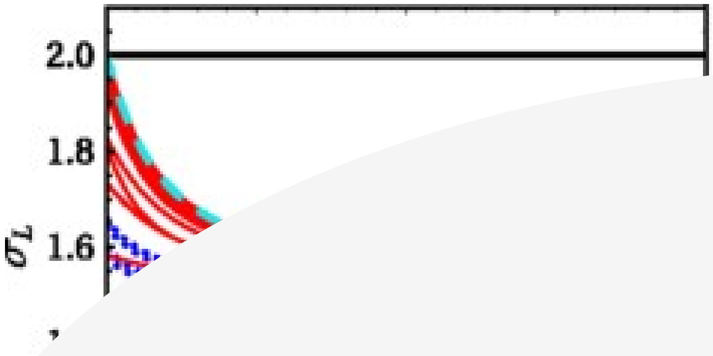


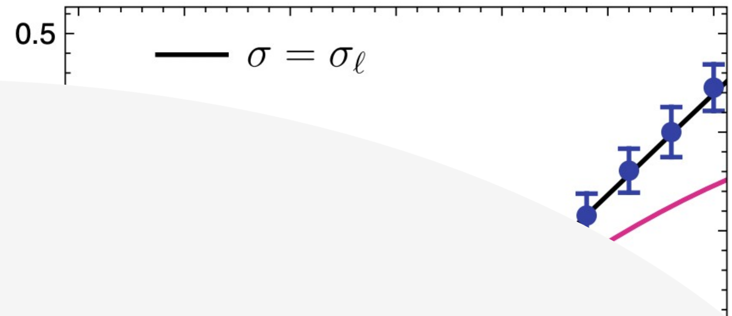
Based on waiting time distribution

- S K Manikandan, D Gupta and S Krishnamurthy, PRL, 124, 120603 (2020)
- P E Harunari, A Dutta, M Polettini, E Roldan, PRX 12, 041026 (2022)

Some other for steady-state systems....

Inferring thermodynamic quantities





In this talk, I will present a method for time-dependent systems
Refs: arXiv:2310.16627, PS and K. Proesmans

Other works:
(1) S. Otsubo, S. Manikandan, T. Sagawa and S. Krishnamurthy Comm. Phys. (2022)
(2) S. Lee, D-K Kim, J. Park, W. Kim, H. Park, and J. S. Lee Phys. Rev. Research (2023)

METHOD

Bound on total entropy production

Our method gives a general bound on $\Delta S_{\mathrm{tot}}(t)$ in terms of moments of x(t)

$$\Delta S_{\mathrm{tot}}(t_f) \geq \frac{k_B}{D} \int_0^{t_f} dt \left[\frac{\dot{\Sigma}^2(t)}{4\Sigma(t)} + \dot{X}_1(t)^2 \right],$$

$$\Sigma(t) = \langle x^2(t) \rangle - \langle x(t) \rangle^2 \qquad X_1(t) = \langle x(t) \rangle$$

Bound on total entropy production

Our method gives a general bound on $\Delta S_{\rm tot}(t)$ in terms of moments of x(t)

Optimisation of the action

$$\mathbb{S}(x, v, t_f) = \Delta S_{\rm tot}(t_f) + \int_0^{t_f} dt \Big[\mu_1(t)\langle x(t)\rangle + \mu_2(t)\langle x^2(t)\rangle\Big]$$

Entropy production — First moment — Second moment

Bound on total entropy production

$$\mathbb{S}\left(x,v,t_f\right) = \int_0^{t_f} dt \int dx \; P(x,t)\left[v^2(x,t) + \mu_1(t)x + \mu_2(t)x^2\right]$$

$$\text{with} \quad v(x,t) = \frac{D}{k_B T}\left[F(x,t) - k_B T \frac{\partial}{\partial x} \ln P(x,t)\right]$$

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left[v(x,t)P(x,t)\right]$$

In general, difficult to carry out this optimisation because P(x,t) depends on the force field F(x,t).

Bound on total entropy production

$$\mathbb{S} = \int_0^{t_f} dt \int dx \; P(x,t) \left[v^2(x,t) + \mu_1(t) x + \mu_2(t) x^2 \right]$$

$$\dot{y}(x,t) = v\left(y(x,t), t\right)$$

$$y(x,0) = x$$

$$\mathbb{S} = \int_0^{t_f} dt \int dx P_0(x) \left[\dot{y}(x,t)^2 + \mu_1(t) y(x,t) + \mu_2(t) y(x,t)^2 \right]$$

JD Benamou and Y Brenier, Numer. Math. (2000)
E Aurell, C Mejía-Monasterio and P Muratore-Ginanneschi, PRL (2011)

Bound on total entropy production

$\delta\mathbb{S} = 0$ gives Euler-Lagrange equation

$$2\ddot{y}(x,t) = \mu_1(t) + 2\mu_2(t)y(x,t).$$

with boundary conditions

$$2\dot{y}(x,t_f) = -\zeta_1(t_f) - 2\zeta_2(t_f)y(x,t_f)$$
$$y(x,0) = x$$

Bound on total entropy production

$$\Delta S_{\rm tot}(t_f) \geq \frac{k_B}{D}\int_0^{t_f} dt \left[\frac{\dot{\Sigma}^2(t)}{4\Sigma(t)} + \dot{X}_1(t)^2\right],$$

$$\Sigma(t) = \langle x^2(t)\rangle - \langle x(t)\rangle^2 \qquad X_1(t) = \langle x(t)\rangle$$

APPLICATION TO
BIT ERASURE EXPERIMENT

Application in Bit erasure

Landauer in 1961 proposed that the minimal thermodynamic cost to erase a bit:

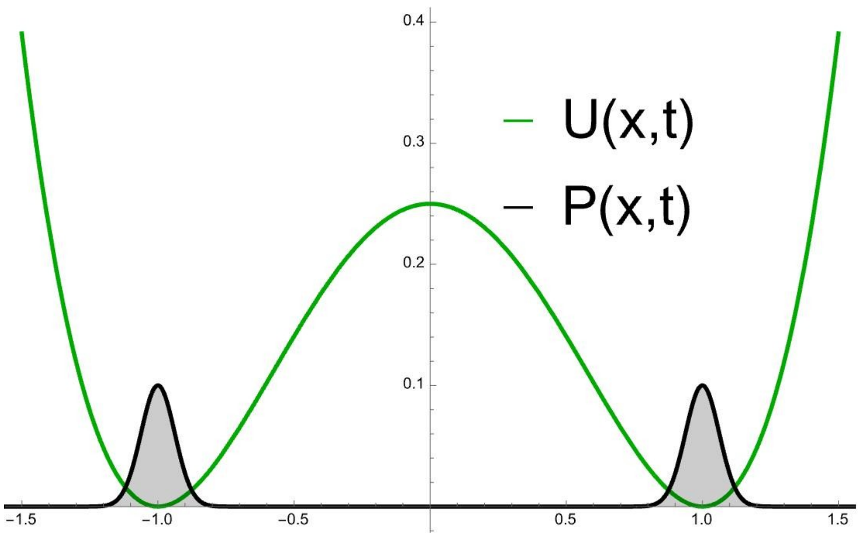
$$W \geq k_B T \ln 2$$

Equality holds only in the quasi-static limit

R. Landauer, IBM Journal of Research and Development, (1961)

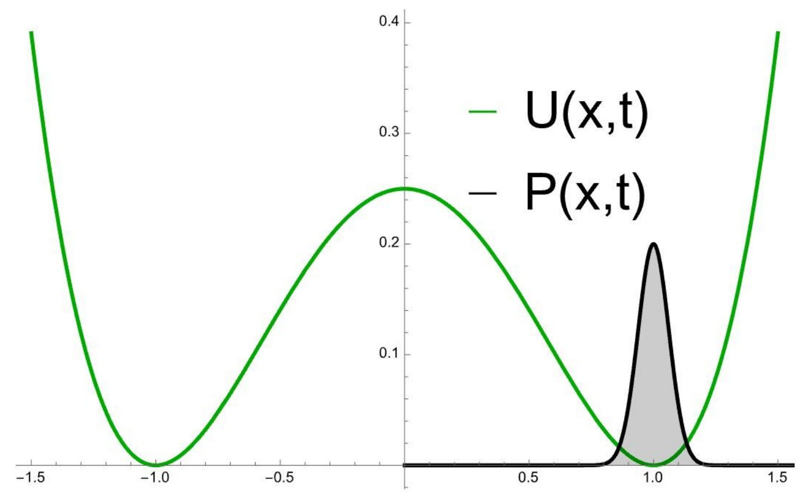
Bit erasure

$\underline{\text{at time } t = 0}$



p(x>0)=p(x<0)=1/2

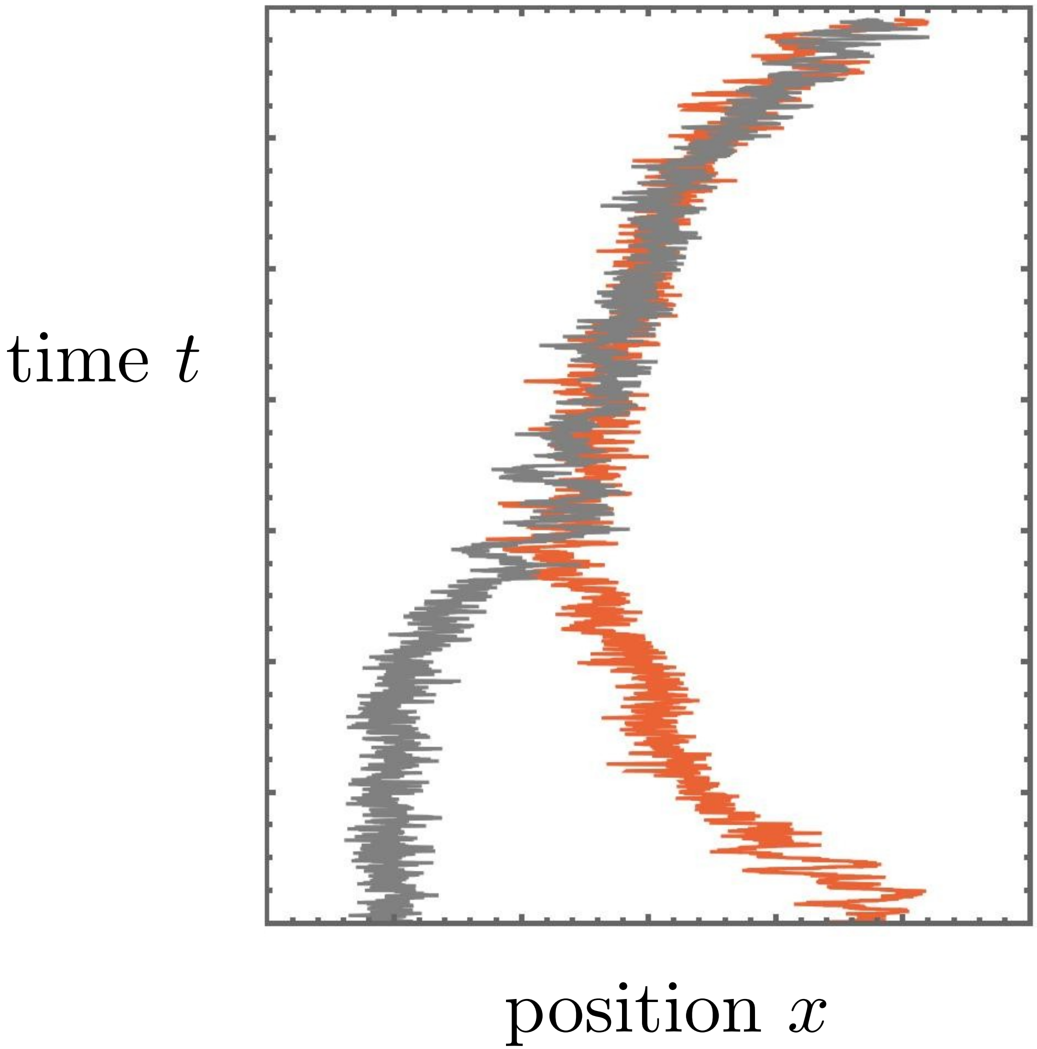
$\underline{\text{at final time } t = t_f}$



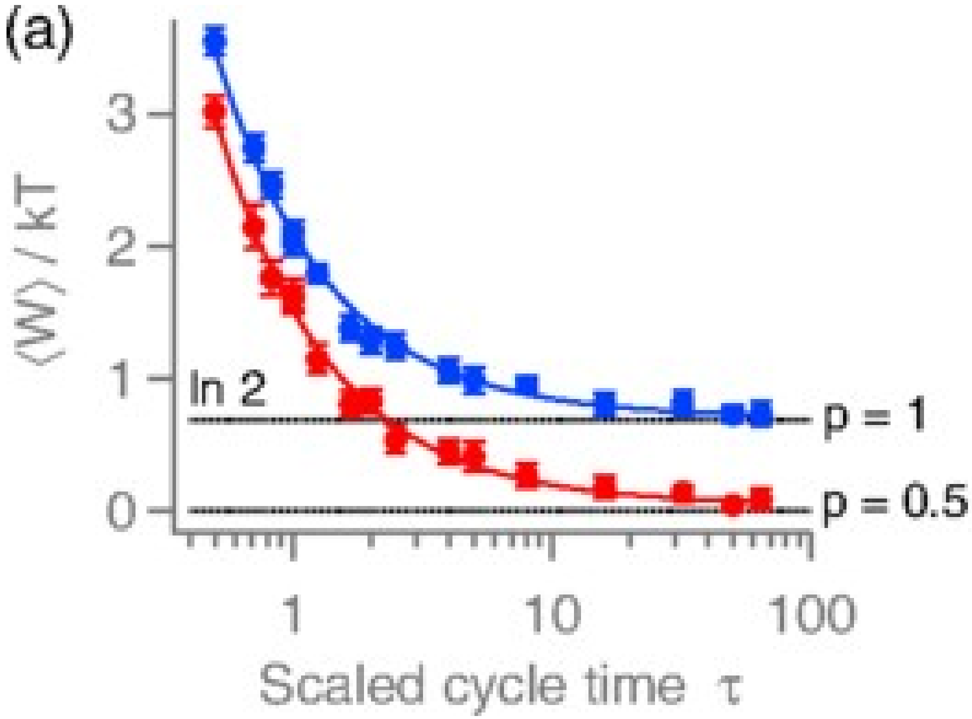
p(x>0)=1, p(x<0)=0

$$U(x,t) = 4E_b \left[-\frac{g(t)}{2} x^2 + \frac{x^4}{4} - A f(t)\, x \right]$$

Bit erasure



Work done



$$W = \int_0^{t_f} \frac{\partial U(x,t)}{\partial t}\, dt$$

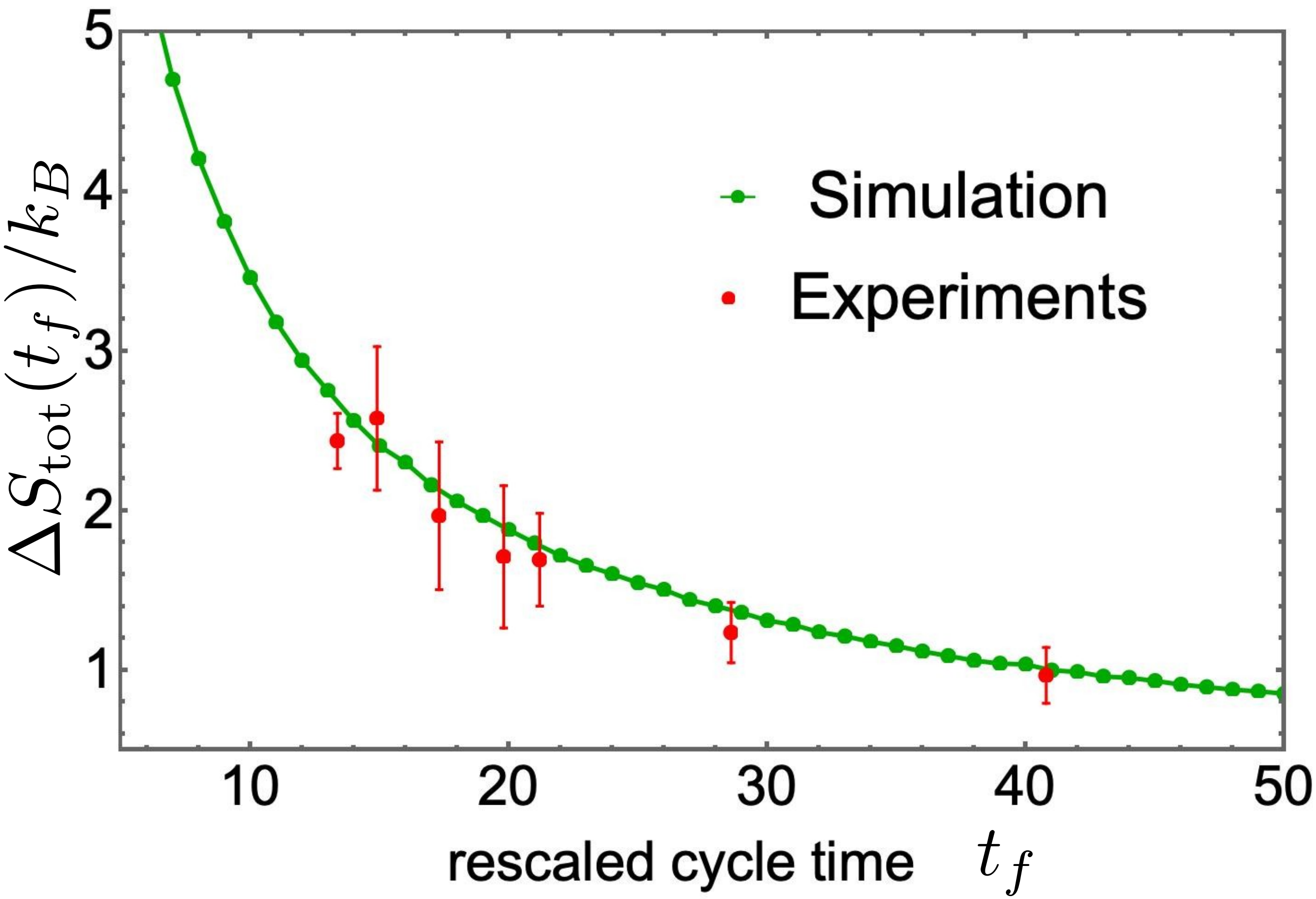
$$\langle W \rangle \geq k_B T \ln 2$$

Y Jun, M Gavrilov, and J Bechhoefer, PRL, 113, 190601 (2014)

A Berut, S Ciliberto et al, Nature, 483 (2012)

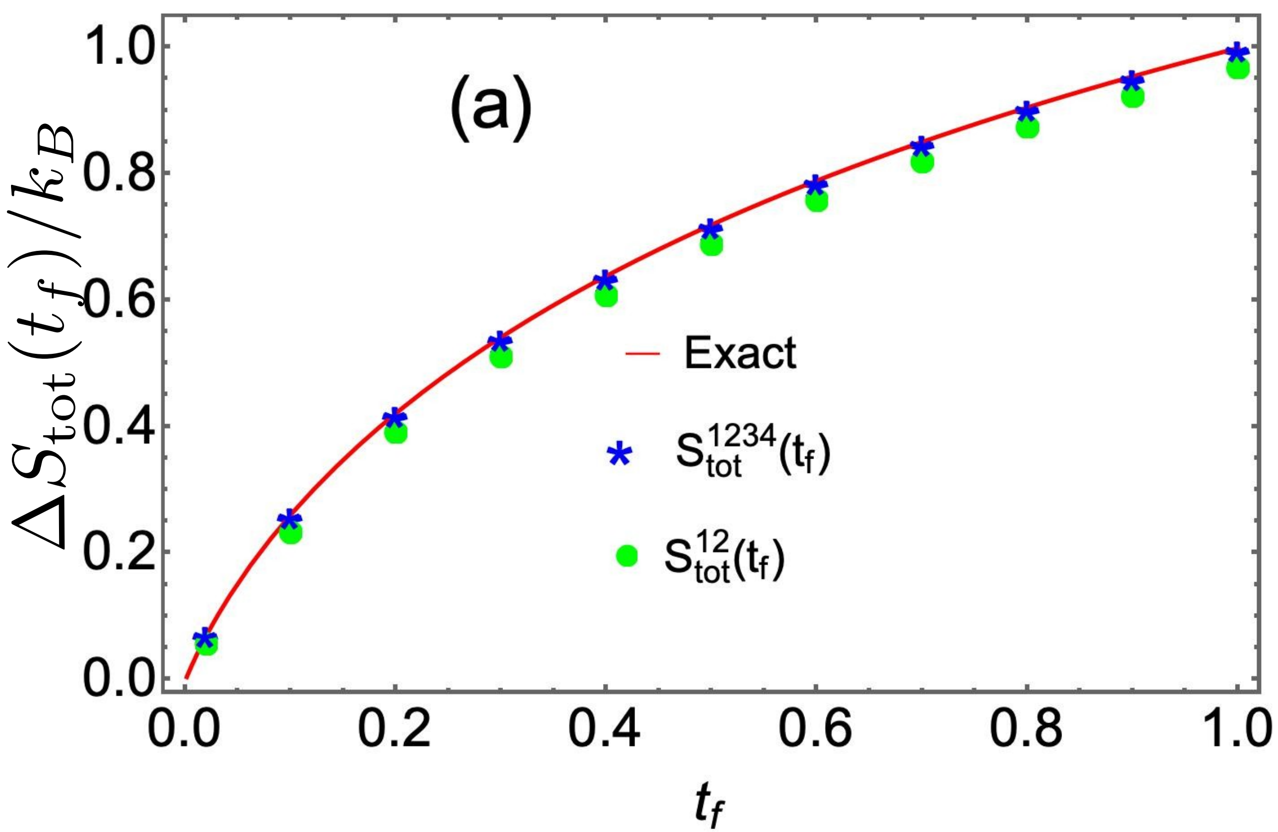
$$\Delta S_{\rm tot}(t_f) \geq \frac{k_B}{D}\int_0^{t_f} dt \left[\frac{\dot\Sigma^2(t)}{4\Sigma(t)} + \dot X_1(t)^2\right],$$

(Inference with < 100 trajectories)



Other examples

$$\frac{dx}{dt} = \sqrt{2D}\ \eta(t), \quad \text{with } P(x_0) \sim e^{-x_0^4}$$



Summary

- We derived a general lower bound on the mean total entropy production for time-dependent systems in terms of the moments.

- We applied this bound to infer total entropy production for bit erasure experiment and found an excellent match with simulation

- Can be extended to general moments and also to higher dimensions

Refs:

PS and K Proesmans arXiv:2310.16627

Acknowledgement:

J. Bechhoefer and P. Basak, Simon Fraser University, Canada

Thank you

Other examples

$$\frac{dx}{dt} = \sqrt{2D}\ \eta(t), \quad \text{with } P(x_0) \sim e^{-x_0^4}$$