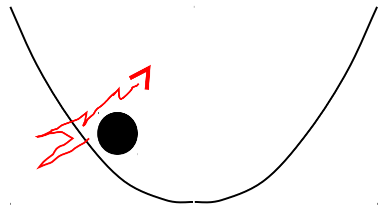
Jarzynski equality for a system governed by Tsallis statistics



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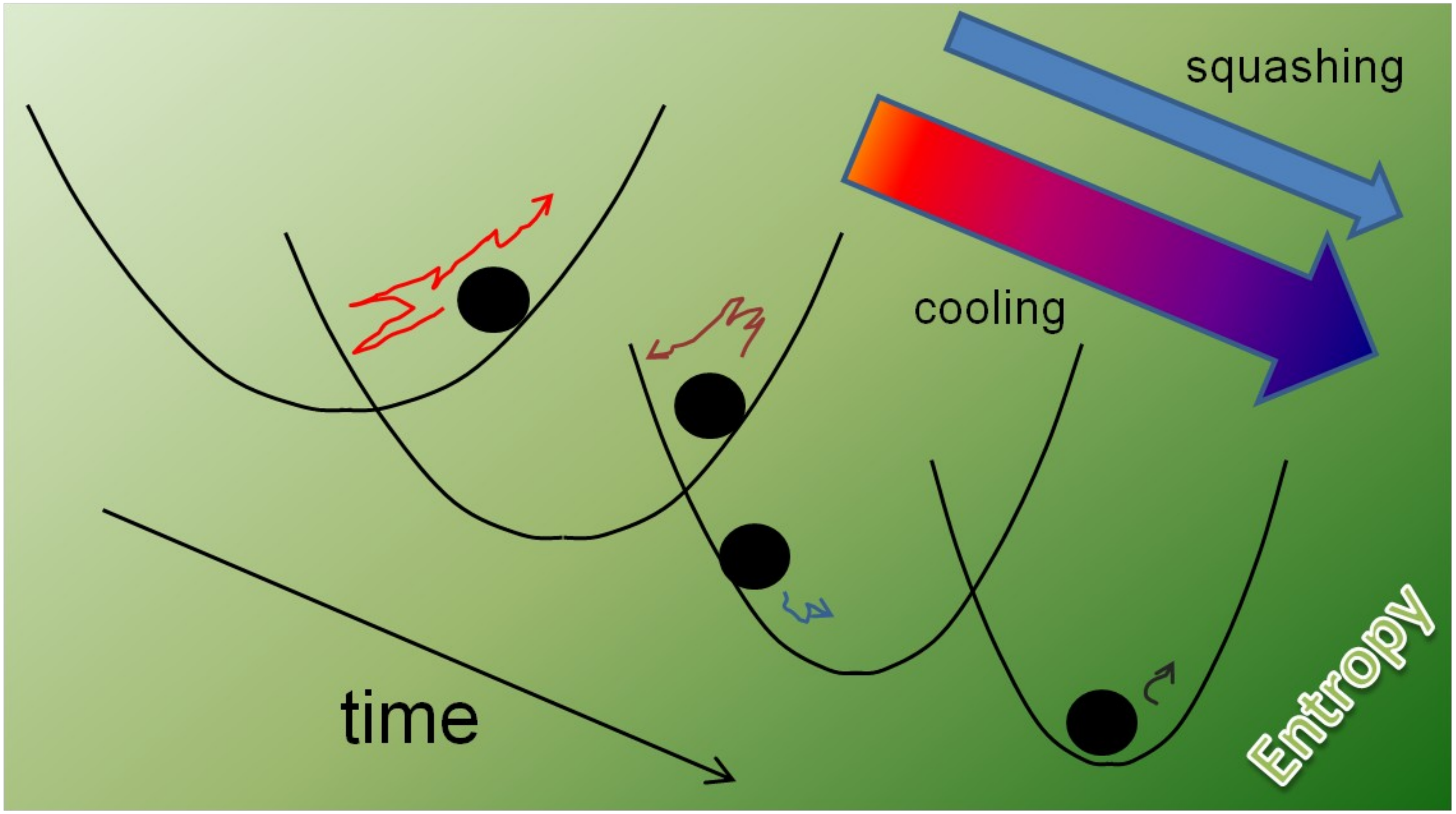
Summary

- Jarzynski equality etc
- Tsallis entropy and statistics
- Dynamical maximisation of uncertainty in stochastic thermodynamics
- Nonisothermal tethered Brownian motion
  - and a Jarzynski equality and Crooks relation for disturbances to the stationary state!

Driven thermodynamic processes



Jarzynski equality

$$\left\langle \exp\left(-\Delta W / kT\right)\right\rangle = \exp\left(-\Delta F / kT\right)$$

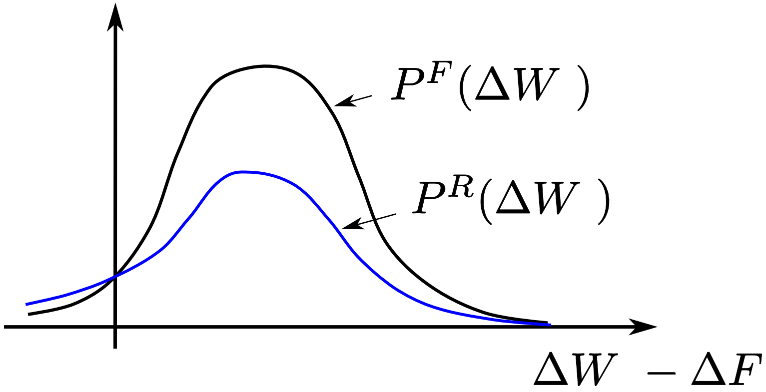
$$\Delta W = \int_0^\tau \frac{\partial \phi(x(t), \lambda(t))}{\partial \lambda} \frac{d\lambda}{dt} dt \qquad \Delta F = F(\lambda(\tau)) - F(\lambda(0))$$

e.g. $$\phi(x, \kappa(t)) = \frac{1}{2}\kappa(t) x^2$$

Start in canonical equilibrium; average over paths.

Crooks relation

$$\frac{P^F(\Delta W)}{P^R(-\Delta W)} = \exp\left(\frac{\Delta W - \Delta F}{kT}\right)$$



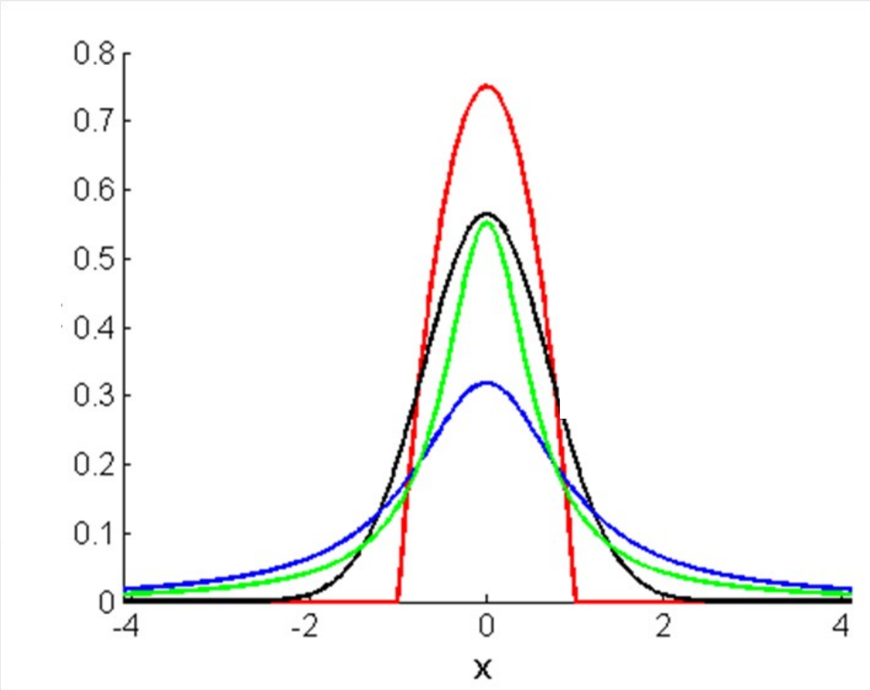
- Start in equilibrium
- Compress system and do work
- Expand and receive work back

Tsallis statistics

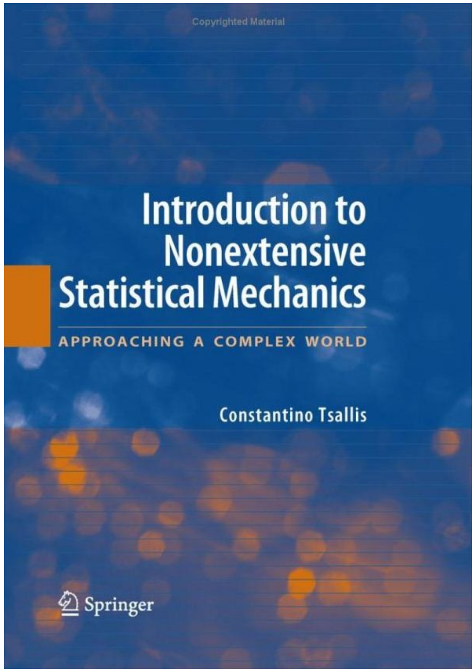
- Distributions that differ from those of canonical Gibbs-Boltzmann equilibrium
- The *q*-exponential:

$$p(x) \propto \exp_q(-U(x)/kT)$$

$$\propto \left(1-(1-q)U(x)/kT\right)^{\frac{1}{1-q}}$$



Origin of Tsallis statistics

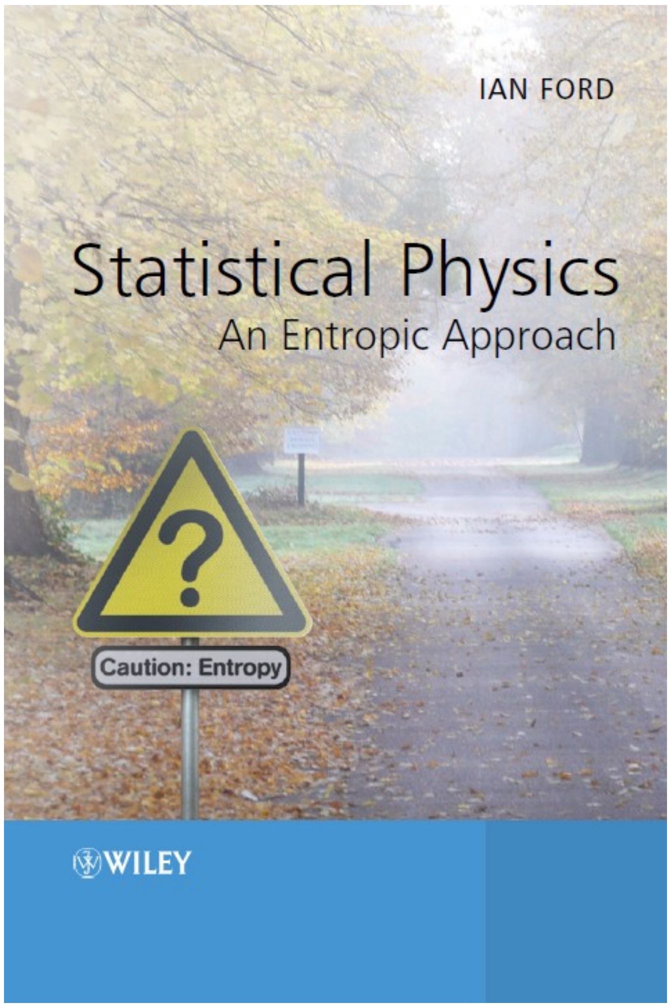


- Constrained maximisation of the Tsallis entropy:

$$S_{\text{Tsallis}} = \frac{1 - \sum p^q(x)}{q-1}$$

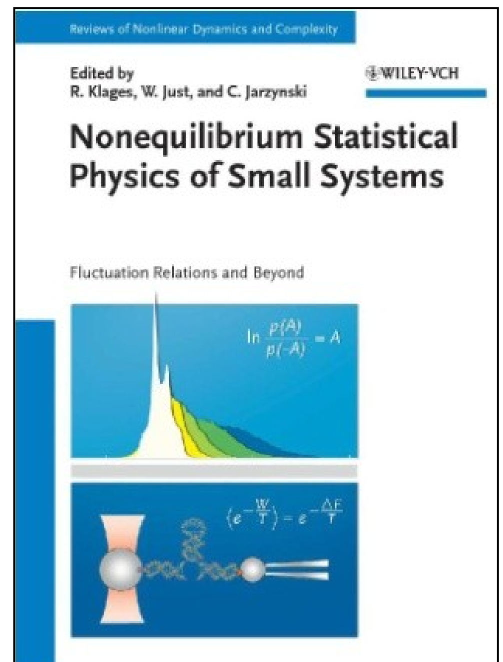
- But why?
- And why are constraints ‘generalised’ or ‘escort’ averages?

A dynamical viewpoint on entropy maximisation in canonical equilibrium



Fluctuation relations: a pedagogical overview

with Richard Spinney, in



A dynamical viewpoint on entropy maximisation in canonical equilibrium

$$\frac{dS_{\mathrm{tot}}}{dt} = \frac{dS_{\mathrm{sys}}}{dt} + \frac{dS_{\mathrm{med}}}{dt}$$

$$S_{\mathrm{sys}} = -k\int p \ln p \, dx$$

$$dS_{\mathrm{med}} = \frac{d\langle Q_{\mathrm{med}}\rangle}{T} = -\frac{d\langle Q_{\mathrm{sys}}\rangle}{T}$$

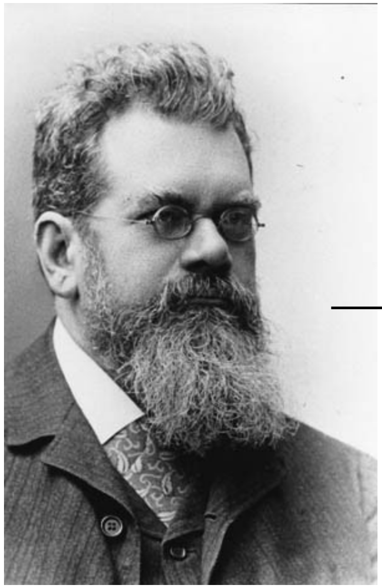
$$dE_{\mathrm{sys}} = dQ_{\mathrm{sys}}$$

$$\frac{dS_{\mathrm{tot}}}{dt} = \frac{d}{dt}\left(S_{\mathrm{sys}} - \frac{1}{T}\langle E_{\mathrm{sys}}\rangle \right)$$

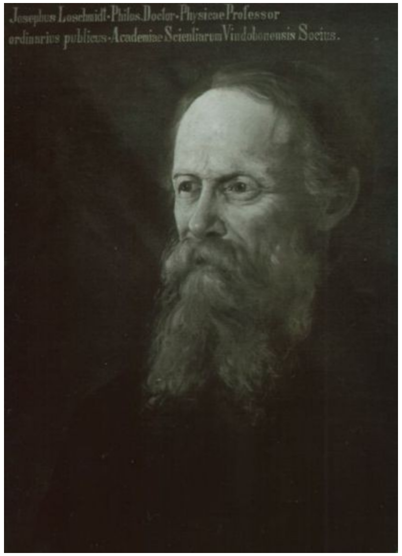
$$\Updownarrow$$

$$\delta\left(S_{\mathrm{sys}} - \beta\sum E_{\mathrm{sys}}(x_i)\,p(x_i) - \alpha\sum p(x_i) \right) = 0$$

Dynamics of entropy



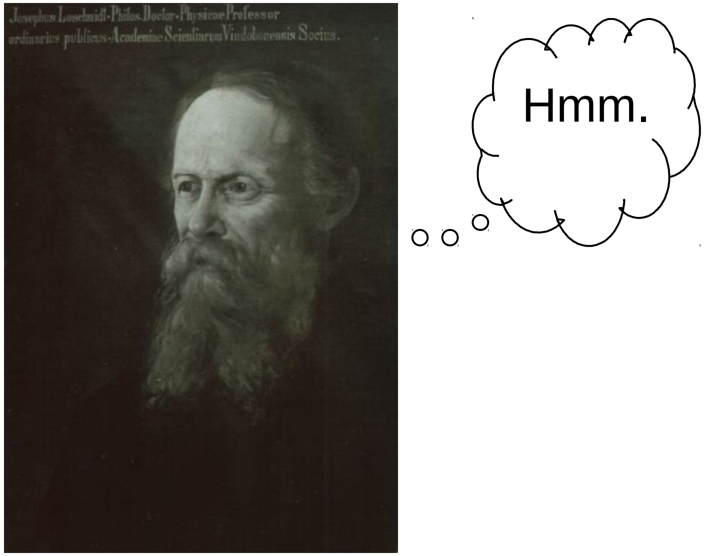
Loschmidt,
I’ve derived the
H-theorem!



Not
happy

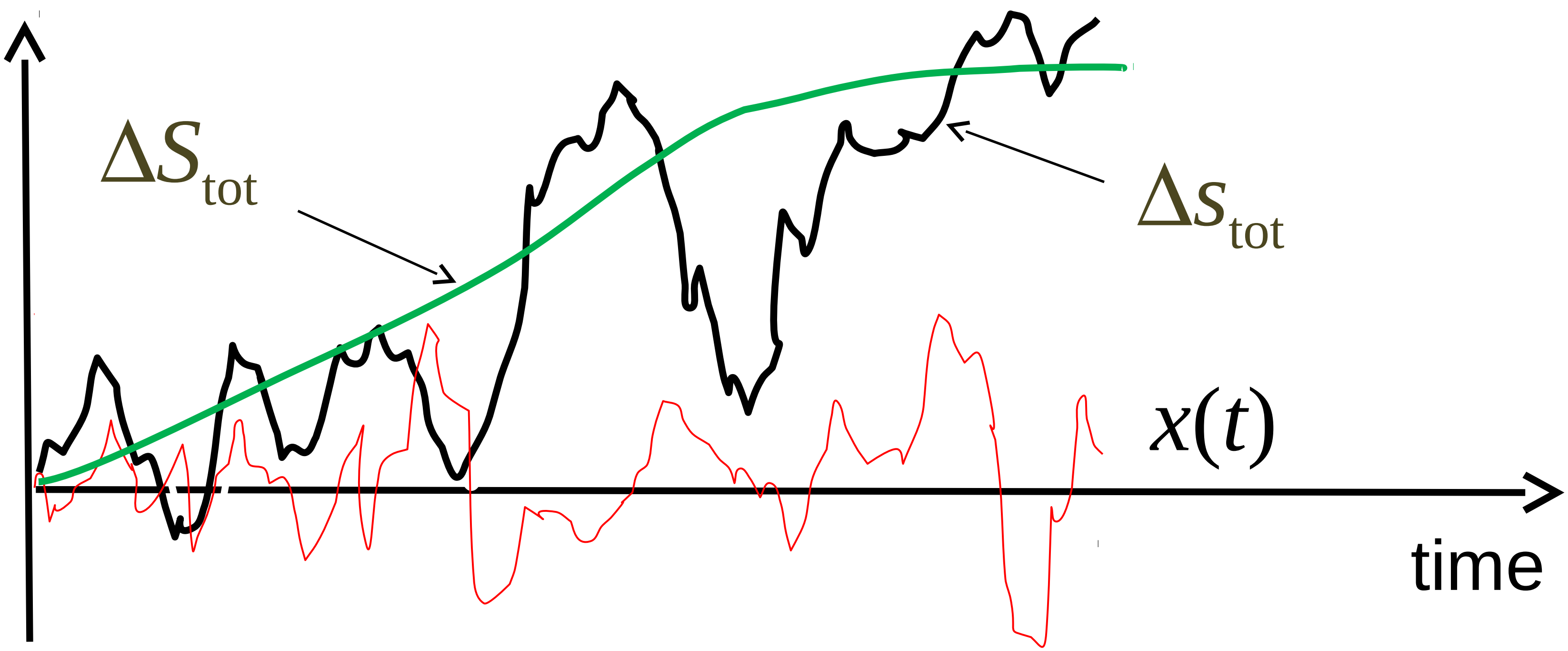
Stochastic thermodynamics

- Breaks time reversal invariance in the <u>model</u> dynamics
  - because the model is incomplete
- Entropy change:
  - evidence from a thermodynamic process of the failure to respect time reversal invariance

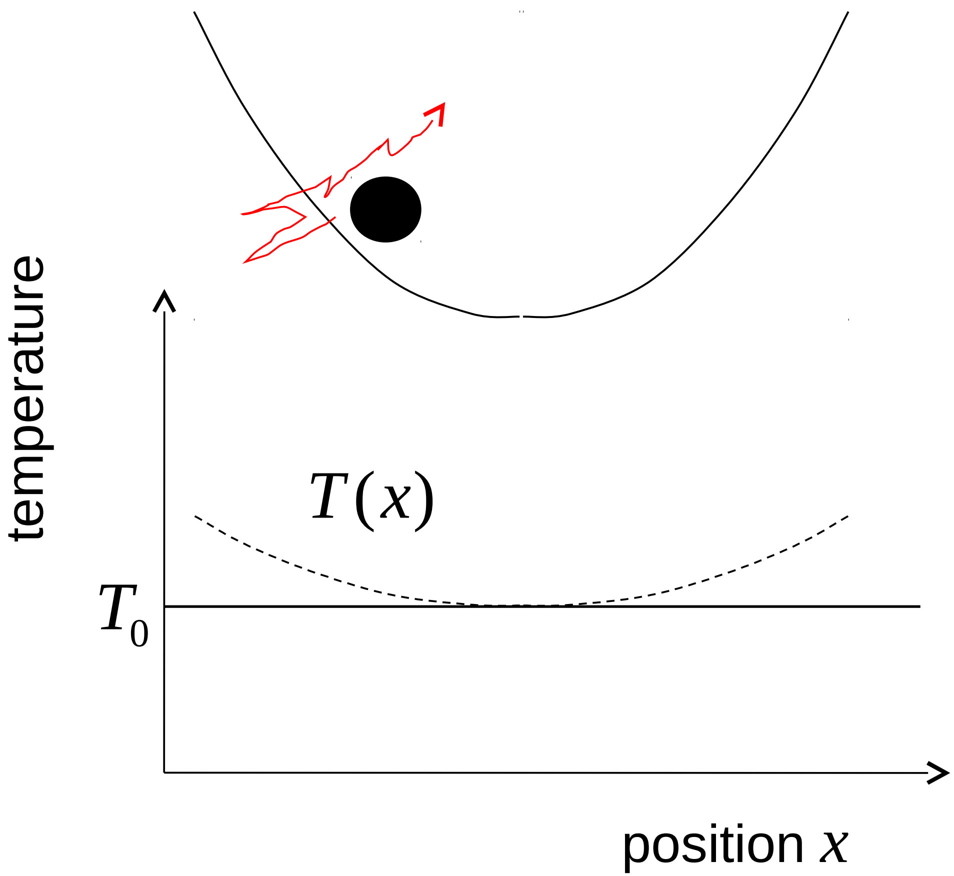


Stochastic thermodynamics (Sekimoto,Seifert)

- Stochastic dynamics (e.g. Brownian motion)
- Path-dependent total entropy production Δs_{tot}



Trapped Brownian particle in a nonisothermal medium



trap potential:

force $F(x) = -\kappa(t)x$

$$T(x) = T_0\left(1 + \frac{\kappa_T x^2}{2kT_0}\right)$$

Full Brownian dynamics:

- Stochastic differential equations for position, velocity and entropy production:

$$dx = v\,dt$$

$$dv = -\gamma v\,dt + \frac{F(x)}{m}dt + \sqrt{\frac{2kT(x)\gamma}{m}}\,dW_t$$

$$ds_{\text{tot}} = \cdots$$

Overdamped Brownian dynamics:

$$\frac{dx}{dt} = \frac{\kappa}{m\gamma} x + \sqrt{\frac{2kT(x)}{m\gamma}} \xi(t)$$

$$\frac{dS_{\text{tot}}}{dt} = \frac{d\langle s_{\text{tot}} \rangle}{dt} = 0$$

q-gaussian

$$p(x) \propto \left(1 + \frac{\kappa_T x^2}{2kT_0}\right)^{-\frac{\kappa_T + \kappa}{\kappa_T}}$$

- aspect of equilibrium, though not canonical
  - instead Tsallis

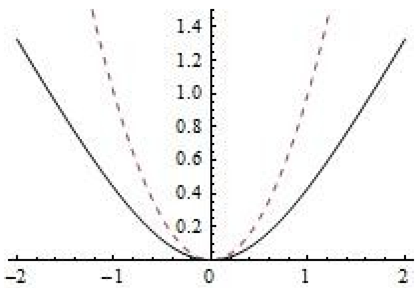
Transform the nonisothermal problem to an isothermal equivalent

$$\frac{dx}{dt} = \frac{\kappa}{m\gamma} x + \left(\frac{2kT(x)}{m\gamma} \right)^{\frac{1}{2}} \xi(t)$$

$$\frac{dy}{dt} = -\frac{1}{m\gamma} \frac{\partial \Phi(y)}{\partial y} + \left(\frac{2kT_0}{m\gamma} \right)^{\frac{1}{2}} \xi(t)$$

$$\frac{dS_{\text{tot}}}{dt} = \frac{d}{dt}\left(S_{\text{sys}} - \frac{1}{T} \langle \Phi \rangle \right)$$

Effective potential



$$\Phi(y) = \left(\kappa + \frac{\kappa_T}{2} \right) \frac{2kT_0}{\kappa_T} \ln\left[\cosh\left[\left(\frac{\kappa_T}{2kT_0} \right)^{\frac{1}{2}} y \right] \right]$$

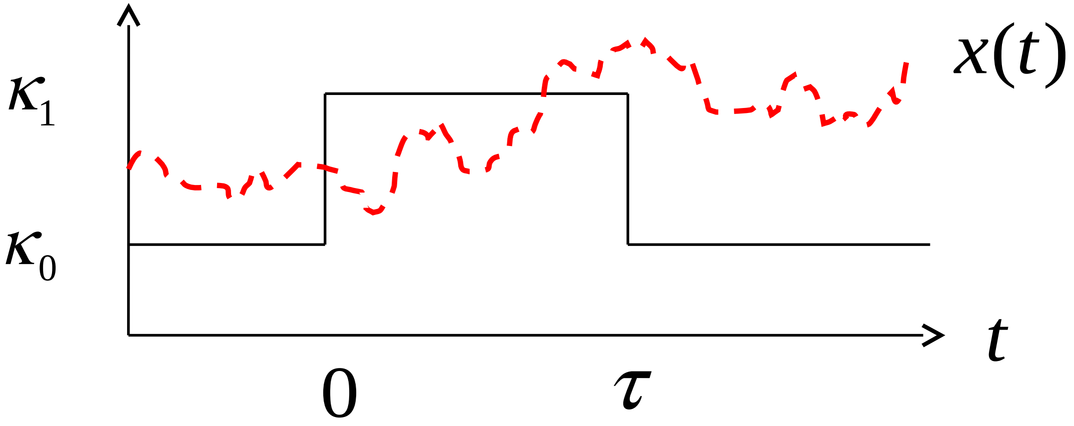
Origin of the Tsallis distribution in this problem

- constrained maximisation of the Shannon entropy
  - for distribution $p(y)$ of variable y
  - modified system potential $\Phi(y)$
- for general overdamped isothermal situations non-Tsallis stationary distributions emerge
- Lift overdamped condition:
  - Prigogine's principle in the stationary state?

Perform work on overdamped nonisothermal oscillator

- step up and step down in spring constant

$$\Delta W = \Delta W_{0\to 1} + \Delta W_{1\to 0} = \frac{1}{2}\left(\kappa_1 - \kappa_0\right)x^2(0) + \frac{1}{2}\left(\kappa_0 - \kappa_1\right)x^2(\tau)$$



Finally: a Tsallis-Jarzynski equality!

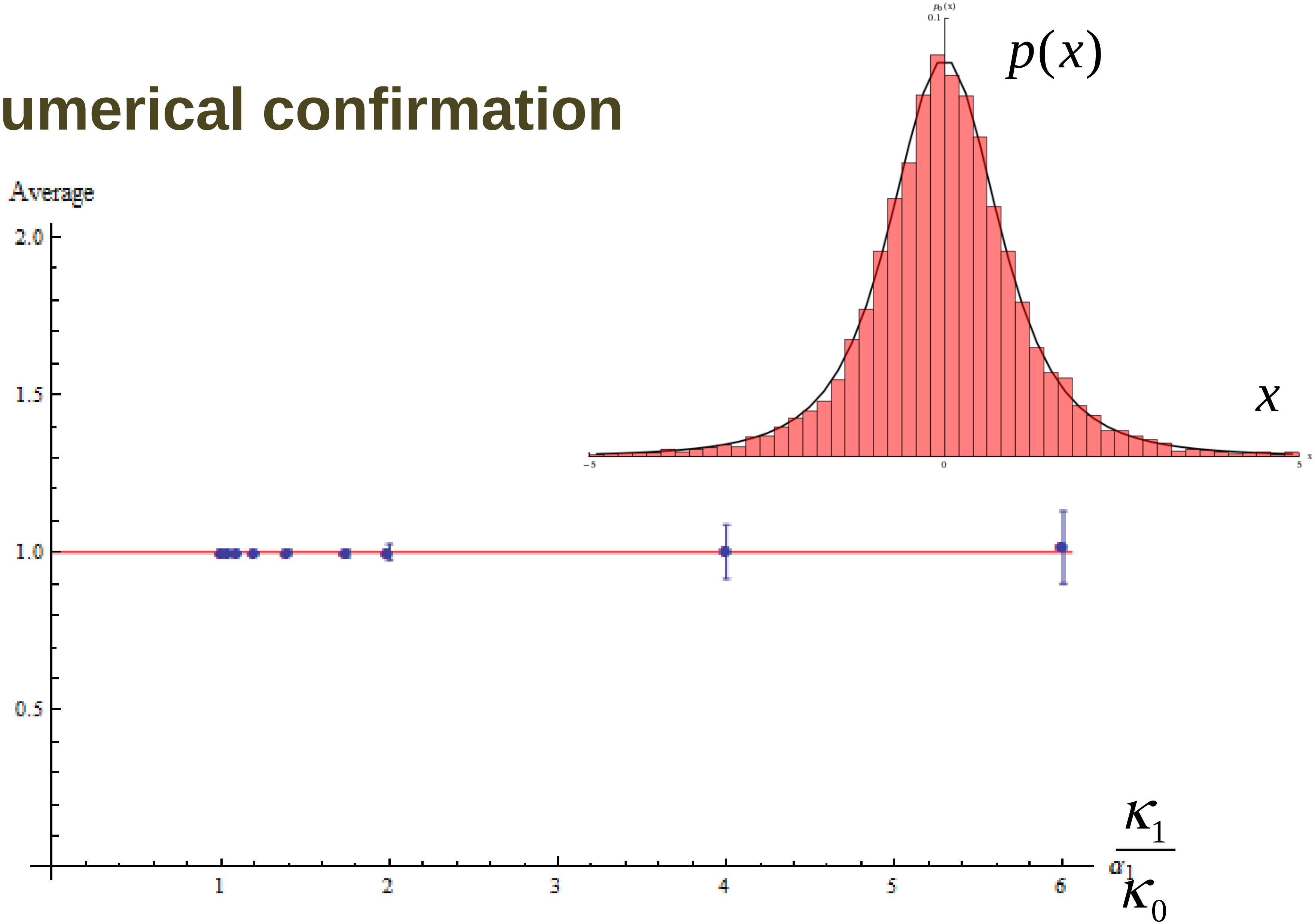
$$\left\langle \exp_{q_+}\left(-\Delta W_{0\to 1}/kT_0\right)\ \exp_{q_-}\left(-\Delta W_{1\to 0}/kT_0\right)\right\rangle = 1$$

with $$q_\pm = 1 \pm \frac{\kappa_T}{\kappa_1 - \kappa_0}$$

Compare with

$$\left\langle \exp\left(-\Delta W/kT\right)\right\rangle = \exp\left(-\Delta F/kT\right) = 1$$

Numerical confirmation



Even a Tsallis-Crooks relation!

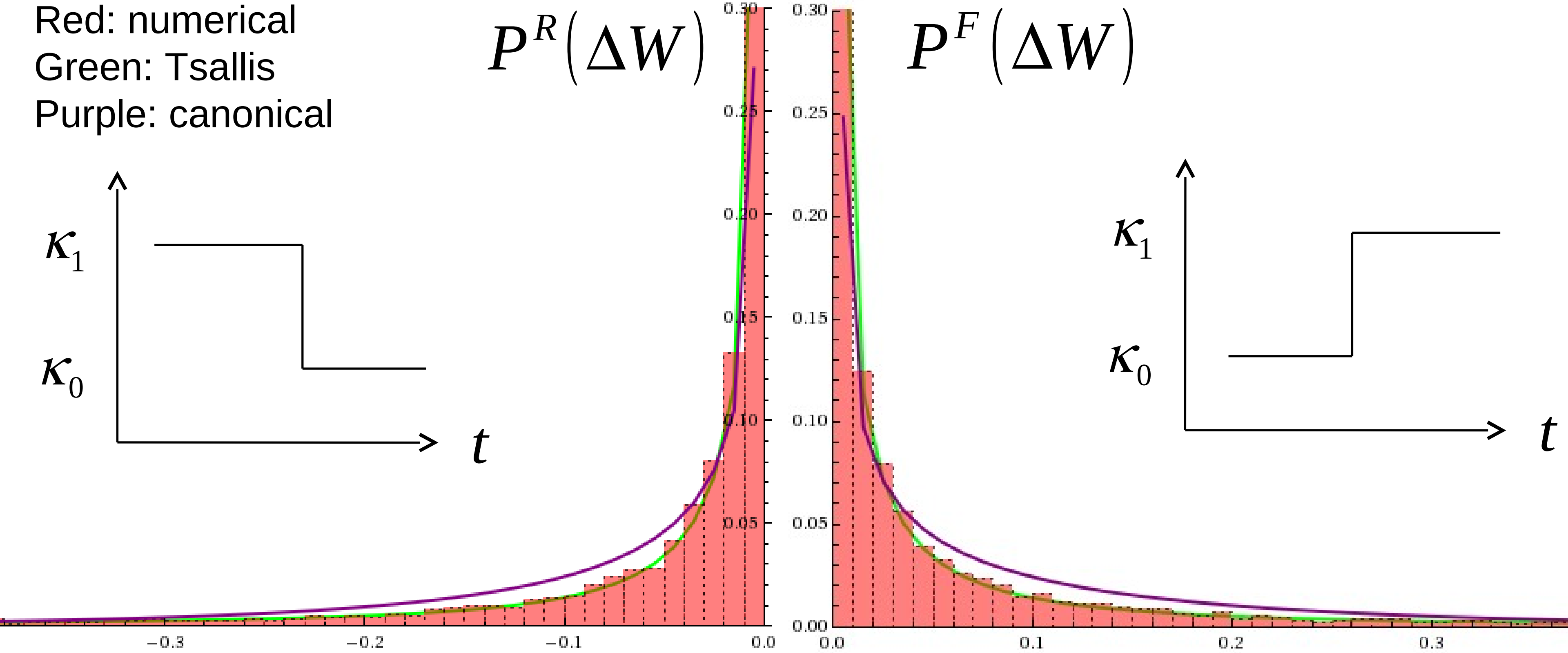
- Work distributions for step-up and step-down processes

$$\frac{P^F(\Delta W)}{P^R(-\Delta W)} = \frac{\Gamma\left(\frac{\kappa_0+\kappa_T}{\kappa_T}\right)}{\Gamma\left(\frac{\kappa_1+\kappa_T}{\kappa_T}\right)} \frac{\Gamma\left(\frac{1}{2}+\frac{\kappa_1}{\kappa_T}\right)}{\Gamma\left(\frac{1}{2}+\frac{\kappa_0}{\kappa_T}\right)} \exp_{q_-}\left(\frac{\Delta W}{kT_0}\right)$$

Compare with $\frac{P^F(\Delta W)}{P^R(-\Delta W)} = \exp\left(\frac{\Delta W - \Delta F}{kT}\right)$

Forward and backward work distributions

Red: numerical
Green: Tsallis
Purple: canonical

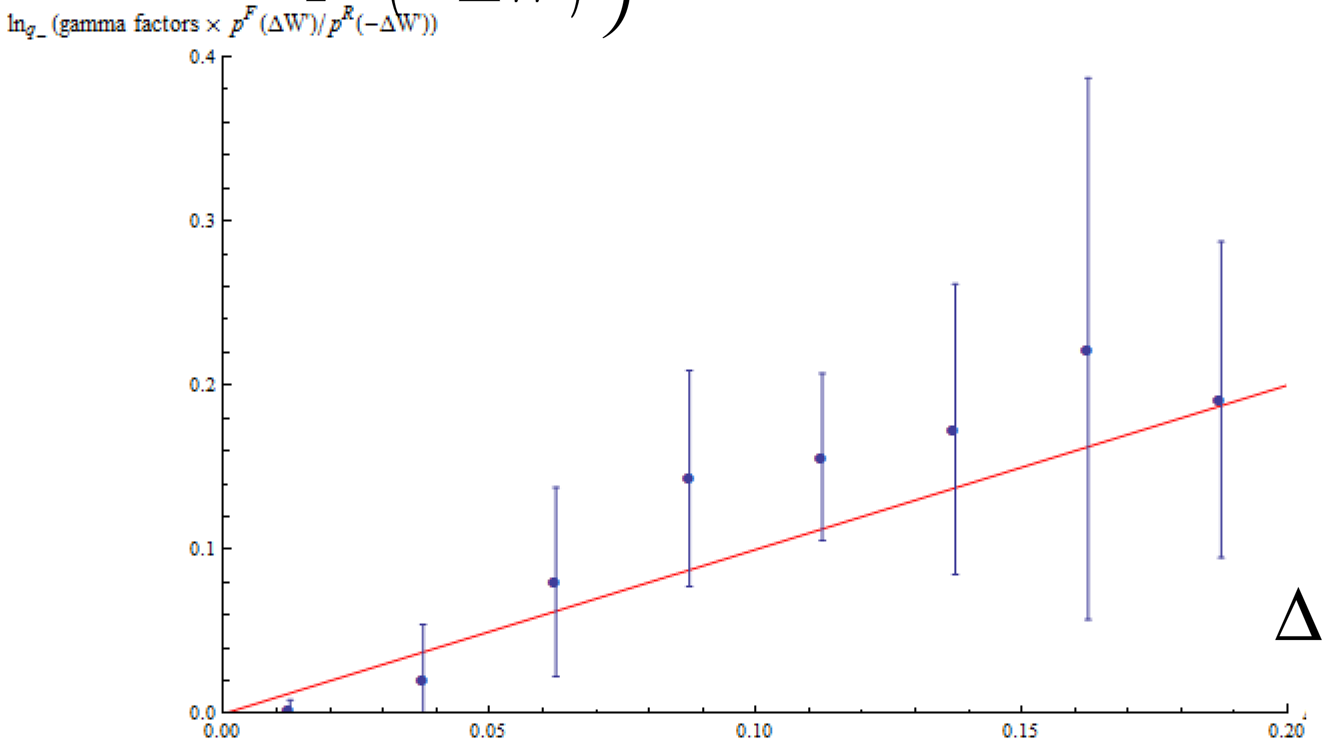


step down

step up

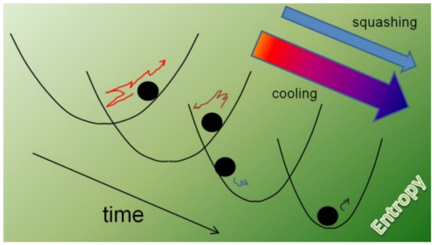
Numerical confirmation

$$\ln_{q_-}\left(\Gamma\text{–factors}\times\frac{P^F(\Delta W)}{P^R(-\Delta W)}\right)$$



$\Delta W / kT_0$

Summary



- Tsallis statistics can describe stationary states of overdamped nonisothermal systems

- Emerge from dynamical maximisation of a Shannon entropy for the equivalent isothermal problem
  - stochastic dynamics maximising the total uncertainty

- Fluctuation relations for special cases have been explored

- Thanks for listening!