Fluctuation relations and second-law-like inequalities for underdamped Langevin systems

M.L. Rosinberg

Laboratoire de Physique Théorique de la Matière Condensée
CNRS and Université. P. et M. Curie, Paris

in coll. with G. Tarjus (Paris) and T. Munakata (Kyoto)

Outline of the talk

A. Integral fluctuation theorem (IFT) for the dissipated heat. Application to the detection of extreme events

Two case studies:
1. Heat flow in harmonic chains
2. Resonator under time-delayed feedback control

For more details, see preprint arXiv:1510.08617

B. Some remarks on time-reversal in non-Markovian systems

For more details, see Phys. Rev. E **91**, 042114 (2015)

Integral fluctuation theorem

We consider an ensemble of N particles with mass m_i $(i = 1, \cdots, N)$ in d dimensions, each one being coupled to a heat reservoir in equilibrium at inverse temperature $\beta_i = 1/T_i$. The dynamics is described by the set of N coupled equations

$$m_i \dot{\mathbf{v}}_i = \mathbf{F}_i([\mathbf{r}], t) - \gamma_i \mathbf{v}_i + \boldsymbol{\xi}_i \ , \tag{1}$$

where $\mathbf{v}_i = \dot{\mathbf{r}}_i$, $\mathbf{r} = (\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)$, $\mathbf{F}_i([\mathbf{r}], t)$ is the total force acting on particle i, γ_i its friction coefficient, and the $\boldsymbol{\xi}_i$'s are Gaussian white noises with zero mean and variances $\langle \xi_{i\mu}(t) \xi_{j\nu}(t') \rangle = 2D_i \delta_{\mu\nu} \delta_{ij} \delta(t - t')$ with $D_i = \gamma_i T_i$ and $\mu, \nu = 1, \cdots, d$.

Let $\mathbf{X}$ denote a trajectory of the system in phase space that starts at the point $\mathbf{x}^0 = (\mathbf{r}, \mathbf{v})_{t=0}$ and is observed during the time interval $[0, t]$. The conditional probability of $\mathbf{X}$ is given by

$$\mathcal{P}[\mathbf{X}|\mathbf{x}^0] \propto \prod_j e^{\frac{d\gamma_j}{2m_j} t} e^{-\beta_j \mathcal{S}_j[\mathbf{X}]}$$

where

$$\beta_j \mathcal{S}_j[\mathbf{X}] = \frac{1}{2D_j} \int_0^t dt' \left[m_j \dot{\mathbf{v}}_j + \gamma_j \mathbf{v}_j - \mathbf{F}_j([\mathbf{r}], t') \right]^2$$

is an Onsager-Machlup action functional and the exponential factors $e^{\frac{d\gamma_j}{2m_j} t}$ come from the Jacobian of the transformations $\boldsymbol{\xi}_j(t) \to \mathbf{r}_j(t)$

The heat dissipated into the bath i during the time interval $[0, t]$ is defined by the functional

$$\mathcal{Q}_i[\mathbf{X}] = \int_0^t dt' \Big[\gamma_i \mathbf{v}_i - \boldsymbol{\xi}_i\big]\mathbf{v}_i = \int_0^t dt' \Big[-m_i \dot{\mathbf{v}}_i + \mathbf{F}_i\big]\mathbf{v}_i$$

Key observation : $\mathcal{Q}_i[\mathbf{X}]$ can be expressed as a logratio of path probabilities *without* referring to time reversal.

Change γ_i for particle i into $-\gamma_i$ but keep the diffusion coefficient D_i fixed. Then

$$\hat{\mathcal{P}}[\mathbf{X}|\mathbf{x}^0] \propto e^{-\frac{d\gamma_i}{2m_i}t} e^{-\beta_i \hat{\mathcal{S}}_i[\mathbf{X}]} \prod_{j \neq i} e^{\frac{d\gamma_j}{2m_j}t} e^{-\beta_j \mathcal{S}_j[\mathbf{X}]}$$

where $\beta_i \hat{\mathcal{S}}_i[\mathbf{X}] = \beta_i \mathcal{S}_i[\mathbf{X}]_{\gamma_i \to -\gamma_i}$ and $e^{-\frac{d\gamma_i}{2m_i}t}$ comes from the Jacobian associated with the equation for particle i.

Take the ratio of the two path probabilities $\Rightarrow$ $$\frac{\mathcal{P}[\mathbf{X}|\mathbf{x}^0]}{\hat{\mathcal{P}}[\mathbf{X}|\mathbf{x}^0]} = e^{\frac{d\gamma_i}{m_i}t} e^{\beta_i \mathcal{Q}_i}$$

Integrate over all paths: $\Rightarrow$ IFT:

$$\langle e^{-\beta_i \mathcal{Q}_i} \rangle_0 = \int \mathcal{D}\mathbf{X}\, e^{-\beta_i \mathcal{Q}_i[\mathbf{X}]} \mathcal{P}[\mathbf{X}|\mathbf{x}^0] = e^{\frac{d\gamma_i}{m_i}t}$$

Jensen's inequality $\Rightarrow$ $$\beta_i \langle \mathcal{Q}_i \rangle_0 \geq -d(\gamma_i/m_i)t$$

Generalization:

$$\langle e^{-(\beta_i \mathcal{Q}_i + \beta_j \mathcal{Q}_j)} \rangle_0 = e^{d(\frac{\gamma_i}{m_i} + \frac{\gamma_j}{m_j})t}$$, etc....

Overdamped dynamics (simple result **only** for linear forces)

$$\langle e^{-\beta \mathcal{Q}_i} \rangle_0 = e^{\mu_i \alpha_i t} \text{ where } \alpha_i = \sum_{\mu=1}^{d} \partial F_{i\mu}/\partial r_{i\mu}$$

(can be checked for all linear overdamped models in the literature)

Application to the detection of extreme events

We now show that the IFT has interesting consequences for the pdf's of the stochastic heat and related quantities. We assume that the system has reached a NESS and focus on the long-time limit.

Let $P_A(A) = \langle \delta(\mathcal{A}[\mathbf{X}] - A) \rangle$ denote the pdf of the time-integrated quantity $\mathcal{A}$, *e.g.*, the heat $\mathcal{Q}$, where the average is over all possible trajectories with an initial state drawn from the stationary distribution p_{st}.

As $t \to \infty$, $P_A(A = at) \sim e^{-I_A(a)t + o(t)}$

and $Z_A(\lambda, t) \equiv \langle e^{-\lambda \mathcal{A}[\mathbf{X}]} \rangle_{st} \sim e^{\mu_A(\lambda) t}$

$I_A(a)$ is the LDF and $\mu_A(\lambda)$ is the SCGF, given by the largest eigenvalue of the appropriate Fokker-Planck operator.

In practice, one often writes

$$Z_A(\lambda, t) \sim e^{\mu_A(\lambda)t} \sim g_A(\lambda)e^{\mu(\lambda)t}$$

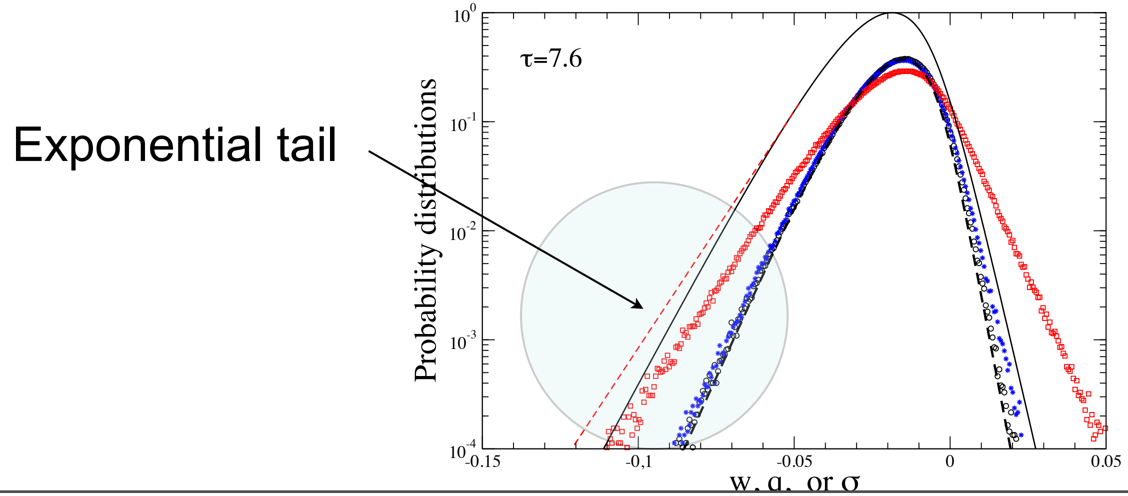
where $\mu(\lambda)$ is obtained by neglecting temporal boundary terms (e.g. by solving the equations of motion by Fourier transform), and $g_A(\lambda$ arises from an average over the initial and final states.

If $\mu(\lambda)$ satisfies the symmetry $\mu(\lambda) = \mu(a-\lambda)$, the LDF $I(a)$, defined from the Legendre transform of $\mu(\lambda)$, has the "Gallavotti-Cohen" symmetry $I(-a)-I(a) = c\,a$ (where c is some constant), and $P_A(A)$ then obeys the "standard" stationary-state FT

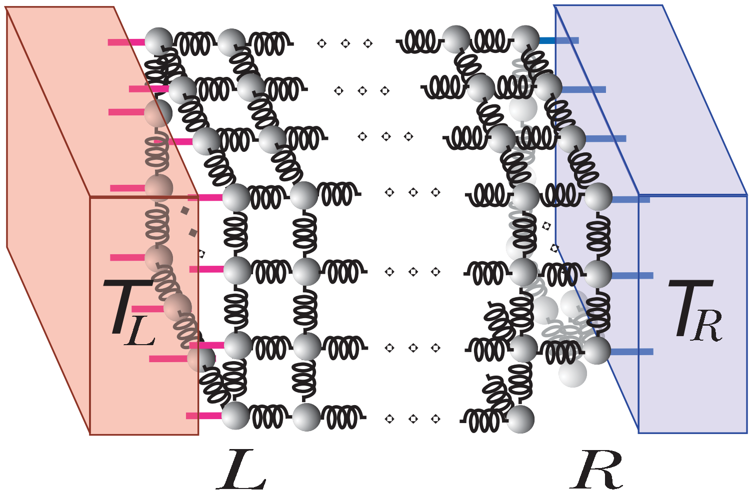
$$\frac{P_A(A = at)}{P_A(A = -at)} = e^{c\,at+o(t)}$$

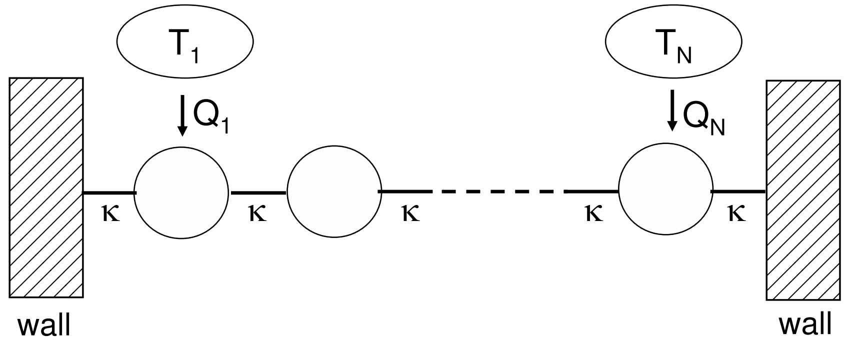
However, if the pre-exponential factor [specifically $g_Q(\lambda)$] has a singularity (e.g. a pole) in the region of the saddle-point integration, the leading contribution to the large deviation function comes from the pole (i.e. it is not the Legendre transform of $\mu(\lambda)$).

The "Gallavotti-Cohen symmetry" of the LDF (cf. van Zon-Cohen 2003) is then violated and the FT has not the "standard" form. This is due to rare (but non-negligible) events that give rise to exponential tails in the pdf of Q.

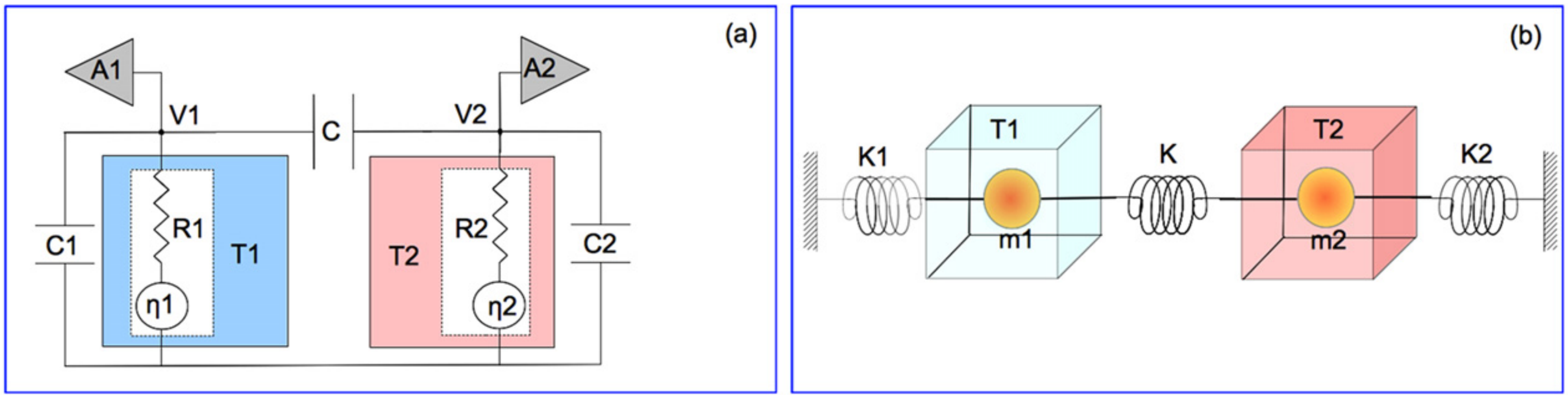


Heat conduction in harmonic chains





From K. Saito and A. Dhar, PRE **83**,041121 (2011) and Kundu et al., J. Stat. Mech. P03007 (2011)



From S. Ciliberto et al. J. Stat. Mech. P12014 (2013)

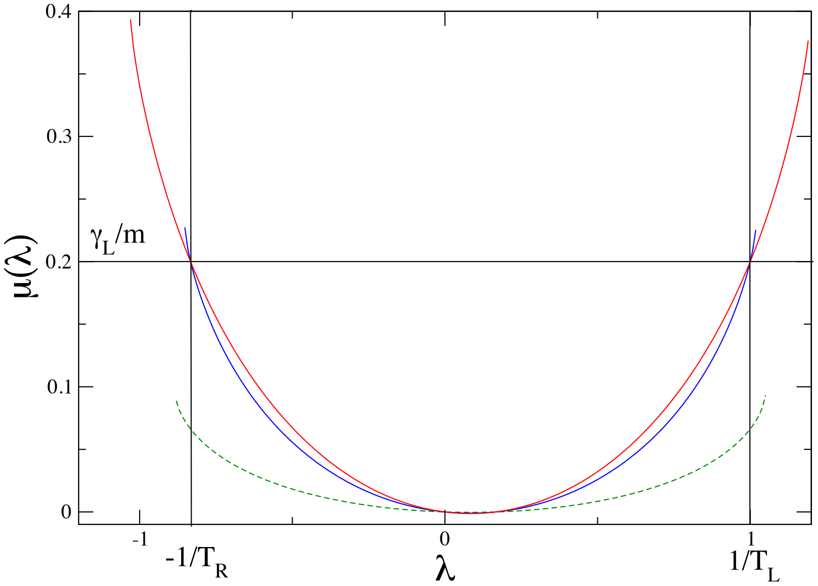
Equations of motion:

$$m\dot{v}_1 = k(u_2 - 2u_1) - \gamma_L v_1 + \xi_1$$
$$m\dot{v}_i = k(u_{i+1} + u_{i-1} - 2u_i)\,, \quad i = 2, \cdots, N-1$$
$$m\dot{v}_N = k(u_{N-1} - 2u_N) - \gamma_R v_N + \xi_N\ ,$$

Characteristic function:

$$\langle e^{-\lambda \mathcal{Q}_L}\rangle_{st} \sim e^{\mu_Q(\lambda)t} \sim g_Q(\lambda) e^{\mu(\lambda)t}$$

The IFT $\langle e^{-\beta_L \mathcal{Q}_L}\rangle_{st} = e^{\frac{\gamma_L}{m}t}$ implies that $\mu_Q(\beta_L) = \gamma_L/m$. Therefore, one could naively think that $\mu(\beta_L)$ is also equal to γ_L/m. However, this is not always true.



$\mu(\lambda)$ for $N = 3$ and different values of the spring constant k ($\gamma_L = 0.2, \gamma_R = 1, T_L = 1, T_R = 1.2$).

For $k < k_c = 0.6$, $\mu(\beta_L) < \gamma_L/m$!

One can understand these results but focusing on the behavior of the auxiliary "hat" dynamics ($\gamma_L \to -\gamma_L$):

ONE CAN SHOW THAT:

$$\mu(\beta_L) = \int \frac{d\omega}{2\pi} \ln \frac{|\det \hat{\boldsymbol{\chi}}(\omega)|}{|\det \boldsymbol{\chi}(\omega)|}$$

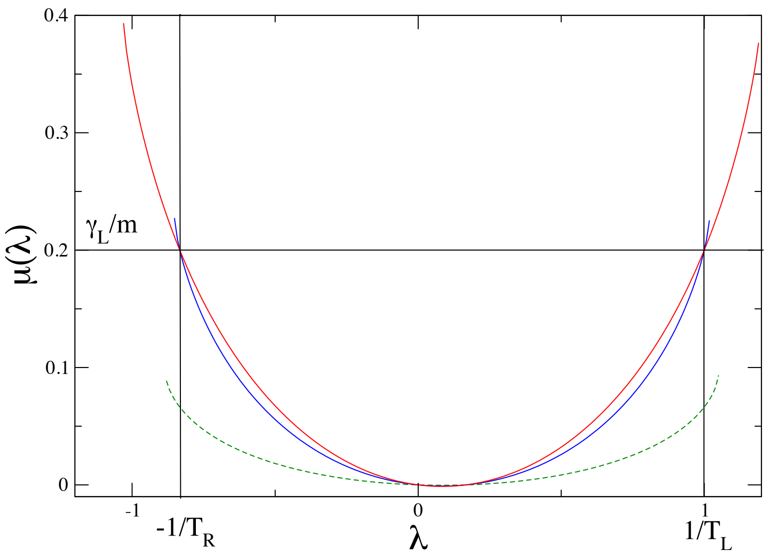
where $\boldsymbol{\chi}(\omega)$ is the matrix formed by the response functions of the N harmonic oscillators and $\hat{\boldsymbol{\chi}}(\omega)$ is formally defined by changing the sign of γ_L in $\boldsymbol{\chi}(\omega)$.

Two cases may happen:

1) $k > k_c$: the auxiliary hat dynamics "converges", *i.e.*, the system reaches a steady state independent of initial conditions. Then, the elements of the matrix $\hat{\boldsymbol{\chi}}(\omega)$ are the Fourier transform of *bona fide* causal response functions and $\det \hat{\boldsymbol{\chi}}(\omega)$ is analytic in the upper half of the complex ω-plane.

→ $\mu(\beta_L) = \mu_A(\beta_L) = \gamma_L/m$

2) $k < k_c$: the hat dynamics does not converge. The elements of $\hat{\boldsymbol{\chi}}(\omega)$ are *not* the Fourier transform of causal response functions and det $\hat{\boldsymbol{\chi}}(\omega)$ has also poles in the upper half complex plane. Then, $\mu(\beta_L) < \gamma_L/m$ as can be seen in the figure.



Pole in the prefactor $g_Q(\lambda)$ for $\lambda = 1/T_L$

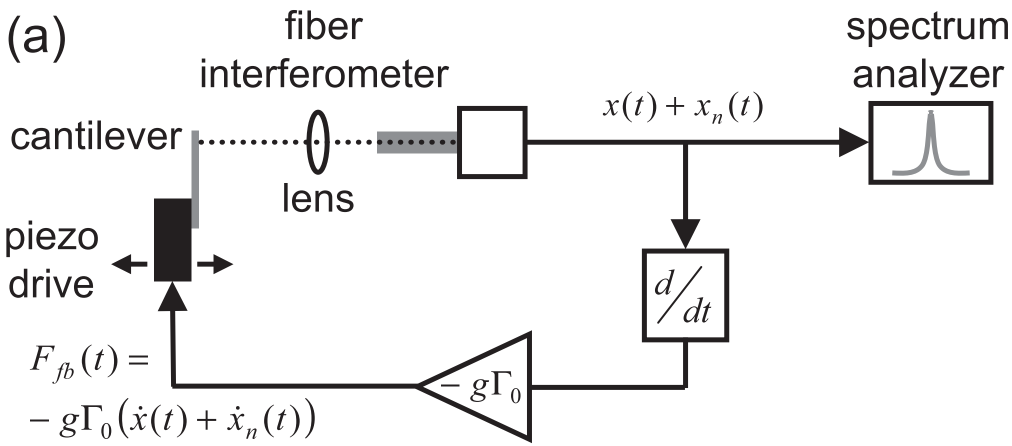
(more precisely, boundary layer as $t \to \infty$).

Therefore we have a simple criterion for predicting whether or not there is an exponential tail in the left-wing of the pdf of the heat (i.e. Q flowing *to* the system), which makes large fluctuations more likely.

Resonator under time-delayed feedback control

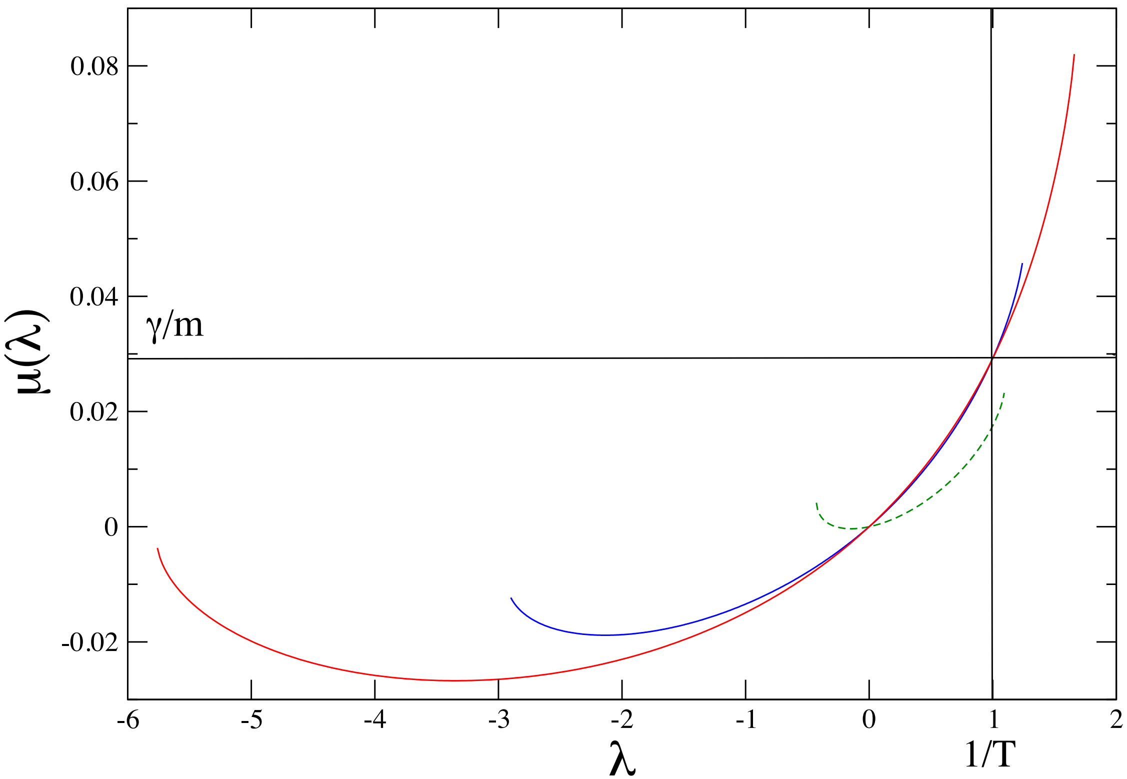
$$m\dot{v}_t = -kx_t + k'x_{t-\tau} - \gamma v_t + \sqrt{2\gamma T}\xi_t$$

This equation faithfully describes the dynamics of nano-mechanical resonators (e.g. the cantilever of an AFM) used in feedback cooling (cold damping) setups. For properly chosen values of the delay τ the feedback force $F_{fb} = k'x(t-\tau)$ reduces thermal fluctuations: $T_{eff} \ll T$.



Relevant control variables: gain k'/k or delay τ

One can repeat the same analysis and use the behavior of the system under the auxiliary dynamics (with $\gamma \to -\gamma$) to predict the possible existence of a singularity in the characteristic functions of the heat or of the work done by the feedback force at $\lambda = 1/T$



$\mu(\lambda)$ for different values of τ (the oscillator quality factor is $Q_0 = \sqrt{mk}/\gamma = 34.2$ and $k'/k = 0.25$).

Time-reversal and second-law-like inequality

Because of non-Markovian character of the continuous feedback control, the operation of time reversal becomes non trivial. In order to express the heat as log-ratio of path probabilities, one must change τ into $-\tau$. This auxiliary dynamics is acausal !

$$m\dot{v}_t = -\gamma v_t + F(x_t) + F_{fb}(x_{t+\tau}) + \sqrt{2\gamma T}\,\xi(t)$$

$$\frac{\mathcal{P}[\mathbf{X}|\mathbf{Y}]}{\tilde{\mathcal{P}}[\mathbf{X}^\dagger|\mathbf{x}_i^\dagger, \mathbf{Y}^\dagger]} = \frac{\mathcal{J}}{\tilde{\mathcal{J}}[\mathbf{X}]} e^{\beta Q[\mathbf{X},\mathbf{Y}]}$$

Generalized local detailed balance equation

Y trajectory in the time interval $[-\tau, 0]$,

$\tilde{\mathcal{J}}[\mathbf{X}] =$ non-trivial Jacobian due to the violation of causality

in general path dependent

In the stationary state, this leads to another second-law-like inequality (see Phys. Rev. E **91**, 042114 (2015)):

$$\frac{\dot{\mathcal{W}}_{ext}}{T} \leq \dot{\mathcal{S}}_{\mathcal{J}}$$

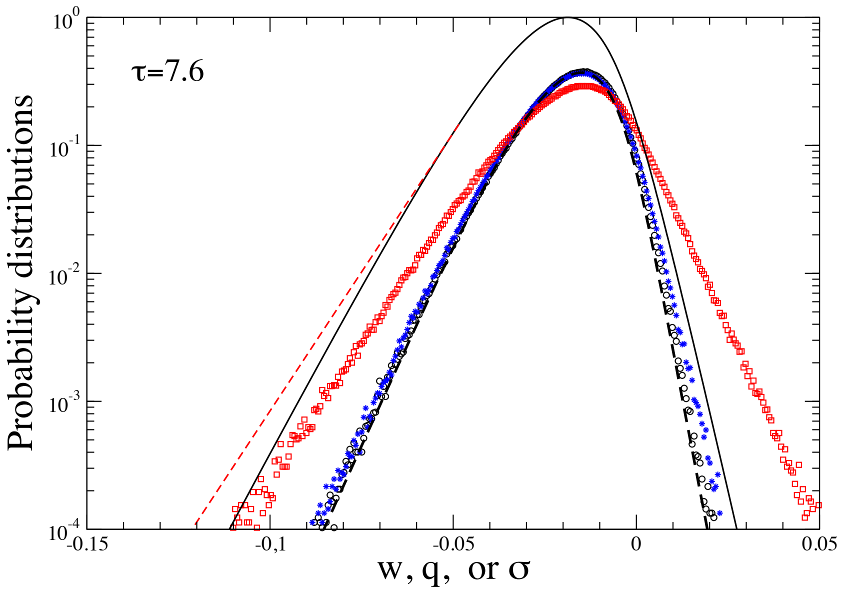
($\dot{W}_{ext}$: extracted work rate)

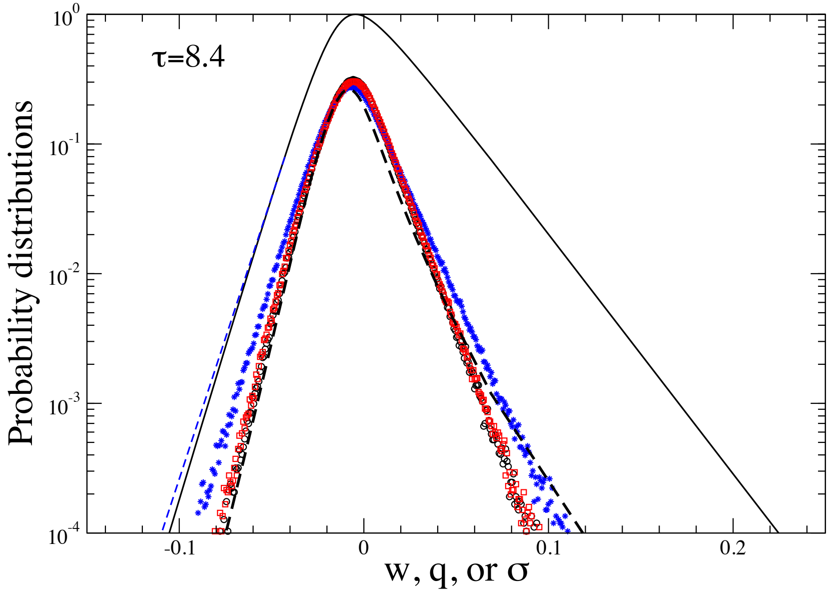
with $$\dot{\mathcal{S}}_{\mathcal{J}} := \lim_{t\to\infty} \frac{1}{t}\langle \ln \frac{\mathcal{J}}{\tilde{\mathcal{J}}[\mathbf{X}]}\rangle_{st}$$

FLUCTUATIONS:

With this non-Markovian dynamics, one can thus define *two* auxiliary dynamics: $\gamma \to -\gamma$ and $\tau \to -\tau$. They can be used to study the occurrence of extreme events in *different* regions of the parameter space. Although the dynamics $\tau \to -\tau$ is acausal, it can still lead to stationary state !

Probability distribution functions for the heat, the work and the (pseudo) entropy production for two different values of the delay:





Rosinberg M. L., Tarjus G., and Munakata T., in preparation.

Thank you for your attention !