Stochastic Thermodynamics of Langevin systems under time-delayed feedback control

M.L. Rosinberg

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

LPTMC, CNRS and Université. P. et M. Curie, Paris

Both practical and theoretical interest:

- Time-delayed feedback processes are ubiquitous in biological regulatory networks and engineering. These systems are typically «autonomous» machines that operate in a nonequilibrium steady state (NESS) where work is permanently extracted from the environment.

- The non-Markovian character of the dynamics raises issues that go beyond the current framework of stochastic thermodynamics and that do not exist when dealing with a discrete (non-autonomous) feedback control.

Main theme of the talk: Because of the delay, the time-reversal operation becomes highly non-trivial. However, one cannot understand the behavior of the system (in particular the fluctuations) without referring to the unusual properties of the reverse process.

TALK ROADMAP

A. SECOND LAW-LIKE INEQUALITIES: (bounds for the average extracted work)

For more details, see PRL **112**, 180601 (2014) and Phys. Rev. E **91**, 042114 (2015).

B. FLUCTUATIONS (work, heat, entropy production): large-deviation functions and fluctuation relations

For more details, see cond-mat. arXiv soon...

A. SECOND-LAW-LIKE INEQUALITIES

Langevin equation:

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

with $F_{fb}(t) = F_{fb}(x_{t-\tau} + \cancel{\eta_{t-\tau}})$

- Inertial effects play an important role in human motor control and in experimental setups involving mechanical or electromechanical systems.
- Deterministic feedback control: no measurement errors

Stochastic Delay Differential Equations (SDDEs) have a rich dynamical behavior (multistability, bifurcations, stochastic resonance , etc.). However, we will only focus on the steady-state regime.

Consequences of non-Markovianity

1) The full description of the time-evolving state of the system in terms of pdf's requires the knowledge of the whole Kolmogorov hierarchy $p(x,v,t), p(x_1,v_1,t_1;x_2,v_2,t_2), \text{ etc.}$

There is an infinite hierarchy of Fokker-Planck (FP) equations that has no close solution in general.

The definition of the Shannon entropy depends on the level of description. There is no unique entropy-balance equation from the FP formalism (nor unique second-law-like inequality), but a set of equations and inequalities.

2) The time-reversal operation is non-trivial and leads to another second-law-like inequality (in this sense, one looses the nice consistency of stochastic thermodynamics).

3) Preparation effects are crucial due to the memory of the dynamics.

⇨ We will only focus on the steady-state regime and on the asymptotic behavior in the long-time limit (we will not consider transients).

Second-law-like inequalities obtained from the FP description

FP equation for the one-time pdf:

$$\partial_t p(x,v,t) = -\partial_x J^x(x,v) - \partial J^v_v(x,v)$$

where

$$J^x(x,v,t) = vp(x,v,t)$$

$$J^v(x,v,t) = \frac{1}{m}[-\gamma v + F(x) + \bar{F}_{fb}(x,v,t)]p(x,v,t) - \frac{\gamma T}{m^2}\partial_v p(x,v,t)$$

and

$$\bar{F}_{fb}(x,v,t)] := \frac{1}{p(x,v,t)}\int_{-\infty}^{\infty} dy F_{fb}(y)p(x,v,t;y,t-\tau)$$

is an effective time-dependent force obtained by formally integrating out the dependence on the variable $y_t := x_{t-\tau}$

➢ Corresponding Shannon entropy

$$S^{xv}(t) = \int dx\, dv\, p(x,v,t) \ln p(x,v,t)$$

d/dt +FP equation => Entropy balance equation:

$$\frac{d}{dt} S^{xv}(t) = \dot{S}_i^{xv}(t) - \frac{\dot{Q}(t)}{T} \boxed{- S_{pump}^{xv}(t)}$$

where $\dot{Q}(t) = \frac{\gamma}{m}(m\langle v_t^2 \rangle - T)$ heat exchanged with the bath

$\dot{S}_i^{xv}(t) = \frac{m^2}{\gamma T} \int dx dv\, \frac{[J_{irr}^v(x,v)]^2}{p(x,v,t)} \geq 0$ non-negative «EP» rate

and $\boxed{\dot{S}_{pump}^{xv}(t) = -\frac{1}{m} \langle \partial_v \bar{F}_{fb}(x,v,t) \rangle}$

«Entropy pumping» rate that describes the influence of the continuous feedback. The effective force contributes to the balance equation because it is velocity - dependent (i.e., it contains a piece which is antisymmetric under time-reversal).

- In the steady state regime, one then obtains a second-law-like inequality

$$\boxed{\frac{\dot{\mathcal{W}}_{ext}}{T} \leq \dot{\mathcal{S}}^{xv}_{pump}} \qquad (\dot{\mathcal{W}}_{ext} = -\dot{\mathcal{Q}})$$

  - one can extract work from the heat bath if

$$\dot{\mathcal{S}}^{xv}_{pump} > 0$$

  - (this depends on the delay, among other things)

Similarly, by working in momentum space only, and defining the Shannon entropy as

$$S^v(t) = \int dx\, dv\, p(v,t) \ln p(v,t)$$

one obtains another inequality

$$\boxed{\frac{\dot{\mathcal{W}}_{ext}}{T} \leq \dot{\mathcal{S}}^{v}_{pump} \leq \dot{\mathcal{S}}^{xv}_{pump}}$$

The entropy pumping rates have no direct interpretation in terms of information-theoretic measures, but one can also consider information flows that reveal how the exchange of information between the system and the controller is affected by the time delay, e.g.

$$\dot{I}^{xv;y}_{flow,v}(t) := \int dx\, dv\, dy\, \partial_v J^v(x,v,t;y,t-\tau) \ln \frac{p(x,v,t;y,t-\tau)}{p(x,v,t)p(y,t-\tau)}$$

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

Second-law-like inequality obtained from time reversal

In the case of non-autonomous feedback control with measurements and actions performed step by step at regular time intervals (e.g. Szilard engines), one can record the measurement outcomes and define a reverse process that does not involve any measurement nor feedback (see recent review in Nature Phys. **11**, 131, 2015). This is not possible when the feedback is implemented continuously.

One must also reverse the feedback

The feedback force then depends on the future ! The «conjugate» dynamics is acausal.

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

Generalized local detailed balance equation:

$\mathcal{P}[\mathbf{X}|\mathbf{Y}]$ probability to observe $\mathbf{X}=\{x_s\}_0^t$ given the previous path $\mathbf{Y}=\{x_s\}_{-\tau}^0$

$$\mathcal{P}[\mathbf{X}|\mathbf{Y}] \propto \mathcal{J}\, e^{-\beta S[\mathbf{X},\mathbf{Y}]}$$

$S[\mathbf{X},\mathbf{Y}] =$ Onsager-Machlup action functional

$$S[\mathbf{X},\mathbf{Y}] = \frac{1}{4\gamma}\int_0^t ds\, \left[m\ddot{x}_s + \gamma \dot{x}_s - F(x_s) - F_{fb}(x_{s-\tau})\right]$$

$\mathcal{J}$ path-independent Jacobian (contains the factor $e^{\frac{\gamma}{2m}t}$)

Fluctuating heat:

$$q[\mathbf{X},\mathbf{Y}] = \int_0^t ds\, [\gamma v_s - \sqrt{2\gamma T}\xi_s] \circ v_s$$
$$= -\int_0^t ds\, [m\dot{v}_s - F(x_s) - F_{fb}(x_{s-\tau})] \circ v_s$$

The heat is odd under time reversal if τ is changed into $-\tau$

Local detailed balance with continuous time-delayed feedback control:

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

$$\tilde{\mathcal{P}}[\mathbf{X}^\dagger|\mathbf{x}_i^\dagger,\mathbf{Y}^\dagger] \propto \tilde{\mathcal{J}}[\mathbf{X}] e^{-\beta \tilde{S}[\mathbf{X}^\dagger,\mathbf{Y}^\dagger]}$$

with $\tilde{S}[\mathbf{X},\mathbf{Y}] = \frac{1}{4\gamma}\int_0^t ds \left[m\ddot{x}_s + \gamma\dot{x}_s - F(x_s) - F_{fb}(x_{s+\tau})\right]$

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

in general path dependent

One can then define a generalized «entropy production» (Kullback-Leibler divergence):

$$\langle R_{cg}[\mathbf{X}]\rangle = \int \mathcal{D}\mathbf{X}\, \mathcal{P}[\mathbf{X}] \ln \frac{\mathcal{P}[\mathbf{X}]}{\tilde{\mathcal{P}}[\mathbf{X}^\dagger]}$$

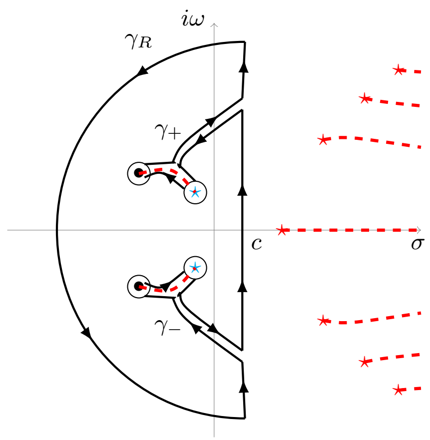
which satisfies an integral fluctuation theorem $\langle e^{R_{cg}[\mathbf{X}]}\rangle = 1$

In the steady state, this leads to another second-law-like inequality:

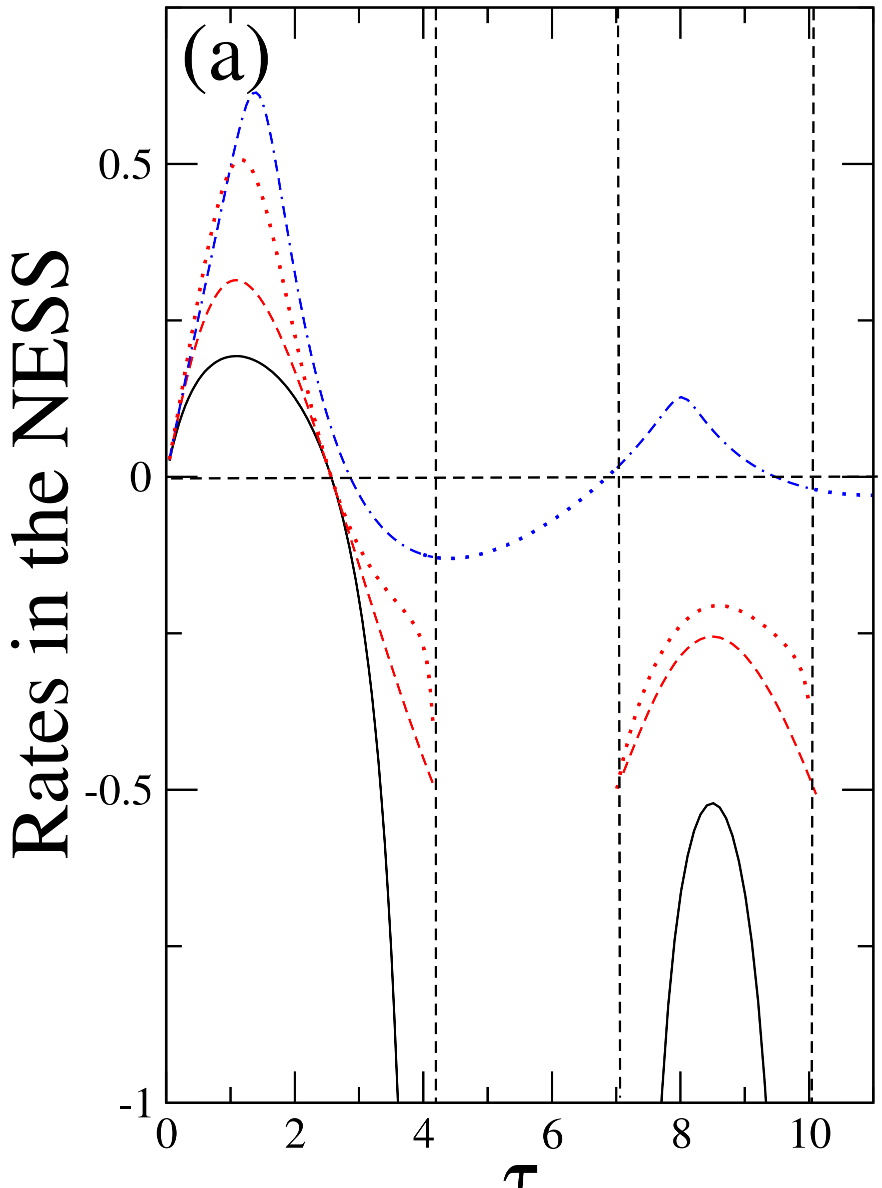
$$\boxed{\frac{\dot{\mathcal{W}}_{ext}}{T} \leq \dot{\mathcal{S}}_{\mathcal{J}}}$$

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

(this quantity can be computed exactly in a linear system but this requires a careful analysis of the «response function» associated to the acausal conjugate Langevin equation in Laplace space.)



Example for a linear system:



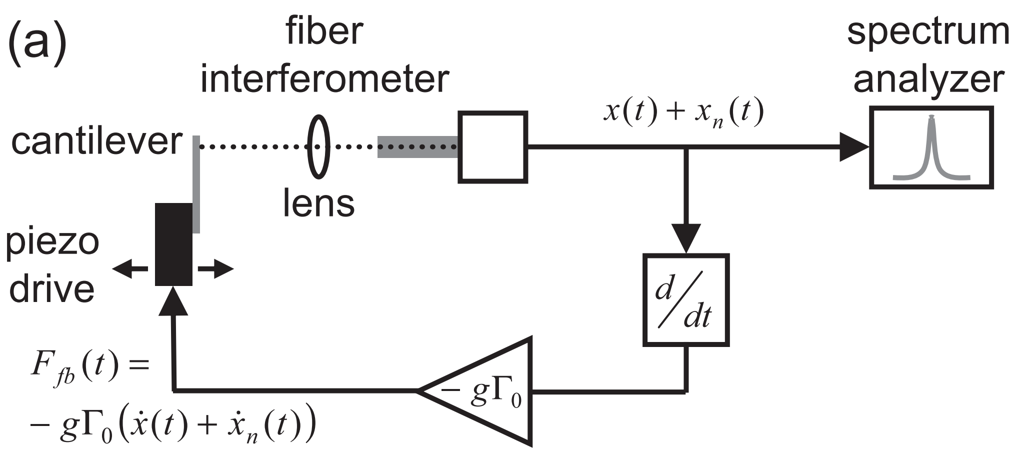
Solid black line: extracted work

red and blue lines: various bounds.

B. FLUCTUATIONS

To be concrete, we will consider a linear Langevin equation, i.e. a stochastic harmonic oscillator submitted to a linear feedback

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



describes accurately the dynamics of nano-mechanical resonators (e.g. the cantilever of an AFM) used in feedback cooling setups.

In reduced units: 3 parameters

$$\dot{v}_t = -x_t - \frac{1}{Q_0} v_t + \frac{g}{Q_0} x_{t-\tau} + \xi_t$$

Quality factor:

$$Q_0 = \omega_0 \tau_0 \ \ (\omega_0 = \sqrt{k/m}, \tau_0 = m/\gamma)$$

Gain: $g = (k'/k) Q_0$

We study the fluctuations of 3 observables:

$$\text{Work:} \quad \beta\mathcal{W}[\mathbf{X},\mathbf{Y}] = \frac{2g}{Q_0^2}\int_0^t ds\, x_{s-\tau} v_s$$

$$\text{Heat:} \quad \beta\mathcal{Q}[\mathbf{X},\mathbf{Y}] = \beta\mathcal{W}[\mathbf{X},\mathbf{Y}] - \Delta\mathcal{U}(\mathbf{x}_i,\mathbf{x}_f)$$

$$= \beta\mathcal{W}[\mathbf{X},\mathbf{Y}] - \frac{1}{Q_0}(x_f^2 - x_i^2 + v_f^2 - v_i^2)$$

$$\text{“Pseudo EP”} \quad \Sigma[\mathbf{X},\mathbf{Y}] = \beta\mathcal{Q}[\mathbf{X},\mathbf{Y}] + \ln\frac{p_{st}(\mathbf{x}_i)}{p_{st}(\mathbf{x}_f)}$$

Quantities of interest: probability distribution functions

$$P_A(A,t) = \langle\delta(A - \beta\mathcal{A}[\mathbf{X},\mathbf{Y}])\rangle_{st}$$

$$= \int d\mathbf{x}_f \int \mathcal{D}\mathbf{Y}\,\mathcal{P}_{st}[\mathbf{Y}] \int_{\mathbf{x}_i}^{\mathbf{x}_f} \mathcal{D}\mathbf{X}\,\delta(A - \beta\mathcal{A}[\mathbf{X},\mathbf{Y}])\mathcal{P}[\mathbf{X}|\mathbf{Y}]$$

and the corresponding moment generating functions

$$Z_A(\lambda,t) = \langle e^{-\lambda\beta\mathcal{A}[\mathbf{X},\mathbf{Y}]}\rangle_{st} = \int_{-\infty}^{+\infty} dA\, e^{-\lambda A} P_A(A,t)$$

Expected long-time behavior of the pdfs: $P_A(A = at) \sim e^{-I_A(a)t}$

where $\sim$ denotes logarithmic equivalence and $I(a)$ is the LDF

Similarly: $Z_A(\lambda, t) \approx g_A(\lambda) e^{\mu_A(\lambda)t}$

where $\mu_A(\lambda) = \lim_{t\to\infty} \frac{1}{t} \ln\langle e^{-\lambda\beta\mathcal{A}[\mathbf{X},\mathbf{Y}]}\rangle_{st}$ is the SCGF

(Scaled Cumulant Generating Function)

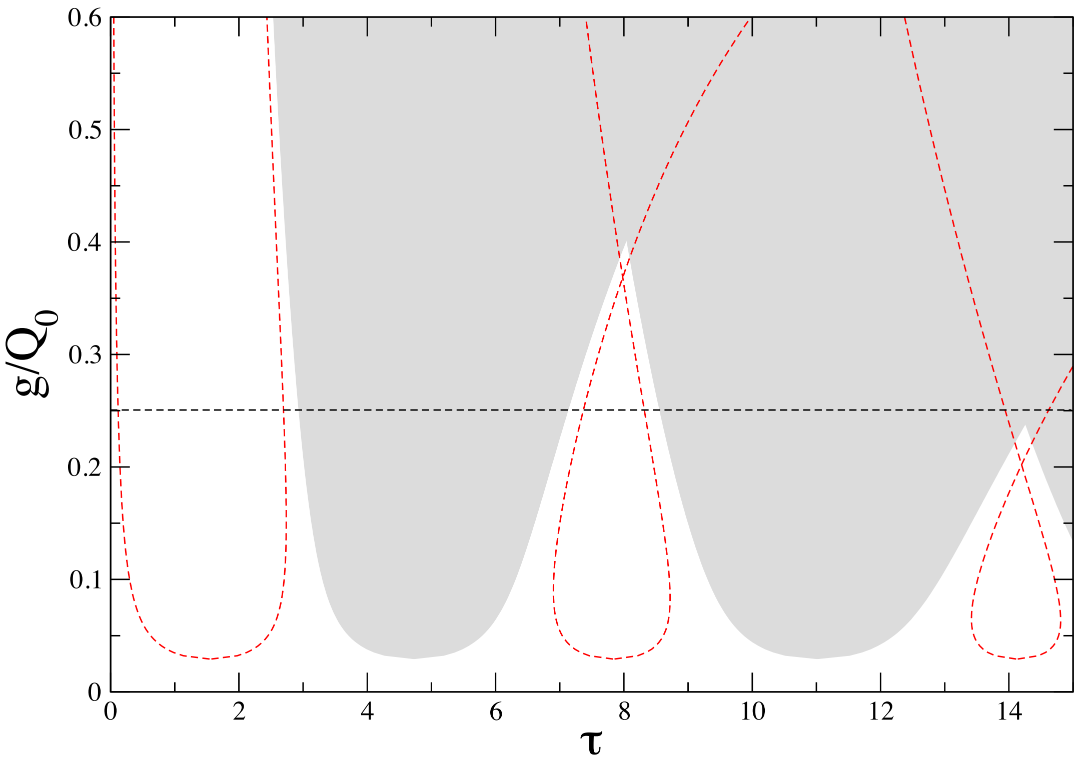
and the pre-exponential factor $g_A(\lambda)$ typically arises from the average over the initial and final states. Here the "initial" state is $\mathbf{Y}$

The 3 observables only differ by «boundary» terms that are not extensive in time. However, since the potential V(x) is unbounded, these terms may fluctuate to order t !

Pole singularities in the prefactors and exponential tails in the pdf's (e.g. for the heat)

Numerical study: $Q_0 = 34.2, g/Q_0 = 0.25$

The quality factor corresponds to the cantilever of the AFM used in recent experiments by Ciliberto *et al* (Eur. Phys. Lett. **89**, 60003 (2010))

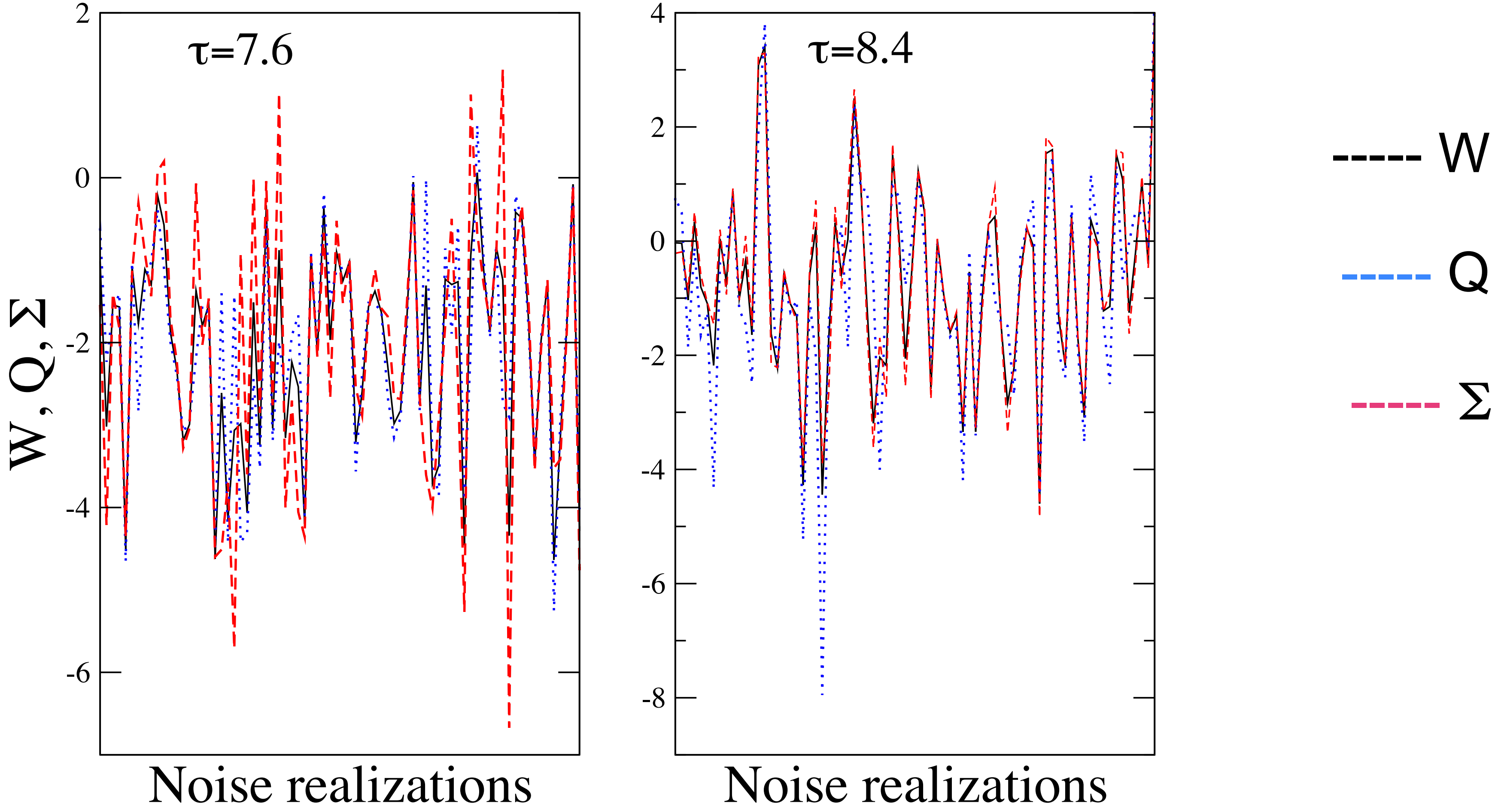


The feedback-controled oscillator has a complex dynamical behavior as a function of the delay or the gain g: multistability regime

As an exemple, we will study the fluctuations in the second lobe where the system can reach a stationary state.

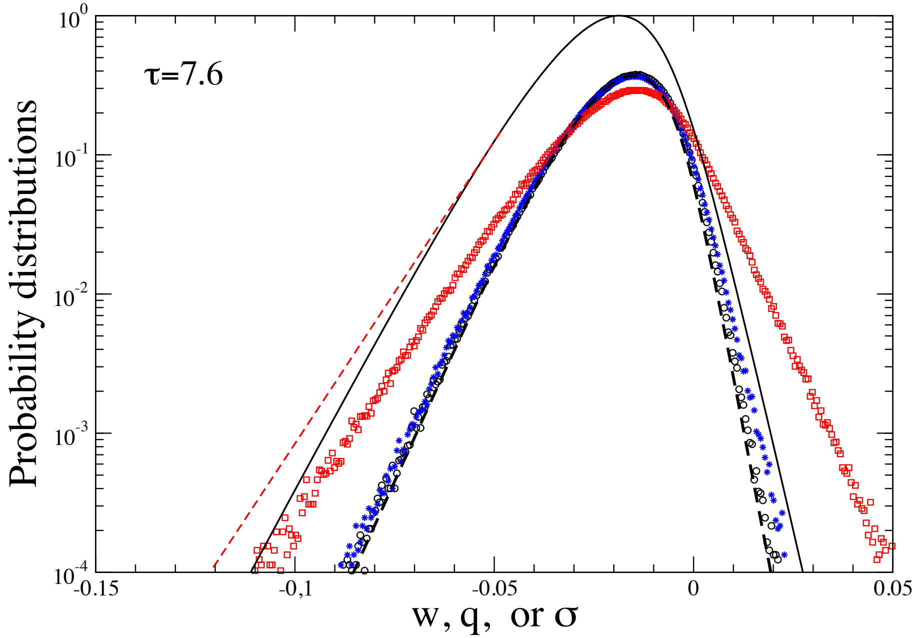
Fluctuations of the 3 observables for different noise realizations:

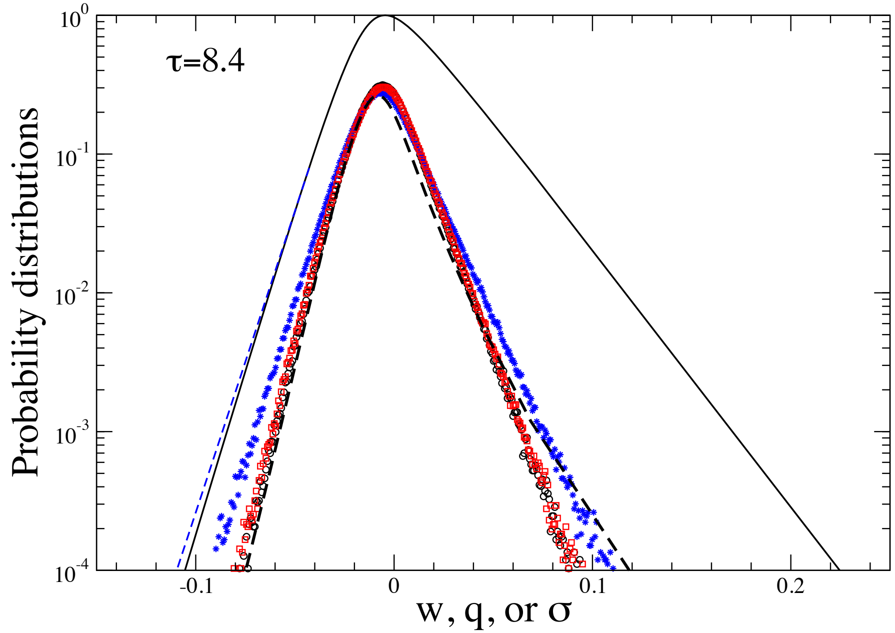
The length of the trajectory is t=100



Boundary terms are still non negligible. Fluctuations are correlated but the qualitative behavior depends on the delay !

Probability distribution functions:





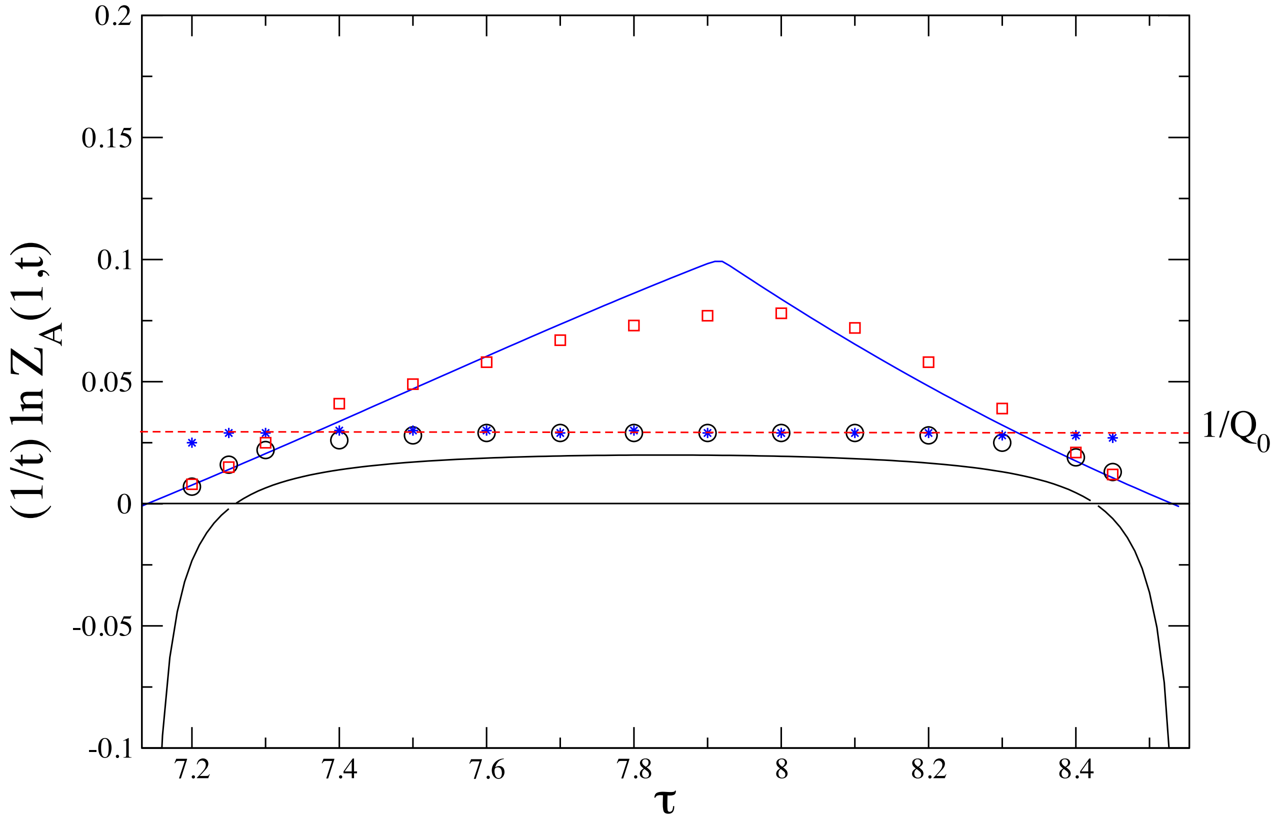
The solid black line the theoretical curve $P_W(W = wt) \sim e^{-I(w)t}$

and the dashed solid line takes into account finite-time corrections.

Main Puzzle: How can we explain the change of behavior of

$P_Q(Q = qt)$ and $P_\Sigma(\Sigma = \sigma t)$ with τ ?

Two origins: 1) Existence of integral fluctuation theorems (IFT):



$$Z_Q(1,t) \equiv \langle e^{-\beta \mathcal{Q}[\mathbf{X},\mathbf{Y}]} \rangle_{st} = e^{\gamma t/m}$$

(exact result for an underdamped Langevin dynamics)

$$Z_\Sigma(1,t) \equiv \langle e^{-\beta \Sigma[\mathbf{X},\mathbf{Y}]} \rangle_{st} \sim e^{\dot{\mathcal{S}}_{\mathcal{J}} t} \quad , t \to \infty$$

(not yet fully proved; some similarity with Sagawa-Ueda relation involving the so-called «efficacy parameter»)

$$(\dot{\mathcal{S}}_{\mathcal{J}} := \lim_{t\to\infty} \frac{1}{t} \ln \frac{\mathcal{J}}{\tilde{\mathcal{J}}})$$

Such IFT's imply a peculiar behavior of the generating functions in the long-time limit:

Pole in the prefactor at $\lambda = 1 \text{ in the limit } t \to \infty$

Boundary layer in the vicinity of $\lambda = 1$ for t large but finite

$$\mu_Q(\lambda = 1) \neq \lim_{\lambda \to 1} \mu_Q(\lambda)$$

But this also depends on the value of the delay !

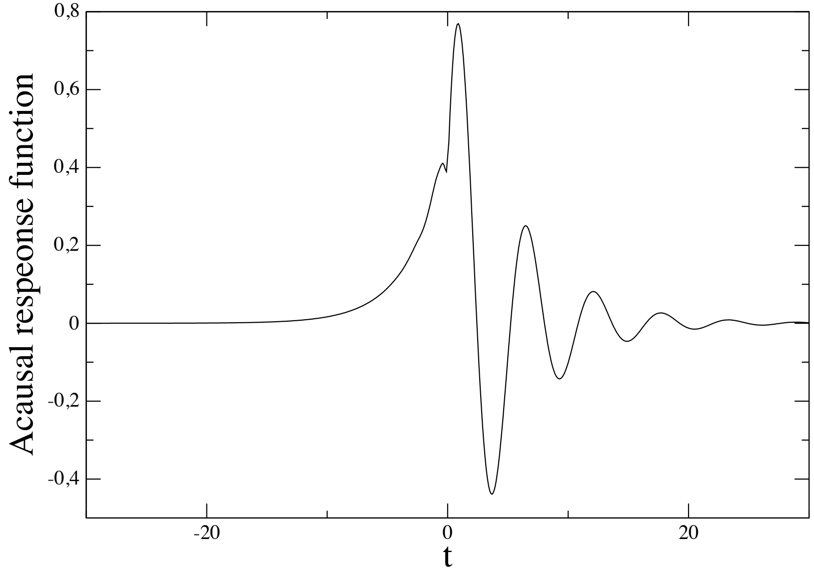
2) The behavior of the pdf's also depends on whether the conjugate, acausal dynamics reaches or does not reach a stationary state.

Inserting the local detailed balance equation into the definition of the generating function, one finds (for instance for the heat)

$$Z_Q(\lambda, t) \sim e^{\dot{\mathcal{S}}_{\mathcal{J}} t} \int d\mathbf{x}_i \int \mathcal{D}\mathbf{Y}\, e^{(1-\lambda)\beta\Delta\mathcal{U}(\mathbf{x}_i,\mathbf{x}_f)} \mathcal{P}_{st}[\mathbf{Y}^\dagger] \int_{\mathbf{x}_i}^{\mathbf{x}_f} \mathcal{D}\mathbf{X}\, e^{-\beta\widetilde{\mathcal{S}}_\lambda[\mathbf{X},\mathbf{Y}]}$$

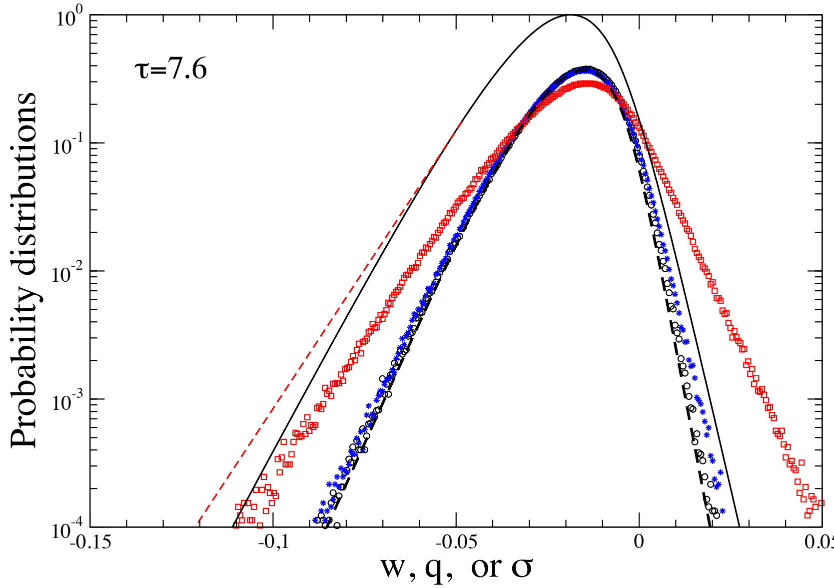
where $\widetilde{\mathcal{S}}_\lambda[\mathbf{X},\mathbf{Y}]$ is the OM action associated with the conjugate Langevin equation

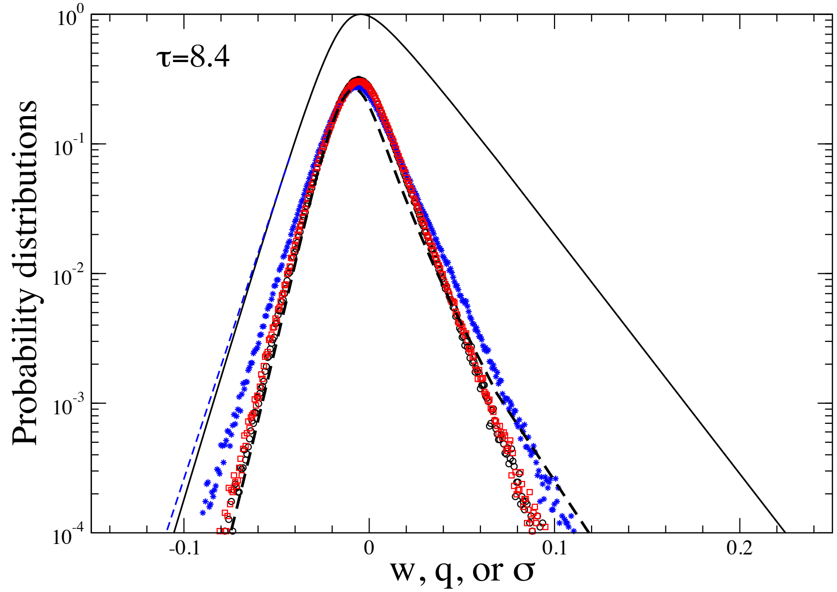
The boundary terms become irrelevant in the long-time limit when the conjugate acausal dynamics reaches a stationary state: no dependence on the state of the system in the far past or the far future .



Acausal response function in the case where the conjugate dynamics reaches a stationary state

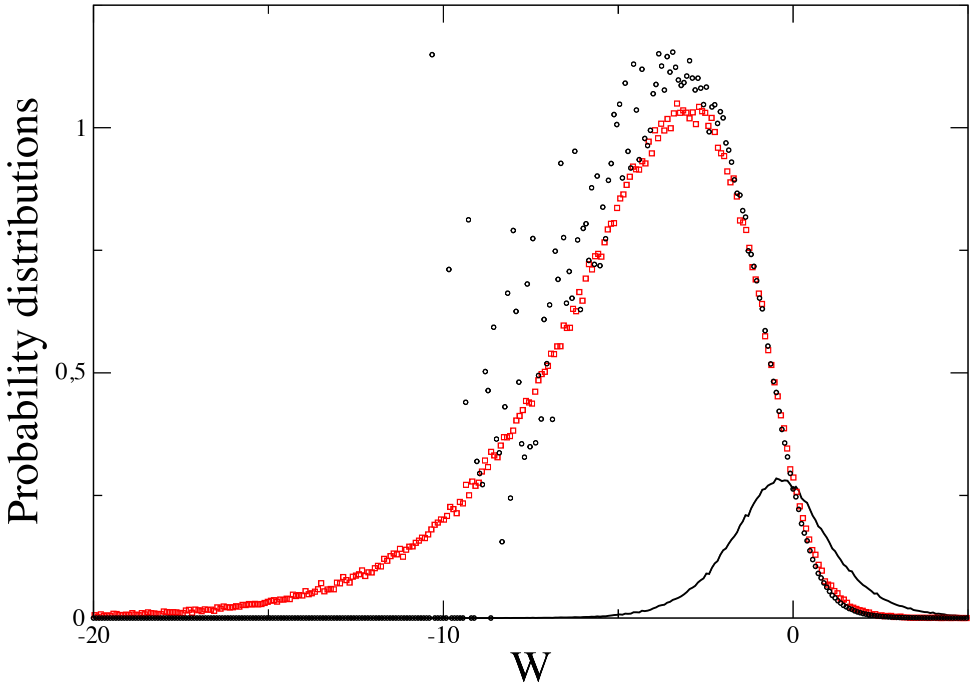
This also depends on the delay and can be related to the position of the poles of the acausal response function in the complex-frequency plane.





Modified Crooks FT for the work: When the acausal dynamics reaches a stationary state, one can show that

$$\frac{P_W(W = wt)}{\widetilde{P}(\widetilde{W} = -wt)} \sim e^{(w+\dot{\mathcal{S}}_{\mathcal{J}})t} \quad , t \to \infty$$



$P_W(W = wt)$

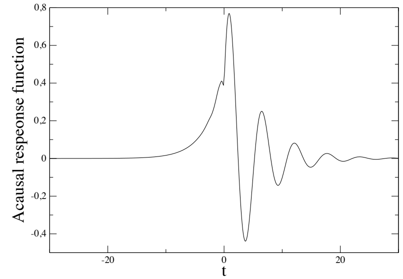
$P_W(W = wt)e^{-wt}$

$\tilde{P}_W(\tilde{W} = -wt)e^{\dot{\mathcal{S}}_{\mathcal{J}}t}$

In the long-time limit, the *atypical* trajectories that dominate $\langle e^{-\beta W} \rangle_{st}$ are the conjugate twins (Jarzynski 2006) of *typical* realisations of the reverse (acausal) process

Alternatively, one can determine the properties of the atypical noise that generates the rare events.

Since the conjugate dynamics converges, the solution of the acausal Langevin equation is



$$\widetilde{x}(t) \approx \int_{-\infty}^{\infty} dt'\ \widetilde{\chi}(t-t')\xi(t')$$

$$= \int_{-\infty}^{t} dt' \widetilde{\chi}_+(t-t)\xi(t') + \int_{t}^{\infty} dt' \widetilde{\chi}_-(t-t')\xi(t')$$

or in the frequency domain: $\widetilde{x}(\omega) \approx \widetilde{\chi}(\omega)\xi(\omega)$

Inserting into the original Langevin equation yields:

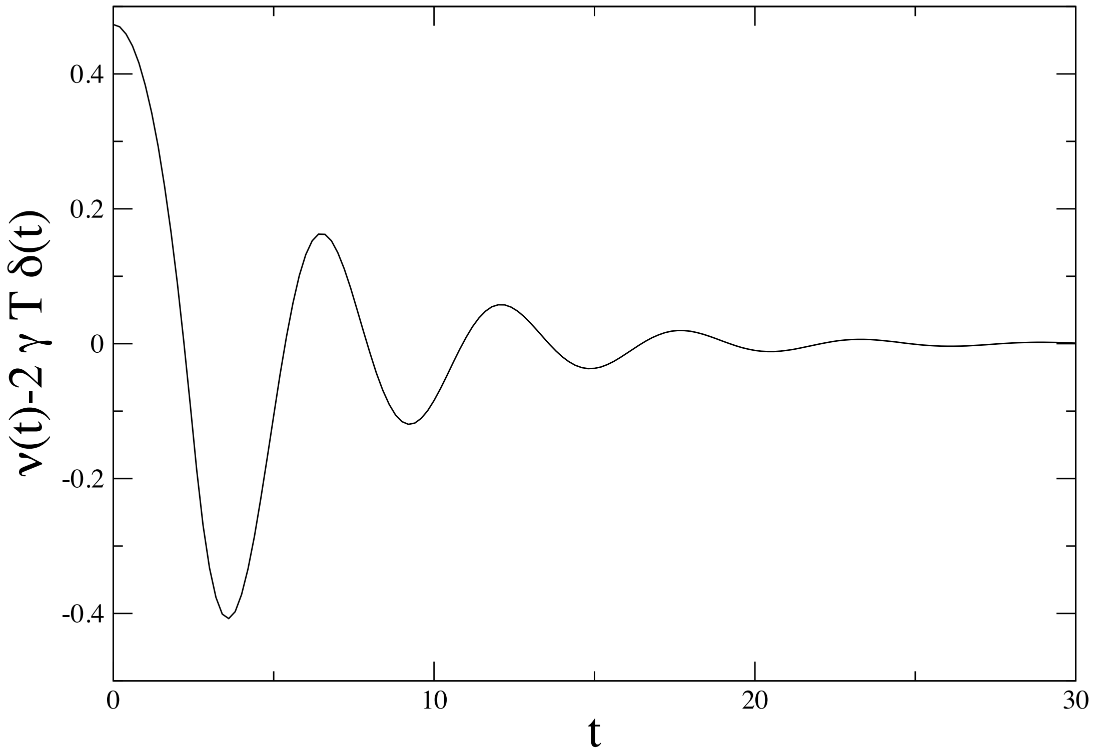
$$\boxed{\xi_{atyp}(\omega) = \frac{\widetilde{\chi}(\omega)}{\chi(\omega)}\xi(\omega)\ .}$$

The atypical noise is colored !

Hence $\langle \xi_{atyp}(t)\xi_{atyp}(t')\rangle = \nu(t-t')$

with $\nu(t) = 2\gamma T\left[\delta(t) + \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi}[|\frac{\widetilde{\chi}(\omega)}{\chi(\omega)}|^2 - 1]e^{-i\omega t}\right]$

Variance of the atypical noise



CONCLUSION

One can extend the framework of stochastic thermodynamics to treat non-Markovian effects induced by a time-delayed feedback. This introduces a new and interesting phenomenology .

Experimental tests ?

Thank you for your attention !