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New Frontiers in Non-equilibrium Physics of Glassy Materials

Stochastic Thermodynamics of Langevin systems under time-delayed feedback control

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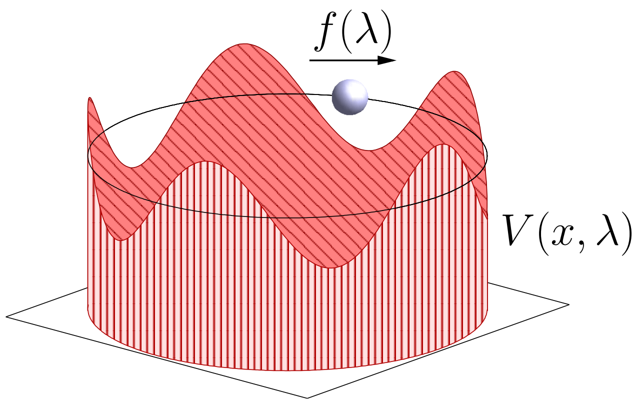
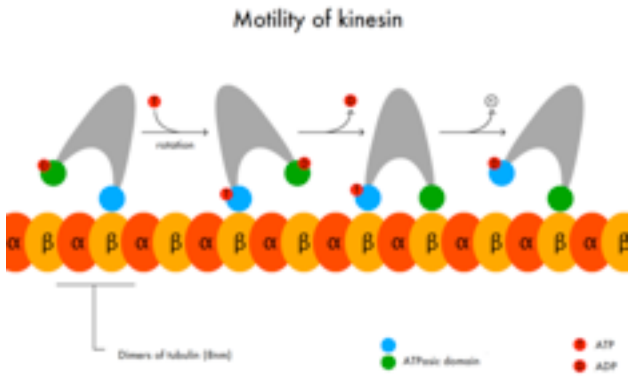
Purpose of Stochastic Thermodynamics:

Extend the basic notions of classical thermodynamics (work, heat, entropy production...) to the level of individual trajectories.





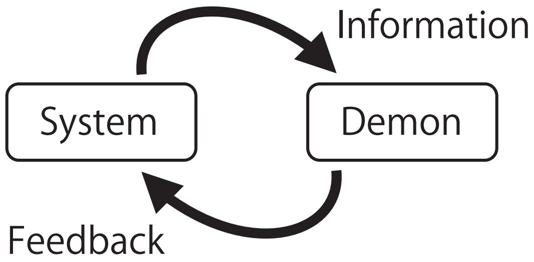
The observed systems

. have only a few degrees of freedom → fluctuations play a dominant role and observables are described by probability distributions.

. are in contact with one or several heat baths

. stay far from equilibrium because of mechanical of chemical «forces».

Thermodynamics of feedback control («Maxwell's demon»):



Purpose: Extend the second law of thermodynamics and the fluctuation theorems in the presence of information transfer and control

Two types of control:

1) Feedback is implemented *discretely* by an external agent through a series of loops initiated at a sequence of predetermined times, e.g. Szilard engines (non-autonomous machines). See recent review in Nature Phys. 11, 131 (2015).

2) Feedback is implemented *continuously*, in real time. Time-lags are then unavoidable (or chosen on purpose). Normal operating regime: NESS in which heat and work are permanently exchanged with the environment (autonomous machines).

- The non-Markovian character of the dynamics (which is neither due to coarse-graining nor to the coupling with the heat bath) raises issues that go beyond the current framework of stochastic thermodynamics and that do not occur when dealing with discrete feedback control.

Main message: Because of the time-delayed feedback control, the relation between dissipation and time-reversibility becomes highly non-trivial (the reverse process is quite unusual). However, in order to understand the behavior of the system (in particular the fluctuations of the observables, e.g. the heat), one must refer to the properties of the reverse process.

Time-delayed Langevin equation:

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

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

- Inertial effects play an important role in human motor control and in experimental setups involving nano-mechanical resonators (e.g., feedback cooling)
- 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.

Second-law-like inequalities

The full description of the time-evolving state of the system in terms of pdf's requires the knowledge of the whole Kolmogorov hierarchy $p(x,v,t), p(x_1,v_1,t;x_2,v_2,t-\tau)$, 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, e.g. $S^{xv}(t) = \int dx\, dv\, p(x,v,t) \ln p(x,v,t)$

There is no unique entropy-balance equation from the FP formalism (and no unique second-law-like inequality in the steady state), but a set of equations and inequalities.

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

The «entropy pumping» rate describes the influence of the continuous feedback. One can extract work from the bath if the entropy puming rate is positive

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

Local detailed balance equation:

relates the heat exchanged with the bath along a given stochastic trajectory to the conditional probabilities of observing the trajectory and its time-reversed image.

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

$\mathcal{P}[\mathbf{X}|\mathbf{Y}]$ 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 $e^{\frac{\gamma}{2m}t}$)

By simply reversing time, and taking the logratio of the probabilities, one does not recover the heat because the heat is not odd under time reversal !

To recover the heat, one must also reverse the feedback

i.e. change τ into $-\tau$!

This defines a conjugate, *acausal* Langevin dynamics:

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

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

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

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

From the local detailed balance equation, one can derive another second-law-like inequality in the stationary state

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

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 new upper bound to the extracted work is different from the one involving the entropy pumping rate.

FLUCTUATIONS

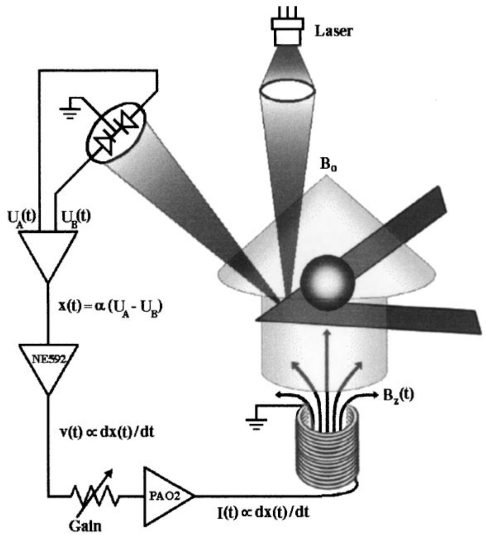
To be concrete, we now consider a linear Langevin equation, i.e. a stochastic harmonic oscillator submitted to a linear feedback

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

3 independent parameters: Q_0, g, τ

$Q_0 = \omega_0 \tau_0 \ \ (\omega_0 = \sqrt{k/m}, \tau_0 = m/\gamma)$ (Quality factor of the resonator)

Active feedback cooling of the cantilever of an AFM (Liang et al. 2000)



This equation faithfully describes the dynamics of nano-mechanical resonators (e.g. the cantilever of an AFM) in the vicinity of the resonance frequency.

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 characteristic (or 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)

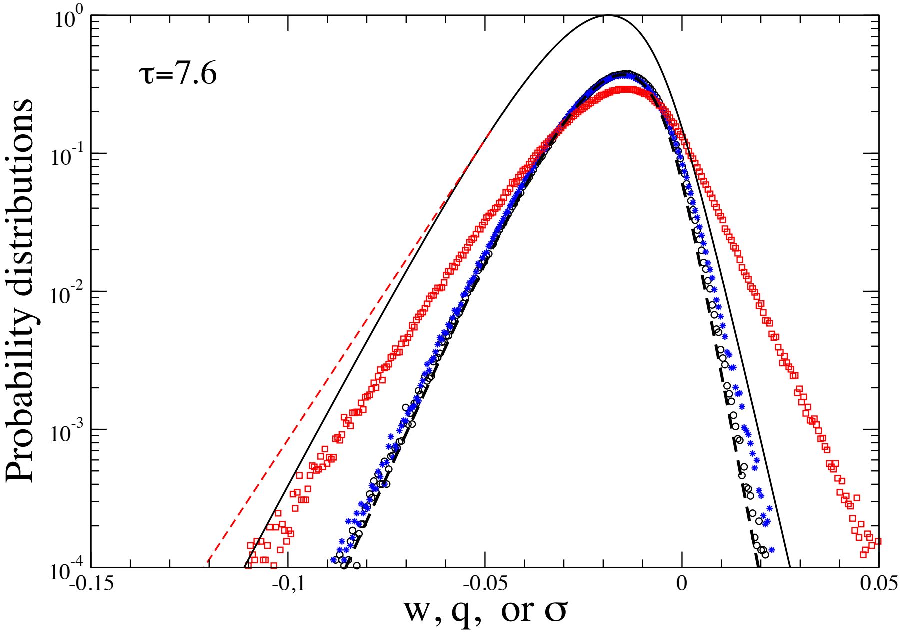
and the pre-exponential factor $g_A(\lambda)$ typically arises from the average over the initial and final states. Here the "initial" state is $\mathbf{Y}$

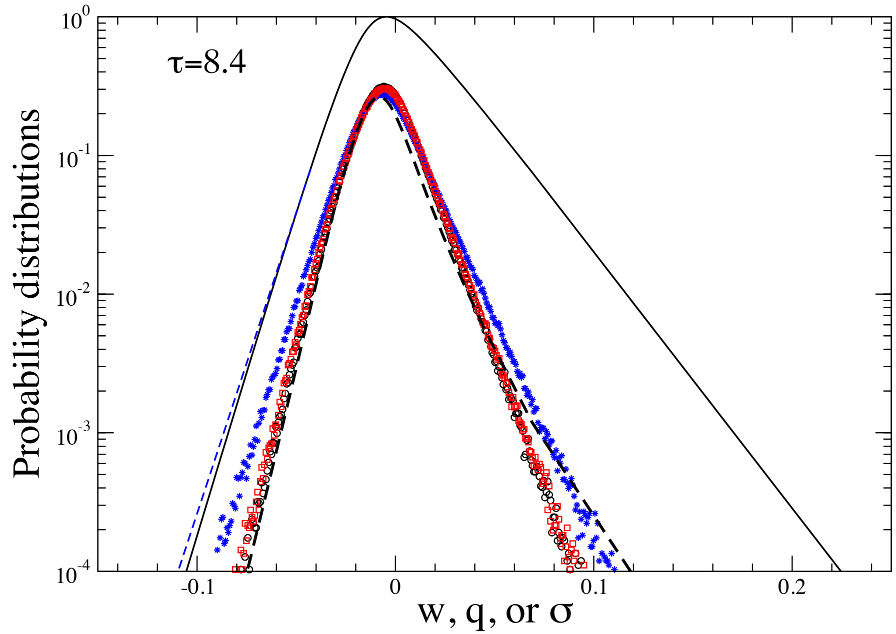
The 3 observables only differ by temporal «boundary» terms that are not extensive in time. However, since the potential V(x) is unbounded, these terms may fluctuate to order t !

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

Probability distribution functions: $Q_0 = 34.2, g/Q_0 = 0.25$

Length of the trajectory: t=100





∘∘∘ W, ∘∘∘ Q, ∘∘∘ Σ

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

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

Two (related) explanations:

1) Existence of exact sum-rules (IFT= integral fluctuation theorems)

. For the heat:

$$\boxed{\langle e^{-\beta\mathcal{Q}}\rangle_{st} = e^{\gamma t/m}}$$

valid at *all* times and for *any* underdamped Langevin dynamics

. For the «pseudo» entropy production:

$$\boxed{\langle e^{-\beta\Sigma}\rangle_{st} \sim e^{\dot{\mathcal{S}}_{\mathcal{J}} t}}$$

$$\text{where } \dot{\mathcal{S}}_{\mathcal{J}} := \lim_{t\to\infty} \frac{1}{t} \ln \frac{\mathcal{J}}{\tilde{\mathcal{J}}} \text{ is a function of } \tau$$

valid only asymptotically (somewhat related to Sagawa-Ueda IFT involving the «efficacy» parameter.

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

What does this mean ?

Although the conjugate dynamics is acausal and therefore cannot be physically implemented, one can still define a response function $\widetilde{\chi}(t-t') = \langle x(t)\xi(t')\rangle$

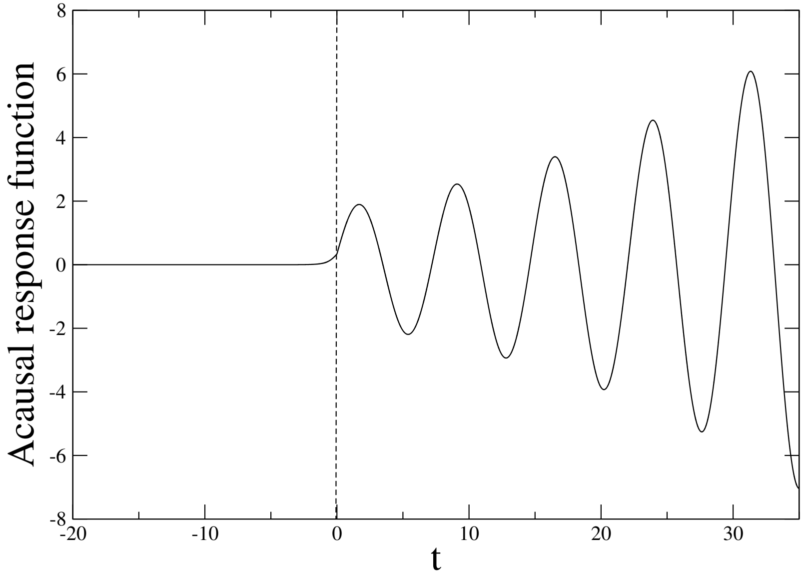
If $\widetilde{\chi}(t) \to 0$ as $t \to \pm\infty$ then

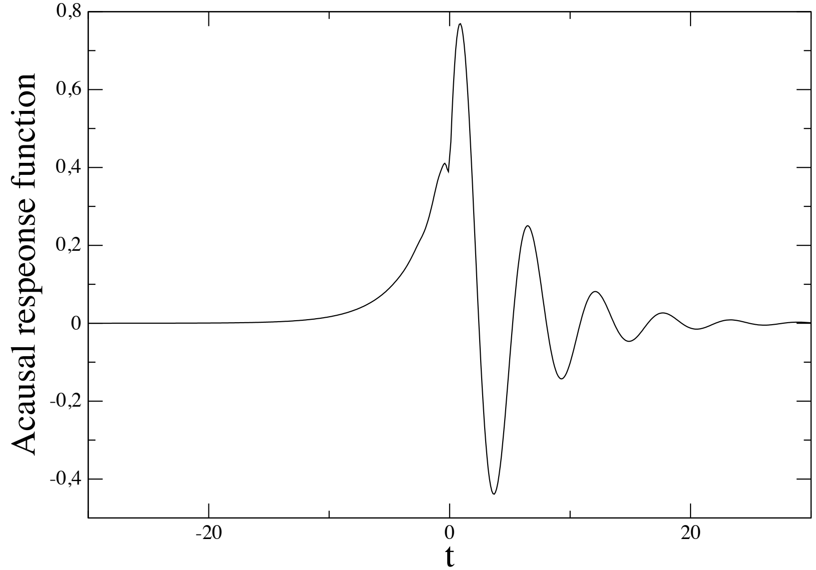
$$x(t) \approx \int_{-\infty}^{\infty} dt' \, \widetilde{\chi}(t-t')\xi(t')$$

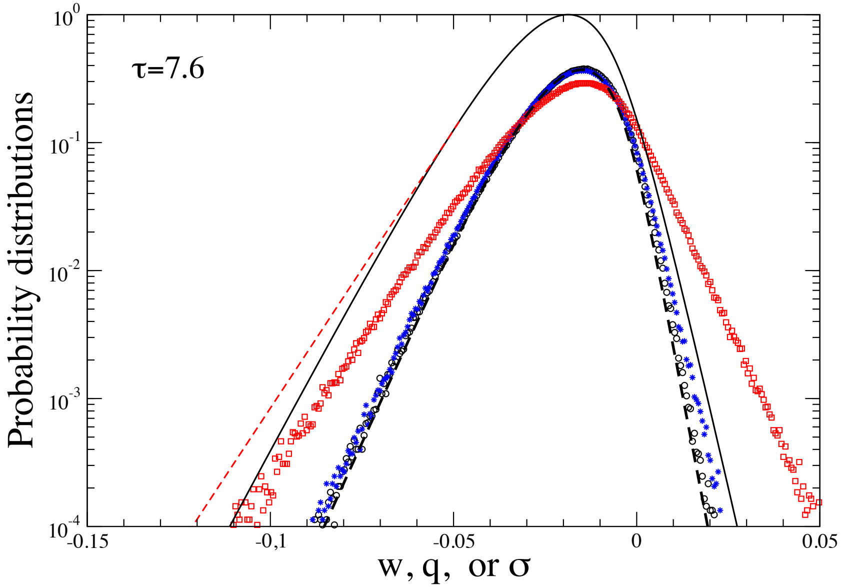
$$= \int_{-\infty}^{t} dt' \widetilde{\chi}_{+}(t-t)\xi(t') + \int_{t}^{\infty} dt' \widetilde{\chi}_{-}(t-t')\xi(t')$$

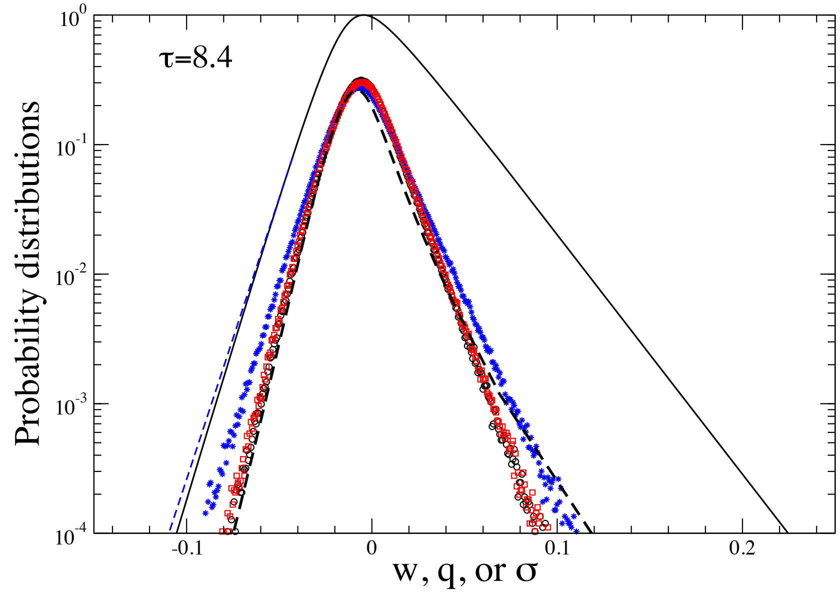
or in the frequency domain: $x(\omega) \approx \widetilde{\chi}(\omega)\xi(\omega)$

In this sense, the acausal dynamics reaches a stationary state that is independent from the initial and final conditions for $t \to \pm\infty$


Acausal response function
t
8
6
4
2
0
-2
-4
-6
-8
-20
-10
0
10
20
30

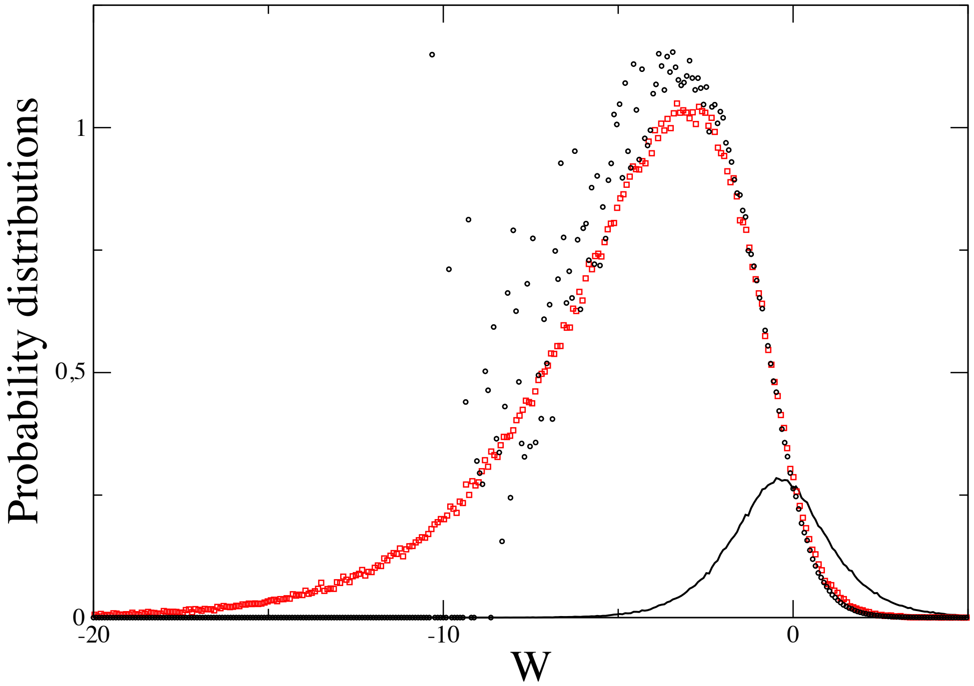

Acausal respeonse function
t
0,8
0,6
0,4
0,2
0
-0,2
-0,4
-20
0
20


τ=7.6
Probability distributions
w, q, or σ
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
-0.15
-0,1
-0.05
0
0.05


τ=8.4
Probability distributions
w, q, or σ
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
-0.1
0
0.1
0.2

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

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



— $P_W(W=wt)$

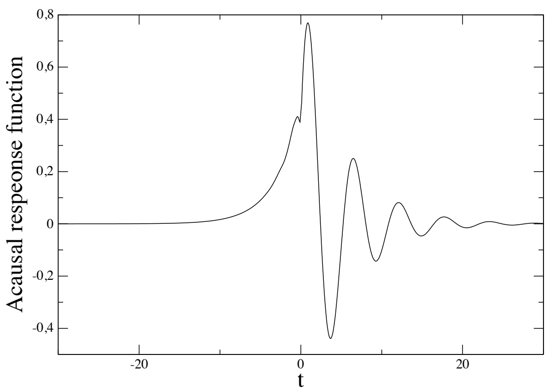
● $P_W(W=wt)e^{-wt}$

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

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



$$x(\omega) \approx \widetilde{\chi}(\omega)\xi(\omega)$$

Inserting into the original Langevin equation yields

$$\chi(\omega)\xi_{atyp}(\omega) \approx \widetilde{\chi}(\omega)\xi(\omega)$$

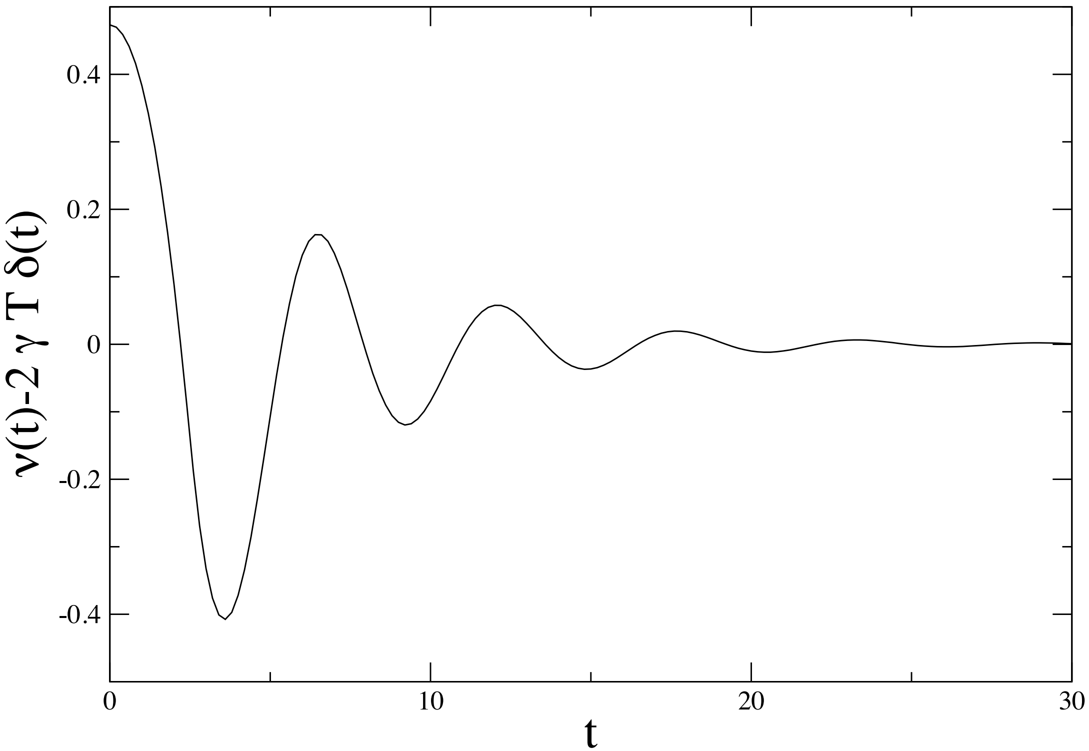
And thus:

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

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



The «atypical» noise that generates the rares events dominating $\langle e^{-\beta W}\rangle_{st}$ is colored !

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 !