Entropy production and fluctuation theorems in stochastic systems with time delay

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(T. Munakata and M.L. R., cond-mat: 1401.0771; T. Munakata, M.L. R., and G. Tarjus, in preparation).

Consider the stochastic delay equation

$$m\ddot{x} + \gamma\dot{x} + ax + bx(t - \tau) = \xi(t)$$

where $\xi(t)$ is a Gaussian white noise, with $<\xi(t)\xi(t')>=2\gamma T\delta(t-t')$

We regard this equation as describing the motion of a Brownian particle (or «system») in contact with a heat bath at temperature T, confined by a harmonic potential, and submitted to a feedback force $F_{fb}(t) \propto x(t - \tau)$

Suppose that the system has reached a nonequilibrium steady state (NESS) where heat is permanently exchanged with the environment.

Questions: Can we define and compute the corresponding entropy production and study its fluctuations ? What is the expression of the 2nd law of thermodynamics ?



$$m\ddot{x} + \gamma\dot{x} - F(x) - F_{fb}(t) = \xi(t)$$

$$F(x) = -\frac{dV(x)}{dx}$$
 conservative force

 $F_{fb}(t)$ feedback control force, that depends on the past state of the system



Feedback control is ubiquitous in physics, biology, and engineering. Information obtained through the measurement modifies the expression of the second law of thermodynamics (Maxwell's demon, Szilard engine, etc...)

Can we quantify this modification ?

This question, at the crossroad of information theory and statistical physics, has been extensively studied in recent years, in the framework of the stochastic thermodynamics of small systems (for a review, see e.g. U. Seifert, Rep. Prog. Phys. **75**, 126001 (2012)). Experiments are now possible.

Relevant application: Active feedback cooling (or cold damping) technique

<u>Objective</u>: reduce the effective noise temperature of (nano-) mechanical oscillators well below their operating temperature



If the resonator frequency is high, the feedback circuit cannot follow instantaneously the system dynamics => The feedback becomes non-Markovian, which degrades the cooling performance.

I) Stochastic thermodynamics (for systems described by a Markov dynamics) : a brief overview

2) Entropy production and fluctuation theorems in the presence of continuous non-Markovian feedback control

3) Application to linear stochastic delay equations

I) Stochastic thermodynamics: a (very) brief reminder

Purpose: extend the thermodynamic concepts of heat, work, entropy to the nano-world and systems that

a) have only a few degrees of freedom so that fluctuations play a dominant role (and observables are described by probability distributions).

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

b) are in contact with heat bath at temperature T (or several baths)





Fluctuation theorems

(e.g. Jarzynski equality, Crooks relation, etc...) These are exact identities obeyed by the probability distribution of an observable (e.g. heat, work, entropy production) integrated over a trajectory during some time t.

We shall focus here on the entropy production.

How can one define the entropy production along a single stochastic trajectory ?

For simplicity consider a process described by the overdamped Langevin equation

$$\dot{x}(t) = F(x_t, \lambda_t) + \xi(t)$$

where the force F depends on some time-dependent protocol $\lambda(t)$ that is repeated many times. For each realization of the noise, the system follows a different path x(s)



One can then define a trajectory-dependent entropy production which is the sum of two contributions:

$$\Delta s_{tot}[\{x_s\}] = \Delta s_m[\{x_s\}] + \Delta s_{sys}$$

where I°
$$\Delta s_m[\{x_s\}] \equiv \frac{q[\{x_s\}]}{T}$$

is the change in the medium entropy, i.e. the heat exchanged with the thermal bath divided by its temperature $\left(k_B=1\right)$.

According to the first law at the level of an individual trajectory, the heat is the work done on the system minus the variation of the internal energy.

$$\Delta s_m[\{x_s\}] \equiv \frac{q[\{x_s\}]}{T} = \frac{1}{T} \int_o^t ds \ F(x_s, \lambda_s) \circ \dot{x}_s$$

and 2°
$$\Delta s_{sys} \equiv -\ln p(x(t)) + \ln(p(x(0)))$$

is the change in the stochastic (Shannon) entropy of the system (Seifert, 1995) defined by $s_{sys}(t) \equiv -\ln p(x(t),t)$

where p(x,t) is the solution of the Fokker-Planck equation evaluated along the trajectory x(t). ONLY VALID FOR A MARKOVIAN DYNAMICS

Then, one can prove that $\Delta s_{tot}[\{x_s\}]$ satisfies an integral fluctuation theorem

(IFT)
$$\langle e^{-\Delta s_{tot}[\{x_s\}]} \rangle = 1$$

By Jensen's inequality, the IFT implies the 2nd Law of thermodynamics:

$$\langle \Delta s_{tot}[\{x_s\}] \rangle \ge 0$$

(but the IFT implies that the entropy production is negative along certain trajectories)

There are also stronger fluctuation relations (detailed fluctuation theorems), such as

$$\frac{P_F(+\Delta s_{tot})}{P_R(-\Delta s_{tot})} = e^{\Delta s_{tot}}$$

Key point: dissipation is related to the time reversibility of the trajectories.

$$\Delta s_m[\{x_s\}] \equiv \frac{q[\{x_s\}]}{T} = \frac{1}{T} \int_o^t ds \ F(x_s, \lambda_s) \circ \dot{x}_s$$

can also be written as the logratio of the probabilities of the trajectory and its time-reversal (for the time-reversed protocol)



Now multiply by the numerator and the denominator by the probabilities of the initial and final states

$$\ln \frac{\mathcal{P}_F[\{x_s\}|x_i]p(x_i)}{\mathcal{P}_B[\{x_s^\dagger\}|x_i^\dagger]p(x_i^\dagger)} = \Delta s_m[\{x_s\}] + \ln \frac{p(x_i)}{p(x_i^\dagger)}$$

$$\Delta s_{tot}[\{x_s\}] = \ln \frac{\mathcal{P}_F[\{x_s\}]}{\mathcal{P}_B[\{x_s\}]}$$



$$\langle e^{-\Delta s_{tot}[\{x_s\}]} \rangle \equiv \int \mathcal{D}x_s \mathcal{P}_F[\{x_s\}] e^{-\Delta s_{tot}[\{x_s\}]} = 1$$

Generalization in the presence of a Markovian, discrete feedback control (Sagawa-Ueda 2010, Horowitz-Vaikuntanthan 2010)

The information obtained through the measurement of the state of the system modifies the IFT and the second law. One finds that

$$< e^{-\Delta S_{tot} - I} >= 1$$

where I is the mutual information between the state of the system and the measurement outcome (depends on the error in the measurement)



Generalized second law

$$\langle \Delta s_{tot}[\{x_s\}] \rangle + \langle I \rangle \ge 0$$

We want to extend this type of results for a non-Markovian and continuous feedback control.

Our study is restricted to the case of a deterministic feedback (no measurement errors). Therefore the mutual information does not come into play. However we expect that

$$< e^{-\Delta S_{tot}} > \neq 1$$

Entropy production and FT for Langevin processes with non-Markovian, deterministic feedback

(T. Munakata and M.L. R., cond-mat: 1401.0771)

(We only focus on the behavior in a nonequilibrium steady state, NESS)

$$m\ddot{x} + \gamma\dot{x} - F(x) - F_{fb}(t) = \xi(t)$$
 e.g., $F_{fb}(t) \propto x(t - \tau)$

Consider a trajectory $\mathbf{X} \equiv \{x_t, \dot{x}_t\}$ during the time interval [-T,T]. Like in Markov systems, we seek to relate the heat or, equivalently, the change in the medium entropy

$$\Delta s_m[\mathbf{X}, \mathbf{X}_-] \equiv \beta \int_{-T}^{T} dt \left[\gamma \dot{x}_t - \xi_t \right] \dot{x}_t$$
$$= -\beta \int_{-T}^{T} dt \left[m \ddot{x}_t - F(x_t) - F_{fb}[\mathbf{X}, \mathbf{X}_-] \right] \dot{x}_t$$

to the time irreversibility of the trajectories, and thus to the probability of ${\bf X}$ and its time reversal (here, ${\bf X}_-$ denotes the trajectory for t<-T, e.g., in the time interval [-T- au,-T])

The probability of observing X for a given initial state $x_i \equiv (x_{-T}, \dot{x}_{-T})$ and a given past trajectory X_{-} is determined by the noise history in the time interval [-T,T] and given by

$$\mathcal{P}[\mathbf{X}|\mathbf{x}_{i},\mathbf{X}_{-}] \propto \left|\mathcal{J}\right| e^{-\beta \int_{-T}^{T} dt \,\mathcal{S}[\mathbf{X},\mathbf{X}_{-}]}$$

where $\mathcal{S}[\mathbf{X},\mathbf{X}_{-}] = \frac{1}{4\gamma} \Big[m\ddot{x}_{t} + \gamma \dot{x}_{t} - F(x_{t}) - F_{fb}[\mathbf{X},\mathbf{X}_{-}] \Big]^{2}$

is a generalized Onsager-Machlup functional and \mathcal{J} is the Jacobian of the transformation from the noise to x. It is independent of x (for $m \neq 0$): this is direct consequence of causality (the Jacobian matrix is lower triangular)

$$\textbf{Time-reversal:} \ \{x^{\dagger}(t), \dot{x}^{\dagger}(t)\} = \{x(-t), -\dot{x}(-t)\} \blacksquare \mathcal{P}[\mathbf{X}^{\dagger}|\mathbf{x}_{i}^{\dagger}, \mathbf{X}_{-}^{\dagger}]$$

In order to recover the heat from the logratio of the probabilities, one must define a new feedback force \tilde{F}_{fb} such that

$$\tilde{F}_{fb}[\mathbf{X}^{\dagger}, \mathbf{X}_{-}^{\dagger}]_{t \to -t} = F_{fb}[\mathbf{X}, \mathbf{X}_{-}]$$

e.g.
$$\tilde{F}_{fb}(t) \propto x(t+\tau)$$
 $\tau \rightarrow -\tau$

The «conjugate» dynamics is non-causal but the corresponding conditiona probability

$$\tilde{\mathcal{P}}[\mathbf{X}^{\dagger}|\mathbf{x}_{i}^{\dagger},\mathbf{X}_{-}^{\dagger}] \propto \left|\tilde{\mathcal{J}}[\mathbf{X}]\right| e^{-\beta \int_{-T}^{T} dt \,\tilde{\mathcal{S}}[\mathbf{X}^{\dagger},\mathbf{X}_{-}^{\dagger}]}$$

with

$$\tilde{\mathcal{S}}[\mathbf{X}^{\dagger}, \mathbf{X}_{-}^{\dagger}] = \frac{1}{4\gamma} \Big[m\ddot{x}_{t} - \gamma \dot{x}_{t} - F(x_{t}) - \tilde{F}_{fb}[\mathbf{X}^{\dagger}, \mathbf{X}_{-}^{\dagger}]_{t \to -t} \Big]$$

is a well-defined mathematical object !

On the other hand, the Jacobian matrix is no longer lower-triangular and $\tilde{\mathcal{J}}[X]$ is in general a nontrivial (positive) functional of the path.

>
$$\Delta s_m[\mathbf{X}, \mathbf{X}_-] = \ln \frac{\mathcal{P}[\mathbf{X}|\mathbf{x}_i, \mathbf{X}_-]}{\tilde{\mathcal{P}}[\mathbf{X}^{\dagger}|\mathbf{x}_i^{\dagger}, \mathbf{X}_-^{\dagger}]} + \ln \frac{\tilde{\mathcal{J}}[\mathbf{X}]}{\mathcal{J}}$$

and we define the total fluctuating entropy production (which measures the actual irreversibility of the trajectory) by $\frac{1}{1-1}$

$$R_{cg}[\mathbf{X}] \equiv \ln \frac{\mathcal{P}_{st}[\mathbf{X}]}{\tilde{\mathcal{P}}_{st}[\mathbf{X}^{\dagger}]}$$

By construction $\langle e^{-R_{cg}[\mathbf{X}]} \rangle_{st} = 1$ \longrightarrow $\langle R_{cg}[\mathbf{X}] \rangle_{st} \ge \mathbf{0}$

Asymptotic relations: when 2T is much larger than the time constant characterizing the non-Markovian feedback (e.g. τ), one can neglect terms non extensive in time when computing expectation values

$$\checkmark \quad \langle R_{cg}[\mathbf{X}] \rangle_{st} \sim \langle \Delta s_m[\mathbf{X}] \rangle_{st} - \langle \ln \frac{\tilde{\mathcal{J}}[\mathbf{X}]}{\mathcal{J}} \rangle_{st}$$

Defining the rates

$$\dot{S}_m = \lim_{T \to \infty} \frac{1}{2T} \langle s_m[\mathbf{X}] \rangle_{st}$$
$$\dot{S}_J = \lim_{T \to \infty} \frac{1}{2T} \langle \ln \tilde{\mathcal{J}}[\mathbf{X}]/J \rangle_{st}$$



Expression of the Jacobian

$$\tilde{\mathcal{J}}[\mathbf{X}] = \det \delta \xi(t) / \delta x(t')$$
 associated to the

conjugate Langevin equation

$$m\ddot{x} + \gamma\dot{x} - F(x) - \tilde{F}_{fb}(t) = \xi(t)$$

$$\tilde{\mathcal{J}}[\mathbf{X}] = \det\left[m\frac{\partial^2}{\partial t^2} + \gamma\frac{\partial}{\partial t} - \frac{\delta\tilde{F}_{tot}(t)}{\delta x(t')}\right]$$

$$\tilde{\mathcal{J}}[\mathbf{X}] = \mathcal{J} \exp \operatorname{Tr} \ln[\delta_{t-t'} - \tilde{M}_{tt'}]$$
$$= \mathcal{J} \exp -\sum_{n=1}^{\infty} \frac{1}{n} \int_{-T}^{T} dt \left\{ \underbrace{\tilde{M} \circ \tilde{M} \circ \dots \tilde{M}}_{n \text{ times}} \right\}_{tt}$$

where

$$\mathbf{re} \quad \tilde{M}(t,t') = \{ G \circ \tilde{F}'_{tot} \}_{tt'} \equiv \int_{-T}^{T} dt'' \ G(t-t'') \tilde{F}'_{tot}(t'',t')$$

G(t) is the Green function for the inertial and dissipative terms in the Langevin equation : $G(t) = \gamma^{-1} [1 - e^{-\gamma t/m}] \Theta(t)$

(see e.g. C. Aron et al., J. Stat. Mech. P11018, 2010)

For linear systems, the Jacobian becomes path-independent !

The operation \circ becomes a convolution and $\ln \tilde{\mathcal{J}}/J$ is proportional to 2T

In the long-time limit, the asymptotic rate $\dot{S}_J = \lim_{T \to \infty} \frac{1}{2T} \langle \ln \tilde{\mathcal{J}}[\mathbf{X}]/J \rangle_{st}$ is then obtained as a Laplace transfom :

$$\dot{S}_{\mathcal{J}} = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds \, \ln[1 - \tilde{M}(s)]$$
$$= -\frac{1}{2\pi i} \sum_{n=1}^{\infty} \frac{1}{n} \int_{c-i\infty}^{c+i\infty} ds \, [\tilde{M}(s)]^n$$

where
$$s = c + i\omega$$
, $\tilde{M}(s) \equiv \int_{-\infty}^{\infty} dt \, \tilde{M}(t) e^{-st} = G(s) \tilde{F}_{tot}'(s)$

$$G(s) = (ms^2 + \gamma s)^{-1}$$
 (bilateral Laplace !!!)

This can be also written as

$$\dot{S}_{\mathcal{J}} = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds \, \ln \frac{G(s)}{\tilde{\chi}(s)}$$

where
$$\tilde{\chi}(s) = [G(s)^{-1} - \tilde{F}'_{tot}(s)]^{-1} = [ms^2 + \gamma s - \tilde{F}'_{tot}(s)]^{-1}$$

Application to a linear stochastic delay equation

$$m\ddot{x} + \gamma\dot{x} + ax + bx(t - \tau) = \xi(t)$$

 $F_{fb}(t) = -bx(t - \tau)$ the feedback force at time t depends on the position at a previous time (no measurement errors)

Remark: at first order $-bx(t - \tau) \approx -bx(t) + (b\tau)\dot{x}(t)$ and one recovers a Markovian dynamics with a velocity-dependent force (standard feedback cooling):

$$m\ddot{x} + (\gamma + \gamma')\dot{x} + (a + b)x = \xi(t)$$
 with $\gamma' = -b\tau$

As a general rule, stochastic time-delayed systems may be regarded as systems with an infinite number of degrees of freedom => infinite hierarchy of Fokker-Planck equations.

$$\partial_t p(x, v, t) = -\partial_x [vp(x, v, t)] + \frac{1}{m} \partial_v \Big[[ax + \gamma v] p(x, v, t) \\ + b \int_{-\infty}^{+\infty} dx_\tau x_\tau p(x, v, t; x_\tau, t - \tau) + \frac{\gamma T}{m} \partial_v p(x, v, t) \Big]$$

However, for a linear system with Gaussian white noise, all stationary probability distributions are Gaussian and can be determined exactly. In particular, $1 + (a+b)a^2 = -2$

$$p_{st}(x,v) \propto e^{-\frac{1}{2}\left[\frac{(a+b)x^2}{T_{eff}^{(x)}} + \frac{mv^2}{T_{eff}^{(v)}}\right]}$$

where $T_{eff}^{(x)} \equiv (a+b) < x^2 >_{st}$ and $T_{eff}^{(v)} \equiv m < v^2 >_{st}$

are effective temperatures whose expressions are obtained by solving the differential equations for the time-correlation functions in the interval $0 \le t \le \tau$

The existence and stability of the stationary solution depends on the delay and on the values of the other parameters. For simplicity, we only consider the case where a NESS exists for *all* values of the delay:



Path probability in the stationary state

The probability of a path is also Gaussian and can be calculated exactly in the overdamped limit m=0

$$\mathcal{P}[\{x_s\}_0^t] \propto \exp\{-\frac{1}{2} \int_0^t ds \int_0^t ds' x(s) S_{xx}^{-1}(s-s') x(s')\}$$

where $S_{xx}^{-1}(t)$ is the operator inverse of the time correlation function $S_{xx}(t) = \langle x(0)x(t) \rangle_{st}$ in the time interval [0,t], defined by

$$\int_{0}^{t} ds'' S_{xx}(s - s'') S_{xx}^{-1}(s'' - s') = \delta(s - s')$$
$$S_{xx}(t) = Ae^{-\omega_{0}|t|} + Be^{\omega_{0}|t|} \quad \text{for} \quad t \le \tau$$

This integral equation can be solved analytically (it is in fact easier to consider the corresponding discretized matrix equation, generalizing a classical result of Doob (1942) for the Ornstein-Uhlenbeck process). The result is

with

$$\mathcal{P}[\{x_s\}_0^t] \propto \exp\{-\frac{1}{4T}\int_0^t ds[\dot{x}_s + \omega_0 x_s]^2 - \frac{\omega_0}{2T}\frac{[Ae^{-\omega_0 t}x_0 - Bx_t]^2}{A^2 e^{-2\omega_0 t} - B^2}\}$$

which is «almost» an Onsager-Machlup action functional, with an additional dependence of the initial and final states that reflects the non-Markovian character of the process.

The path probability can then be computed in the time interval $\tau \leq t \leq 2\tau$ using

$$\mathcal{P}[\{x_s\}_{\tau}^t] = \mathcal{P}[\{x_s\}_{\tau}^t | \{x_s\}_{0}^{\tau}] \mathcal{P}[\{x_s\}_{0}^{\tau}]$$

with

$$\mathcal{P}[\{x_s\}_{\tau}^t | \{x_s\}_{0}^{\tau}] \propto e^{-\frac{\beta}{4\gamma} \int_{\tau}^t ds \left[\gamma \dot{x}_s + ax_s + bx_{s-\tau}\right]^2}$$

etc...

Entropy production: In the stationary state, the probabilities of a trajectory and its time-reversal are identical !

$$\square \square \frac{\mathcal{P}[\mathbf{X}]}{\mathcal{P}[\mathbf{X}^{\dagger}]} = 0$$

This ratio cannot be a proper definition of the entropy production !

On the other hand
$$R_{cg}[\mathbf{X}] \equiv \ln \frac{\mathcal{P}_{st}[\mathbf{X}]}{\tilde{\mathcal{P}}_{st}[\mathbf{X}^{\dagger}]}$$
 is non zero !

For instance, in the long-time limit, one finds

$$\lim_{T \to \infty} \frac{1}{2T} \langle R_{cg}[X] \rangle = \frac{b^2}{2a} [1 - e^{-2a\tau} + 2a\tau e^{-2a\tau}] + \mathcal{O}(b^3)$$

Calculation of the Jacobian for the conjugate, non-causal Langevin equation :

$$m\ddot{x} + \gamma\dot{x} + ax + bx(t+\tau) = \xi(t)$$

$$\dot{S}_{\mathcal{J}} = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds \, \ln \frac{G(s)}{\tilde{\chi}(s)}$$

$$G(s) = (ms^2 + \gamma s)^{-1}$$
$$\tilde{\chi}(s) = [ms^2 + \gamma s + a + be^{s\tau}]^{-1}$$

Rem: There are 2 poles on the I.h.s. of the complex s-plane and an infinity of poles on the r.h.s. = signature of non-causality



$$\dot{S}_{\mathcal{J}} = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds \ln \frac{ms^2 + \gamma s + a + be^{s\tau}}{ms^2 + \gamma s}$$

 τ -expansion :

$$\dot{S}_{\mathcal{J}} = \frac{b}{m}\tau - \frac{b\gamma}{2m^2}\tau^2 + \frac{b(\gamma^2 - am - 4bm)}{6m^3}\tau^3 + \mathcal{O}(\tau^4)$$

I) Check of the generalized second law $S_m \geq S_{\mathcal{T}}$ One has $\dot{S}_m = rac{\gamma}{m} [\beta T_{eff}^{(v)} - 1]$ where $T_{eff}^{(v)} \equiv m < v^2 >_{st}$ 2) Check of the $\dot{S}_{m} - \dot{S}_{J}$ 0.05 asymptotic relation Rates in the NESS 0 $\langle \frac{\mathcal{J}[\mathbf{X}]}{I} e^{-\Delta s_{tot}[\mathbf{X}]} \rangle_{st} \sim \mathcal{O}(1)$ -0.05 Ś m -0.1 $\dot{S}_{\mathcal{J}} = \lim_{T \to \infty} \frac{1}{2T} \ln \langle e^{-\Delta s_{tot}} \rangle_{st}$ $\dot{S}^{}_{J}$ Positive feedback (b<0) -0.15 -0.2 5 The rates \dot{S}_m , $\dot{S}_{\mathcal{J}}$ and $\dot{R}^{\tau} = \dot{S}_m - \dot{S}_{\mathcal{J}}$ as a function of τ for $m = 1, \gamma = 1, a = 0.5$ and b = -0.25. The open circles are obtained from the equation $\dot{S}_{\mathcal{J}} \approx -\frac{1}{2T} \ln \langle e^{-\Delta s_{tot}} \rangle_{st}$ using T = 10 and averaging over 10^6 independent simulations of the Langevin equation with Heun's method and a time step $\Delta t = 10^{-3}$.

Conclusion

We have extended the framework of stochastic thermodynamics to Langevin systems submitted a continuous non-Markovian (e.g. timedelayed) feedback control.

By studying the nature of the time-reversal breaking in the action functional of the path space measure, we have identified the unusual mathematical mechanism that contributes to the positivity of the entropy production.