Théorèmes et relations de fluctuations enjeux expérimentaux et théoriques.

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Introduction

There are only a very few results valid for systems driven arbitrarily far from equilibrium:

- Fluctuation Theorems / Fluctuation Relations,
- Jarzynski and Crooks equalities.

These results deal with:
Chaos & Dyn. Systems / Non-eq. Stat. Phys / Thermodynamics

Outline

Fluctuation Relations

For a given quantity $A(t)$, and a time τ :

$$A_\tau(t) = \frac{1}{\tau}\int_t^{t+\tau} A(t)dt'$$

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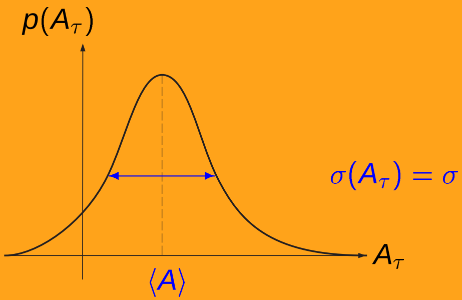
$\forall\tau$ in transient states starting at equilibrium (TFT)
for $\tau \to \infty$ in steady states (SSFT)

A simple picture...

$$A_\tau(t) = \frac{1}{\tau}\int_t^{t+\tau} A(t)dt'$$



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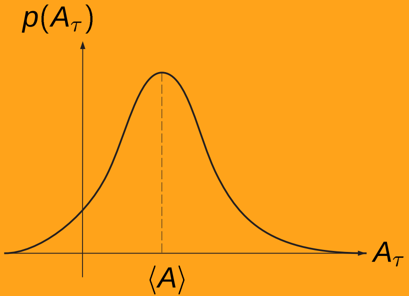
$$\ln\left(\frac{p(A_\tau = +a)}{p(A_\tau = -a)}\right)$$



FT/FR examine the symmetry of the pdf $p(A_\tau)$ of $\{A_\tau\}_\tau$ around 0 :

$$p(A_\tau = +a) \qquad \text{vs.} \qquad p(A_\tau = -a)$$

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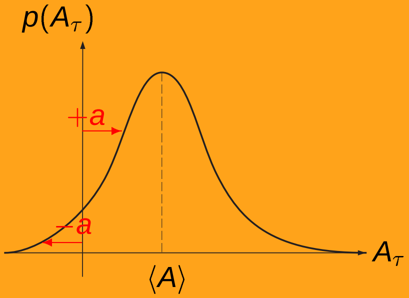

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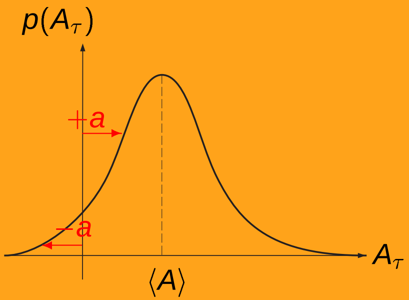
$$\ln\left(\frac{p(A_\tau = +a)}{p(A_\tau = -a)}\right) \propto a$$



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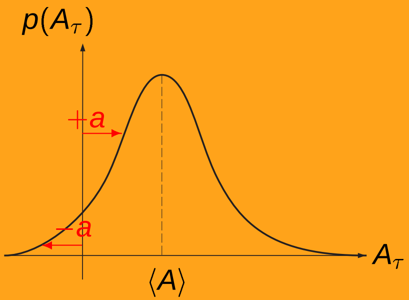

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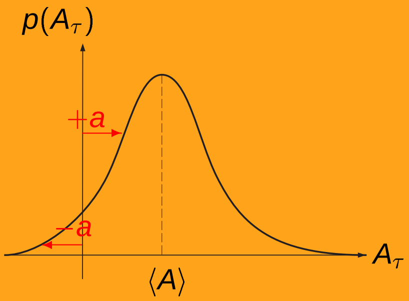
$$\ln\left(\frac{p(A_\tau\!=\!+a)}{p(A_\tau\!=\!-a)}\right) = \Gamma_A a\tau$$



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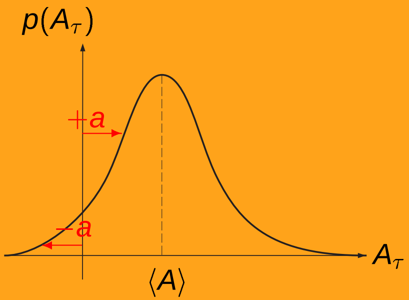

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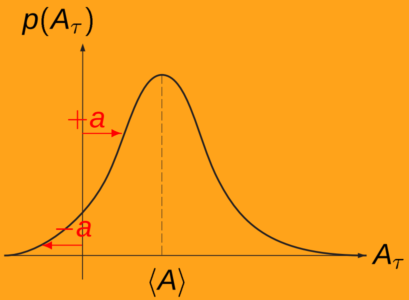

valide

- $\forall\tau$ si transitoire à partir d'un état d'équilibre (TFT)
- pour $\tau\to\infty$ si état stationnaire hors équilibre (SSFT)

History : 2 theorems

1993: first observation (A=shear stress)

Evans, Cohen, Morriss - Phys. Rev. Lett. **71** p2401 (1993) (times cited: 220)

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Gallavotti, Cohen - J. Stat. Phys. **80** (5-6) p931-970 (1995) (times cited: 208)

Gallavotti - Math. Phys. Electron. J. **1** p12 (1995) (times cited: unknown)

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1994: Evans-Searles derivation (TFT)

Evans, Searles - Phys. Rev. E **50** (2) p1645 (1994) (times cited: 103)

Evans, Searles - Adv. Phys. **51** p1529 (2002) (times cited: 77)

Evans, Searles, Rondoni - Phys. Rev. E **71** 056120 (2005) (times cited: 7)

GC Fluctuation Theorem : a statement

We define:

$\sigma \equiv$ phase space contraction rate (of a dynamical system)

$\sigma_\tau \equiv \frac{1}{\tau} \int_t^{t+\tau} \sigma(t')dt'$

$\sigma_+ \equiv \lim_{\tau\to\infty} \sigma_\tau$, asymptotic average value

$y \equiv \frac{\sigma_\tau}{\sigma_+}$, reduced variable, of p.d.f. $p_\tau(y)$

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"Gallavotti-Cohen FT"

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Chaotic Hypothesis : mixing of trajectory is strong enough in phase space. ("Anosov like systems", less restrictive...)

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Valid at arbitrary distance from equilibrium
(no need to be on the linear response branch)

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Green-Kubo relations can be derived from
$\{\mathrm{FT} + \text{central limit theorem}\}$ (both FTs)

Stochastic systems

Different derivations

Kurchan - J. Phys. A **31** p3719 (1998)

Lebowitz, Spohn - J. Stat. Phys. **95** p333 (1999)

Crooks - Phys. Rev. E **60** p2721 (1999)

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Langevin equation

Farago - J. Stat. Phys. **107** p781 (2002)

van Zon, Cohen - Phys. Rev. Lett. **91** 110601 (2003)

van Zon, Cohen - Phys. Rev. E **67** 046102 (2003)

van Zon, Cohen - Phys. Rev. E **69** 056121 (2004)

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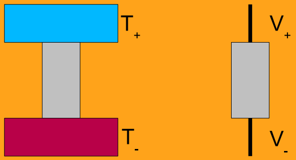

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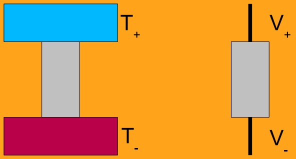

Fourier's law / Fick's law / Ohm's law
Numerically interesting : thermostated systems and their variants

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History : experiments

Deterministic systems

Ciliberto, Laroche J. Physique **74** p2694 (1998) (convection) (times cited: 40)

Aumaitre, Fauve *et al* - Eur. J. Phys. B **19** p449 (2001) (numer.) (times cited: 37)

Aumaitre, Fauve - Europhysics Letters **12** p822 (2003) (convection) (times cited: 4)

Feitosa, Menon - Phys. Rev. Lett. **92** (2004) (granular materials) (times cited: 20)

Ciliberto, Garnier *et al* - Physica A **340** p240 (2004) (turbulence) (times cited: 9)

Langevin dynamics

Wang, Sevick *et al* - Phys. Rev. Lett. **89** 050601 (2002) (trapped bead) (times cited: 95)

Carberry, Reid *et al* - Phys. Rev. Lett. **92** 140601 (2004) (trapped bead) (times cited: 26)

Garnier, Ciliberto - Phys. Rev. E **71** (6) 060101 (2005) (resistor) (times cited: 4)

Turbulence

turbulent Rayleigh-Bénard convection
- heat flux measured indirectly Ciliberto, Laroche J. Physique **74** p2694 (1998)

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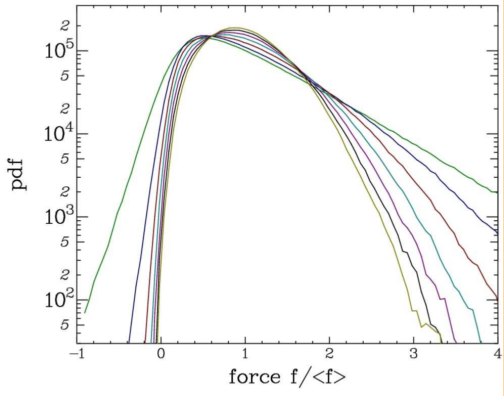
pdfs are non-Gaussian.

An experiment : force in a jet



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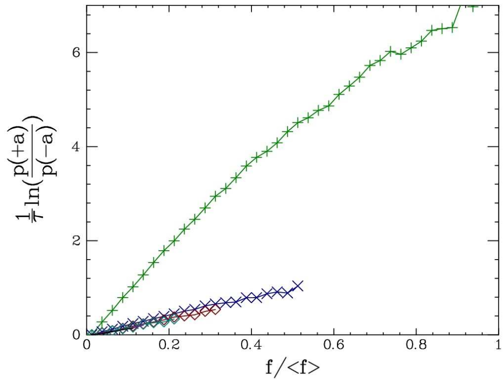

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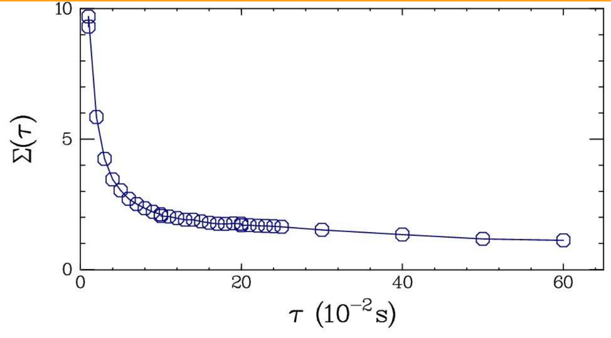

Chaos ?

- Electroconvection in nematics

  Goldburg et al, Phys. Rev. Lett. **87** 245502 (2001)

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  No negative events!

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  Garnier, Wòjcik Phys. Rev. Lett. **96** 114101 (2006)

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- Non-chaotic systems

  Lepri et al. J. Stat. Phys. **99** p857 (2000)

  FT works on transients.

Trapped beads

A Langevin equation, with external force $F_0 = -k(x - x_0)$

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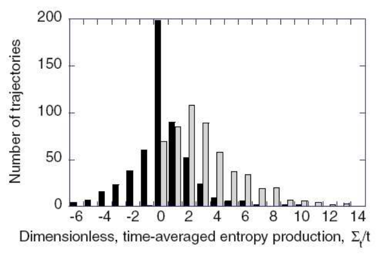

$\tau = 10^{-2}$s
$\tau = 2$s

Other systems described by Langevin dynamics

- Resistor with non-zero intensity.

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- Brownian harmonic ocillator (torsion pendulum)

  Douarche et al - Phys. Rev. Lett. **97** 140603 (2006)

  Joubaud et al - (under writing) this afternoon

Some (experimental) problems

Central limit theorem $\rightsquigarrow \sqrt{\langle y^2 \rangle - \langle y \rangle^2}$ is decreasing as $\frac{1}{\sqrt{\tau}}$

so the large τ limit is hard to get experimentally.

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The closer to equilibrium, the harder... the asymmetry hides in the noise.

Mean $\langle A \rangle$ or $\langle y \rangle = 1$ cannot be shifted at will...

The slope is fixed by the FT

For a Gaussian distribution, TF/FR implies

$$\frac{2\langle A\rangle}{\sigma_A} = 1$$

(using correct units of course).

Sinaï scaling function

$p_\tau(y)$ is the pdf of reduced variable $y \equiv \frac{\sigma_\tau}{\sigma_+}$ Then for large times $\tau \to \infty$, $\exists!$ function $\xi(y)$ such that

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Fluctuation Theorem additionally says that:

$$\ln\left(\frac{p_\tau(y=+a)}{p_\tau(y=-a)}\right) = \pi_+\tau a$$

so

$$\xi(a) - \xi(-a) = a\sigma_+$$

Limit of large τ is trivial ?

If correlations decrease exponentially $\propto e^{-t/\tau_\alpha}$, then when $\tau = 2N\tau_\alpha \to \infty$, one can write $A_\tau = \sum_{i=1}^{N} A_i(t_i)$ with $A_i(t_i) = \frac{1}{2\tau_\alpha} \int_{t_i}^{t_{i+1}} A(t')dt'$ and $t_i = 2i\tau_\alpha$.

And the A_i are independant.

So $p_\tau(y)$ tends to a Gaussian (CLT), and FT is trivial.

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And if $\exists$ algebraic correlations (the case of turbulence) ?
Is it more interesting ?

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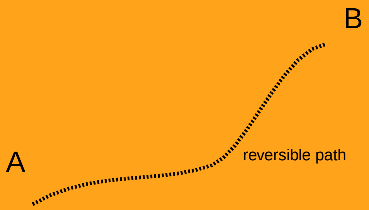

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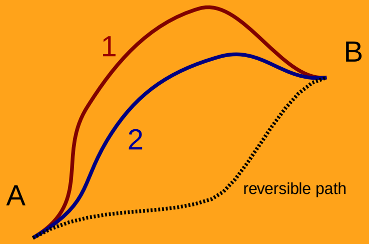

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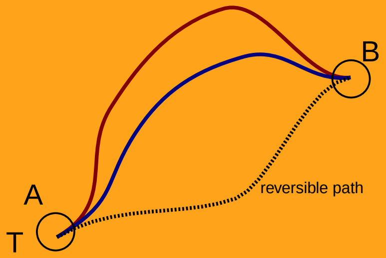

Jarzynski equality : comments

$$\langle \exp\left(-\beta W_J\right)\rangle = \exp\left(-\beta \Delta F_{AB}\right)$$

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  But fluctuations prevent good convergence...
- previous work:
  Born (1920, infinitely slow) Swanzig (1954, infinitely fast)

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- One usually writes $W_{AB} = \triangle F + W^d_{AB}$.
- if $p(W_{AB})$ is Gaussian, then JE says $\triangle F = \langle W_{AB} \rangle - \frac{1}{2}\sigma_{W_{AB}}$.

Bibliography

Jarzynski equality:

Jarzynski Phys. Rev. E **56** (5) p5018-5035 (1997) (times cited: 128)

Jarzynski Phys. Rev. Lett. **78** (14) p2690-2693 (1997) (times cited: 290)

Crooks J. Stat. Phys. **90** (5-6) p1481-1487 (1998) (times cited: 65)

Zwanzig J. Chem. Phys. **22** (8) p1420-1426 (1954) (times cited: 1039)

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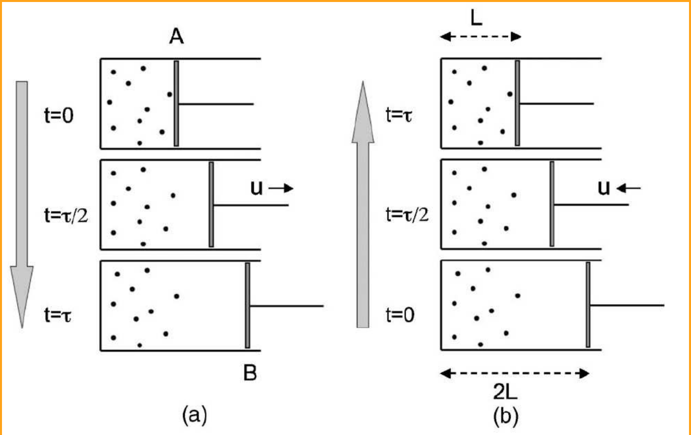
Crooks relation:

Crooks Phys. Rev. E**60** (3) p2721-2726 (1999) (times cited: 92)

Bennett J. Comput. Phys. **22** (2) p245-268 (1976) (times cited: 362)

e.g.: piston expansion (forward = A-B)



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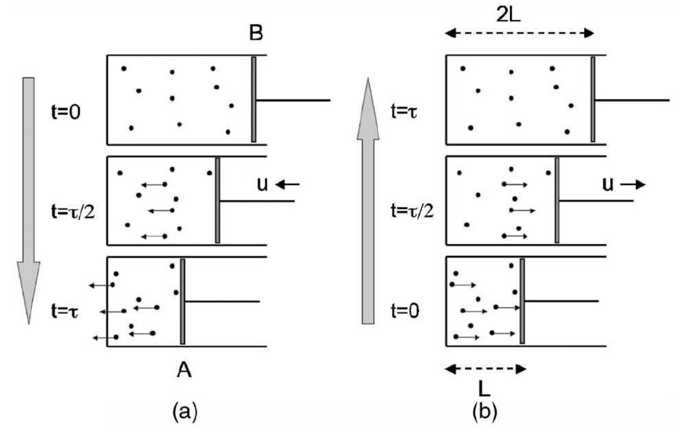

e.g.: piston compression (backward = B-A)

For the forward process (expansion), the heaviest contributions to the exponential average $\langle e^{-\beta W} \rangle_{AB}$ are from the (exotic and very rare) realizations of the reverse process where there is an "antishock" wave.

Jarzynski equality : comments (bis)

$$\langle \exp\left(-\beta W\right)\rangle = \int_A^B \mathrm{d}W\, p(W) e^{-\beta W} = \int_A^B \mathrm{d}W\, g(W)$$

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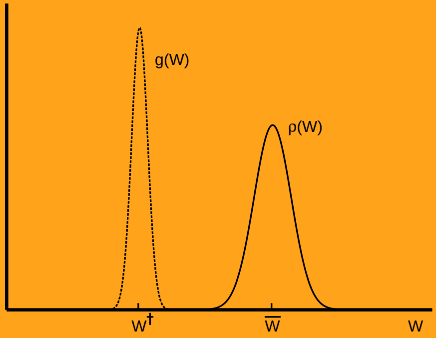

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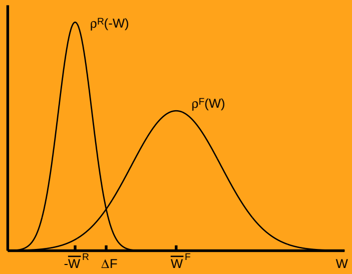

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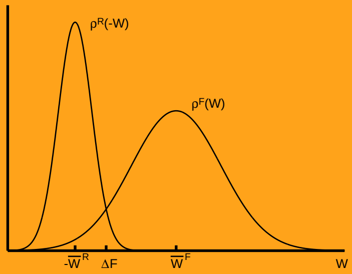

Number of realizations needed for convergence ?

$$N^F \simeq \exp(\beta \bar{W}_d^R)$$

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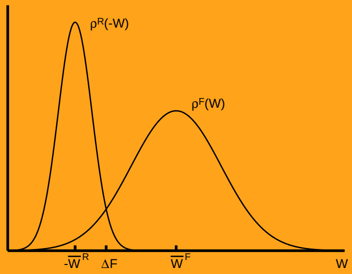

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Of the 2 processes $A - B$ (F) and $B - A$ (R), the convergence of JE will be more rapid for the more dissipative one.

Experiments

Liphardt et al. Science **296** p1832 (2002) (DNA)

Collin et al. Nature London **437** p231 (2005) (DNA)

Douarche et al Europhys. Lett. **70** 593 (2005) (Browian oscillator)

Douarche et al J. Stat. Mech.: Theory Exp. P09011 (2005) (Browian oscillator)

Crooks Relation

$$\frac{p_F(+\omega)}{p_R(-\omega)} = e^{+\omega}$$

p_F is the pdf of ω.
p_R is the pdf of ω when the system is driven in a time-reversed manner.
as a consequence

$$\langle e^{-\omega} \rangle = 1$$

Jarzynski follows from the choice

$$\omega = -\beta \triangle F + \beta W = W^d$$

and starting at equilibrium (!).

Conclusion

- FTs give indications for searching FRs.
- JE can be exploited, but still hard to master.
- Many "new" results, and a growing number of exprimental observations.
- Many differents points of view that can not incompatible.

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$$m\frac{d^2x}{dt^2} = -\alpha\frac{dx}{dt}$$

α : coefficient de frottement fluide (Stokes)

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chaleur : $Q_\tau = W_\tau - \triangle U$ $\qquad U = \frac{1}{2}k(x - x^*)^2$

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Power injected in the R//C system: $\mathcal{P}_{in} = U.I$

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$\mathcal{P} \sim$ *distance from equilibrium* $\quad \mathcal{P}/k_B T \sim$ *entropy production*

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