Lagrangian Pictures of Non-Equilibrium

Workshop : Steady-states, fluctuations and dynamics of non-equilibrium systems

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Introduction

The quest of a theory of non equilibrium systems progress step by step...

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Lagrange : Fluid dynamics should be simpler in the Lagrangian frame moving with the fluid

Main result

All systems are in equilibrium in the Lagrangian frame of it's mean local velocity
Chetrite, R., Gawędzki, K. : *Eulerian and Lagrangian pictures of non-equilibrium diffusions* , arXiv :0905.4667

Equilibrium system : Caracterization

The gibbs density is an invariant reversible density (i.e for Markov process : detailed balance)

$$\exp(-\beta H(x))P_s^t(x,y) = \exp(-\beta H(y))P_s^t(y,x)$$

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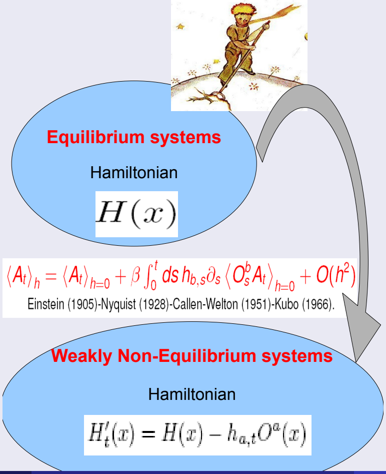
Weakly Non-Equilibrium : Fluctuation-Dissipation Theorem(FDT)



Far from equilibrium system : Caracterization

by example : Chetrite, R., Gawędzki, K. : *Fluctuation relations for diffusion process.* Commun. Math. Phys.(2008)

For a markovian system

$$\rho_0(x)P^T(x \to y, W) = \rho_0^r(y)P^{r,T}(y \to x, -W)\exp(W)$$

with :

- ρ_0 the initial density of the forward process.
- ρ_0^r the initial density of the backward process.
- $P^T(x \to y, W)$ is the transition probability with the constraint $W_T = W$ fixing the value of a functional W_T linked to the entropy production.

The stumbling block is the choice of the backward process relative to the forward process.

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Fluctuation relation

- Jarzynski type relation : $\langle \exp(-W_T) \rangle = 1$
- Gallavotti-Cohen type relation : If we have the large deviation regime for W_T : $P^T(x \to y, W = Tw) \sim \exp(-TZ(w))$:

$$Z(w) + w = Z^r(-w)$$

Mathematical setup for describe non-equilibrium dynamics

- Deterministic finite-dimensionnal dynamical systems
- Deterministic infinite-dimensionnal systems
- Random finite-dimensionnal dynamical systems
  (with noise modeling the environment)
- Random infinite-dimensional dynamical systems.
  (like developped turbulence).

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Markovian diffusion process

$$\dot{x} = u_t(x) + \eta_t(x)$$

$u_t(x)$: deterministic(drift) vector field
$\eta_t(x)$: white noise with Stratonovich convention with zero mean and :
$\langle \eta_t^i(x)\,\eta_s^j(y)\rangle = 2\delta(t-s)\,D_t^{ij}(x,y)$

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Exemple : Langevin-Kramers dynamics $u_t(x) = -\Gamma_t \nabla H_t + \Pi_t \nabla H_t + G_t(x)$ and $D_t(x, y) = \frac{1}{\beta}\Gamma_t$.

Instantaneous density function $\rho_t(x) = \langle \delta(x_t - x) \rangle$

- Its evolution is given by the continuity equation (i.e Focker-Planck equation) :

$$\partial_t \rho_t \; + \; div(j_t) = 0$$

with the probability current :
$j_t = (\widehat{u}_t - d_t \nabla)\rho_t$ with $\widehat{u}^i_t = u^i_t - r^i_t$, $r^i_t(x) = \partial_{y^i} D^{ij}_t(x,y)|_{y=x}$ and $d_t(x) = D_t(x,x)$

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- We introduce the "hydrodynamic" velocity v_t such that $j_t(x) = \rho_t(x) v_t(x)$.
It is also the mean symmetric velocity of the process conditioned to be in x :
$v_t(x) = \frac{\lim_{h \to 0} \left\langle \frac{x_{t+h} - x_{t-h}}{2h} \delta(x_t - x) \right\rangle}{\langle \delta(x_t - x) \rangle}$

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Non Equilibrium Steady State (NESS)

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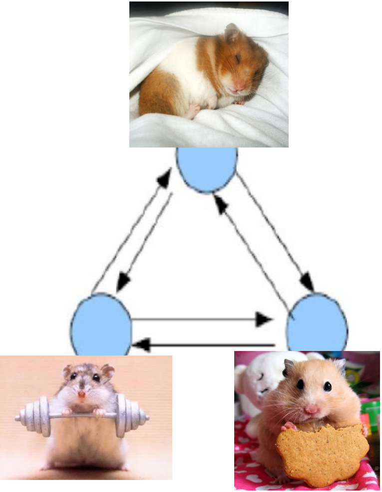
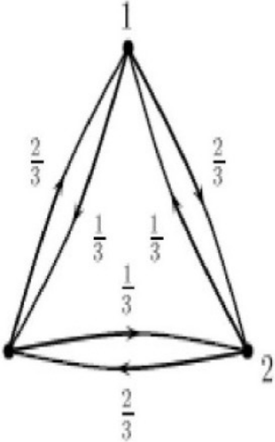
- The process takes the Equilibrium form (non-homogeneous ! !) :

$$\dot{x} = d_t(x) \nabla \ln(\rho) + r_t(x) + \eta_t(x)$$

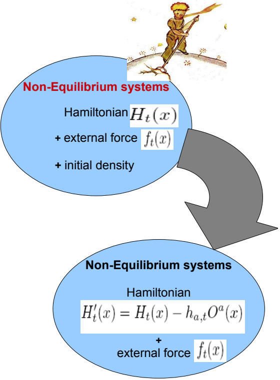
Analogies with 3-state Markov chain : the hamster life





Lagrangian picture : the clue of the modified fluctuation dissipation theorem around a NESS

General idea



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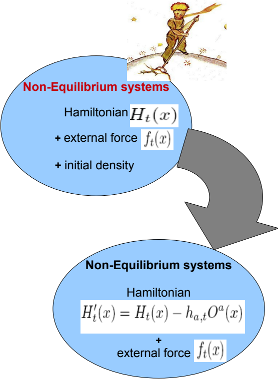

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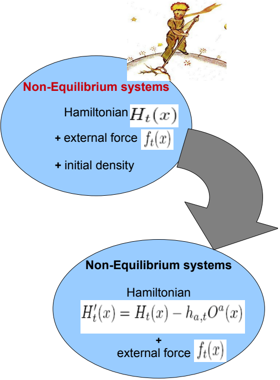

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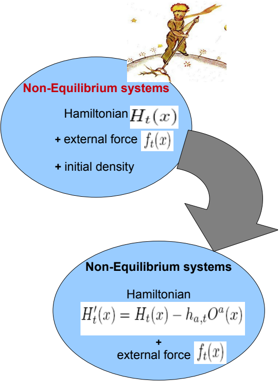

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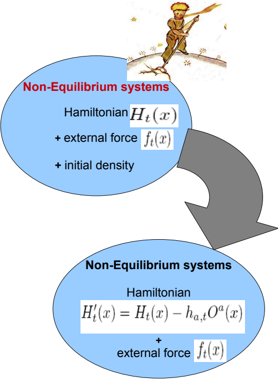

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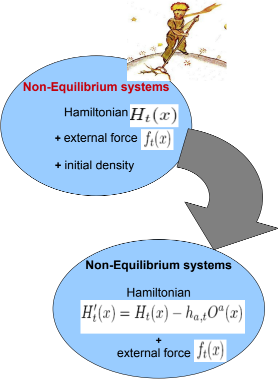

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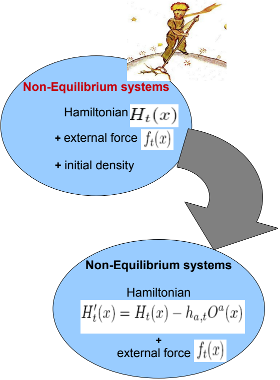

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  In the Lagrangian frame of the mean local velocity v^i the FDT takes the usual form

Experimental validation of the MFDT around a NESS

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For a colloidal particle (diameter $1\mu m$) silicon bead trapped on a circular orbit (radius $4\mu m$) by an optical tweezer. System described by an equation for the angle :
$\frac{d\theta}{dt} = -B\cos(\theta) + F + \eta$ with $B = 0.87\ s^{-1}$, $F = 0.85 s^{-1}$ and $d = 0.025\ s^{-1}$.

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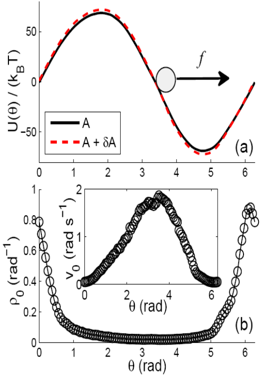

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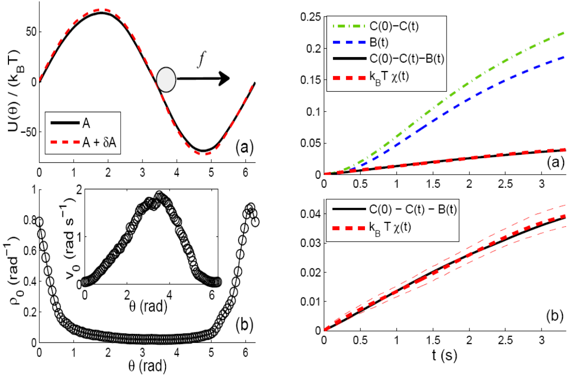

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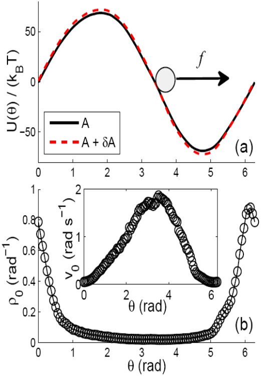

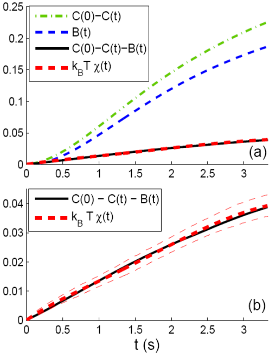

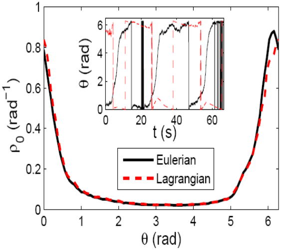

Lagrangian picture : the technical story

Lagrangian frame of mean local velocity

- Let $x \to \Phi_t(x)$ be the Lagrangian flow of v :

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Step 1 : Freeze of the instantaneous density in the Lagrangian frame to the initial time value of the Eulerian frame density

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$$\widetilde{\rho}_t(x) = \left\langle \delta \left(\Phi_t^{-1}(x_t) - x \right) \right\rangle = \langle \delta \left(x_t - \Phi_t(x) \right) \rangle \det \left(\nabla \Phi_t(x) \right) = \rho_t \left(\Phi_t(x) \right) \det \left(\nabla \Phi_t(x) \right)$$

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- 2) the solution of the Cauchy problem for continuity equation is :
$\rho_t(x) = \int dy \delta\left(x - \Phi_t(y)\right) \rho_{t_0}(y) = \det^{-1}\left(\nabla \Phi_t\left(\Phi_t^{-1}(x)\right)\right) \rho_{t_0}\left(\Phi_t^{-1}(x)\right)$

Lagrangian picture : the technical story

Lagrangian frame of mean local velocity

- Let $x \rightarrow \Phi_t(x)$ be the Lagrangian flow of v :

$$\partial_t \Phi_t(x) = v_t(\Phi_t(x)) \text{ and } \Phi_{t_0}(x) = x$$

- In the Lagrangian frame of v the process x_t becomes

$$\widetilde{x}_t = \Phi_t^{-1}(x_t)$$

Step 1 : Freeze of the instantaneous density in the Lagrangian frame to the initial time value of the Eulerian frame density

- 1)
$\widetilde{\rho}_t(x) = \left\langle \delta\left(\Phi_t^{-1}(x_t) - x\right)\right\rangle = \langle \delta\left(x_t - \Phi_t(x)\right)\rangle \det\left(\nabla \Phi_t(x)\right) = \rho_t\left(\Phi_t(x)\right) \det\left(\nabla \Phi_t(x)\right)$
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   - $\Rightarrow \widetilde{\rho}_t(x) = \rho_{t_0}(x)$

Step 2 : Equilibrium form for the diffusion process in the Lagrangian frame ; Long but trivial calculus

$$\dot{\widetilde{x}} = \widetilde{d}_t(\widetilde{x})\nabla \ln(\rho_{t_0}) + \widetilde{r}_t(\widetilde{x}) + \widetilde{\eta}_t(\widetilde{x})$$

with :

- $\widetilde{\eta}^i_t(\widetilde{x}) = \partial_k \left(\Phi_t^{-1}\right)^i (x)\eta^k_t(x)$
- and then : $\widetilde{D}^{ij}_t(\widetilde{x},\widetilde{y}) = \partial_k \left(\Phi_t^{-1}\right)^i (x) D^{kl}_t(x,y)\partial_l \left(\Phi_t^{-1}\right)^j (y)$

Examples of Non Equilibrium diffusion

Relaxing systems with initial quench from temperature T_i to T_f

$\dot{x} = -\Gamma \nabla H + \eta$ with $d = \Gamma T_f$ and the initial density $\rho_i(x) = \frac{\exp(-\frac{H(x)}{T_i})}{Z_i}$

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Overdamped unidimensional harmonic oscillator $H = \frac{k}{2}x^2$

- Effective temperature in the Eulerian frame :
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- Mean local velocity : $v_t(x) = -k\Gamma \frac{1}{1+\frac{T_f}{T_i - T_f}\exp(2k\Gamma t)} x$
- Lagrangian coordinate : $\widetilde{x}_t = x_t \frac{\exp(k\Gamma t)}{1+\frac{T_f}{T_i - T_f}\exp(2k\Gamma t)}$

Linear stochastic equation in the NESS : $\dot{x} = Mx + \eta$ with $\langle \eta_t \eta_s \rangle = 2D\delta(t-s)$

- Invariant density :
  $\rho(x) = \frac{\exp(-\frac{1}{2} x C^{-1} x)}{Z}$ with $C = 2\int_0^\infty \exp(sM) D \exp(sM^T) ds$

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Rouse Polymer in vortical velocity

- $\gamma \dot{x}_i^a = -\partial_{x_i^a} H + \gamma u_i^a(x_i) + \eta_i^a$ with $H = \sum_i \left[\frac{\kappa}{2} (x_i - x_{i+1})^2 + \frac{k}{2} x_i^2 \right]$, $u_i(x) = w x_i \wedge e^3$ and $\langle \eta_{i,t}^a \eta_{j,s}^b \rangle = 2\gamma\beta^{-1} \delta^{ab} \delta_{ij} \delta(t-s)$

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$$\begin{cases} \widetilde{x}_{i,t}^1 = \cos(wt) x_{i,t}^1 + \sin(wt) x_{i,t}^2 \\ \widetilde{x}_{i,t}^2 = \sin(wt) x_{i,t}^1 - \cos(wt) x_{i,t}^2 \\ \widetilde{x}_{i,t}^3 = x_{i,t}^3 \end{cases}$$

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- More complex for Sheared polymer $u_i(x) = s\,(x_i.e_1)\,e_2$ the Lagrangian flow are combination of ellipses.

Non Equilibrium diffusion without Lagrangian pictures

One-dimensional Kardar-Parisi-Zhang equation

$\partial_t h_t(x) = \nu \nabla^2 h_t(x) + \frac{\lambda}{2} \left(\nabla h_t(x)\right)^2 + \eta_t(x)$ with $\langle \eta_t(x) \eta_s(y) \rangle = 2D\delta(t-s)\delta(x-y)$

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$\Rightarrow$ Shocks $\Rightarrow$ No unique global invertible Lagrangian flow $\Rightarrow$ No global Lagrangian frame picture.

Diffusive hydrodynamical limits of lattice particle systems

$$\partial_t n_t + \nabla j_t = 0 \text{ with } j_t(x) = -D\left(n_t(x)\right)\nabla n_t(x) + \eta_t(x, n_t)$$
$$\text{and } \langle \eta_t(x, n)\eta_s(y, n)\rangle = \epsilon\chi(n)\delta(t-s)\delta(x-y)$$

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SSEP : ? ? ? ?

Conclusion

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- Other models of non equilibrium dynamics ?
- Experimental realization of passage to Lagrangian frame ?
- Practical interest ?

Physics is like ♡ : sure, it may give practical results, but that not why we do it.
Richard Feynman

More general equilibrium form (i.e FDT valid) of diffusion process

"Langevin" form

$$\dot{x}_t^i = -\beta d_t^{ij}(x_t)\left(\partial_j H\right)(x_t) + \pi_t^{ij}(x_t)\left(\partial_j H\right)(x_t) - \frac{1}{\beta}\left(\partial_j \pi_t^{ij}\right)(x_t) + r_t^i(x_t) + \eta_t^i(x_t)$$

and the perturbation $H \to H_t = H - h_{t,a}O^a$

General form

$$x_t^i = d_t^{ij}(x_t)\left(\partial_j \ln \rho^e\right)(x_t) - \pi_t^{ij}(x_t)\left(\partial_j \ln \rho^e\right)(x_t) - \left(\partial_j \pi_t^{ij}\right)(x_t) + r_t^i(x_t) + \eta_t^i(x_t)$$

and the perturbed system such that

$$\ln\left(\rho^e\right) \to \ln(\rho^e) + \beta h_{t,a}O^a$$
$$L_{t,h}^{\dagger}\left(\rho^e \exp(\beta h_{t,a}O^a)\right) = 0$$

Equilibrium Langevin equation

$$\dot{x}^i = -\Gamma^{ij}\partial_j V(x) + \zeta_t^i$$

ex : overdampted Brownian particle in a stationary potential : $\gamma \frac{dq}{dt} = -\nabla V + \eta_t$
The Gibbs density $exp(-\beta V)$ is an equilibrium density, the detailed balance and the FDT holds.

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..........BUT..........

if initially, the unperturbed state is not inside the Gibbs density at the température of the bath (ex : Quench), the systeme relax toward the Gibbs density and in this regime the TFD is broken (Cugliandolo, L. F., Kurchan, J., Parisi, G. : *Off equilibrium dynamics and aging in unfrustrated systems.* (1994))

$$\frac{1}{\beta}\frac{\delta}{\delta g_{a,s}}\left\langle x^b_t\right\rangle\Big|_{g=0} = \frac{1}{2}\left(\partial_s - \partial_t\right)\left\langle x^a_s x^b_t\right\rangle_0 - \frac{\Gamma^{bj}}{2}\left\langle x^a_s\left(\partial_j H\right)_t\right\rangle_0 + \frac{\Gamma^{aj}}{2}\left\langle\left(\partial_j H\right)_s x^b_t\right\rangle_0$$

Langevin equation with non conservative external force :

$$\dot{x}^i = -\Gamma^{ij}\partial_j H(x) + \Pi^{ij}\partial_j H(x) + G^i(x) + \zeta_t^i$$

The Gibbs density $exp(-\beta H)$ is no longer an invariant density. There is a new invariant density $\rho^i(x)$, this density has a non zero probability current, it's a NESS. The detailed balance and the FDT fails.

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Most popular analytical NESS : Overdamped motion on a circle

$$\dot{x} = -H'(x) + F + \eta \text{ with } H(x) = H(x+1) \text{ and } F = const$$

Risken, H. : The Fokker Planck Equation, 2^{nd} edition, Springer, Berlin-Heidelberg 1989

Analytical expression for the NESS :

$$\rho^i(x) = \frac{\exp(-\beta H(x))}{Z} \int_0^1 \left(\theta(x-y) + \exp(\beta F)\theta(y-x)\right) \exp\left(\beta\left(H(y) + (x-y)F\right)\right) dy$$

corresponding to a constant probability current : $j = \frac{\exp(\beta F)-1}{\beta Z}$

Backward process

$\frac{dx}{dt} = (u_{t^*,+}(x) - u_{t^*,-}(x) - v_{t^*}(x))$

Non trivial for the markovian generator : $L^r_{t*} = \left(L_t - 2\widehat{u}_{t,+}.\nabla - \nabla.\widehat{u}_{t,+} + \nabla.u_{t,-}\right)$

Functional W

$$W_T = -ln(\rho^r_0)(x_T) + ln(\rho_0)(x_0) + J_T$$

with

$$J_T = \int_0^T \Big(2\widehat{u}_{t,+} \cdot d_t^{-1}(x_t)\,(\dot{x}_t - u_{t,-}(x_t)) - \nabla \cdot u_{t,-}(x_t)\Big)\ dt,$$

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J_T is "the" fluctuating entropy production in the environment relative to the backward process, W_T is "the" fluctuating entropy production when $\rho^r_0(y) = \rho^d_T(y)$

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Natural inversion

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Reversed protocol

Choice : $u_{t,+} = u \leftrightarrow u_{t,-} = 0$
$\Longrightarrow W_T^{tot} = -ln(\rho_0^r)(x_T) + ln(\rho_0)(x_0) + \int_0^T \left(2\widehat{u}_t \cdot d_t^{-1}(x_t) \cdot \dot{x}_t - \nabla \cdot u_t(x_t)\right)\, dt$

Lebowitz-Spohn : *A Gallavotti-Cohen type symmetry in the large deviation functional for stochastic dynamics*. J. Stat. Phys.(1999)

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Deterministic case : $W_T^{nat} = -ln(\rho_0^r)(x_T) + ln(\rho_0)(x_0) - \int_0^T \nabla \cdot u_t(x_t)\, dt$,

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Reversed protocol

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Lebowitz-Spohn : *A Gallavotti-Cohen type symmetry in the large deviation functional for stochastic dynamics*. J. Stat. Phys.(1999)

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We introduce the density "locally invariant" $\rho_t^{li} = \exp(-\varphi_t^{li})$ with : $div(j_t^{li}) = div(\rho_t^{li} v_t^{li}) = 0$.

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The backward process is associated with opposite probability current.

If we choose : $\rho_0(x) = \rho_0^{li}(x)$ et $\rho_0(x) = \rho_N^{li}(x)$. $\Longrightarrow W_T^{ex} = \int_0^T \left(\partial_t \varphi_t^{li}\right)(x_t)dt$.

Langevin equation : exchanged heat, extracted work

$W_T = \varphi_0^r(x_T) - \varphi_0(x_0) + J_T$ with J_T the fluctuating entropy production in the environment. $\Longrightarrow$ fluctuating exchanged heat : $Q_T[x] = -\frac{J_T[x]}{\beta}$.

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$\mathcal{T}_T[x] = \frac{W_T[x]}{\beta} + F_T - F_0 \Longrightarrow$
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- DFR type Crooks :
  $\exp(-\beta H_0(x))P^T(x \to y, \mathcal{T}) = \exp(-\beta H_T(y))P^{r,N}(y \to x, -\mathcal{T})\exp(\beta\mathcal{T})$

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- type Jarzynski :
  $\langle\exp(-\beta\mathcal{T}_T)\rangle = \exp(-\beta(F_T - F_0))$

For each time inversion, there is an extracted work $\Longrightarrow$ source of confusion and arguments.

Multiplicative fluctuation relation, Kraichnan case

Distribution of finite time Lyapunovs exponents

- Writting : $X = O.diag\,(exp(\rho_1), exp(\rho_2), ..., exp(\rho_d))\, O'$ with $O, O' \in O(d)$ and $\rho_1 \geq \rho_2 ... \geq \rho_d$ called stretching exponents.

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- One may often establish the existence of the multiplicative large deviations : $P^T\,(x \to y, \overrightarrow{\rho} = T\overrightarrow{\sigma}) \sim \exp\,(-TZ(\overrightarrow{\sigma}))$

  The rate function Z is an important quantity in transport theory, it determines the rate of decay of transported scalar moments, multi-fractal dimensions of the density....

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- This relation generalizes the usual Gallavotti-Cohen relation because it's for a stochastic dynamics, and it deals with the individual stretching exponents while the usual Gallavotti-Cohen relation deals with the phase space contraction=(sum of stretching exponents)

Why W_T is a good functional for being a non-equilibrium entropy production ?

We define the trajectories :
$[x]_t = x_t$ et $\left[\widetilde{x}\right]_t = x^*_{t^*}$
and the measures on the space of trajectories :
$\int F[x]M[dx] = \int dx \rho_0(x) E_x\left(F[x]\right)$
$\int F[x]M^r[dx] = \int dx \rho^r_0(x) E^r_x\left(F[\widetilde{x}]\right)$
where E_x denotes the expectation in the forward process that starts at x and E^r_x pertains for the backward process. Then DFR $\Rightarrow M^r[dx] = \exp(-W_T[x])M[dx] \mapsto$ so $\langle W_T \rangle = S(\, M|\, M^r)$ with S the relative entropy (Kullback-Leibler).