Production d’entropie dans les systèmes hamiltoniens hors équilibre

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The chain

Anharmonic chain of n oscillators

$$H_S(q,p) \equiv \frac{p^2}{2} + V(q), \quad q,p \in \mathbb{R}^{n \cdot d},$$

with a potential

$$V(q) \equiv \sum_{j=1}^{n} U_1^{(j)}(q_j) + \sum_{j=1}^{n-1} U_2^{(j)}(q_{j+1} - q_j),$$

subject to the following hypotheses:

(H1) Smoothness and stability:

$$C^\infty \ni V = ''\text{quadratic}'' + ''\text{bounded}'' \to \infty.$$

(H2) Effective coupling along the chain: the matrices

$$\mathfrak{M}_j(x) \equiv D^2 U_2^{(j)}(x), \quad j = 1, \cdots, n-1,$$

are uniformly (positive or negative) definite.

The heat baths and the coupling

Two scalar fields ϕ_L, ϕ_R on $\mathbb{R}^d$, with Hamiltonians

$$H_\ell(\phi_\ell, \pi_\ell) \equiv \frac{1}{2} \int \left(|\nabla \phi_\ell|^2 + |\pi_\ell|^2 \right) dx, \quad \ell \in \{L, R\}.$$

Initial conditions are distributed according to the Gibbs (Gaussian) measure

$$Z^{-1} e^{-H_L/kT_L - H_R/kT_R} \, d\phi_L \, d\phi_R \, d\pi_L \, d\pi_R.$$

The coupling of the chain to the baths is provided by

$$H_{int} \equiv q_1 \cdot \int \nabla \phi_L \rho_L \; dx + q_n \cdot \int \nabla \phi_R \rho_R \, dx.$$

The complete Hamiltonian is

$$H \equiv H_{S,ren} + H_L + H_R + H_{int},$$

with a renormalized chain hamiltonian

$$H_{S,ren} \equiv H_S + \frac{1}{2} \left(q_1^2 |\rho_L|_2^2 + q_n^2 |\rho_R|_2^2 \right) .$$

Equation of motion

For appropriate choices of the coupling functions ρ_L and ρ_R, Hamilton's equations can be written as a system of SDE:

$$\begin{aligned} dq &= p\,dt, \\ dp &= -\nabla V(q)\,dt + F\Gamma s\,dt, \\ ds &= -\Gamma s\,dt - F^\top p\,dt - 2T^{1/2}dw, \end{aligned}$$

where

- $s = (s_L, s_R) \in \mathbb{R}^{M\cdot d} \oplus \mathbb{R}^{M\cdot d}$ is an effective field for the chain,
- $\Gamma = \Gamma_L \oplus \Gamma_R$ is a positive definite square matrix,
- $F = F_L \oplus F_R \colon \mathbb{R}^{M\cdot d} \oplus \mathbb{R}^{M\cdot d} \to \mathbb{R}^{n\cdot d}$ is a linear map with range $\{(x_1, 0, \cdots, 0, x_n) |\, x_1, x_n \in \mathbb{R}^d\}$,
- $w = w_L \oplus w_R$ is a $2M \cdot d$–dimensional standard brownian motion,
- $T = T_L \oplus T_R$ is the diagonal temperature matrix on $\mathbb{R}^{M\cdot d} \oplus \mathbb{R}^{M\cdot d}$.

Old and new results

In our first study of this model, we proved:

- The existence of a stationary state for arbitrary temperatures T_L, T_R.
- The uniqueness of the stationary state for small values of $\delta \equiv \left|\frac{T_L - T_R}{T_L + T_R}\right|$.
- Relaxation to the the stationary state (i.e. the mixing property) when it is unique.

Our <u>new</u> <u>results</u> concern:

- Uniqueness (and mixing property) of the stationary state for arbitrary δ.
- Strict positivity of the (Boltzmann) entropy production in the stationary state.
- Relation between Boltzmann and Gibbs entropy production near the stationary state.
- Some heuristics on the Gallavotti/Cohen fluctuation theorem (following Lebowitz/Spohn).

Uniqueness of stationary state

Equation of motion: $dx(t) = b(x(t))\,dt + a\,dw(t)$

$\downarrow\downarrow\downarrow\downarrow$

Markovian diffusion on (extended) phase space X.

By previous results:

- The transition kernel $P^t(x, dy)$ has a smooth den sitiy.
- Any stationary state, i.e. any measure μ such that

$$\mu(Y) = \int P^t(x, Y)\,\mu(dx),$$

has a smooth density.

Uniqueness of the sationary state μ
$\Uparrow$
supp$P^t(x, \cdot) = X$

Stroock-Varadhan Theorem

Equation of motion: $dx(t) = b(x(t))\,dt + a\,dw(t)$

$\downarrow\downarrow\downarrow\downarrow$

Control problem: $\dot{x}(t) = b(x(t)) + au(t)$

$\downarrow\downarrow\downarrow\downarrow$

Controled path: $\varphi_x^u(t)$

$\downarrow\downarrow\downarrow\downarrow$

Support in function space: $\overline{\{\varphi_x^u | \, u \in C([0,\tau])\}}$

$\downarrow\downarrow\downarrow\downarrow$

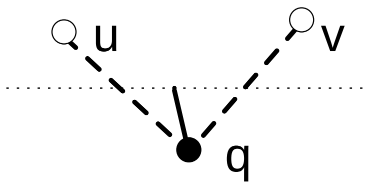
Accessible points: $Y_\tau(x) \equiv \{\varphi_x^u(\tau) | \, u \in C([0,\tau])\}$

$\downarrow\downarrow\downarrow\downarrow$

$$\boxed{\textbf{supp} P^\tau(x,\cdot) = \overline{Y_\tau(x)}}$$

Control of a single oscillator

$$\ddot{q} = f(q) - u - v$$



<u>Conditioning</u>:

- $q(0), \dot{q}(0), q(\tau), \dot{q}(\tau)$ are prescribed.
- $u\colon [0,\tau] \to \mathbb{R}^d$ is prescribed.
- $v^{(\alpha)}(0), v^{(\alpha)}(\tau)$ are prescribed for $\alpha \leq M$.

<u>Solution</u>:

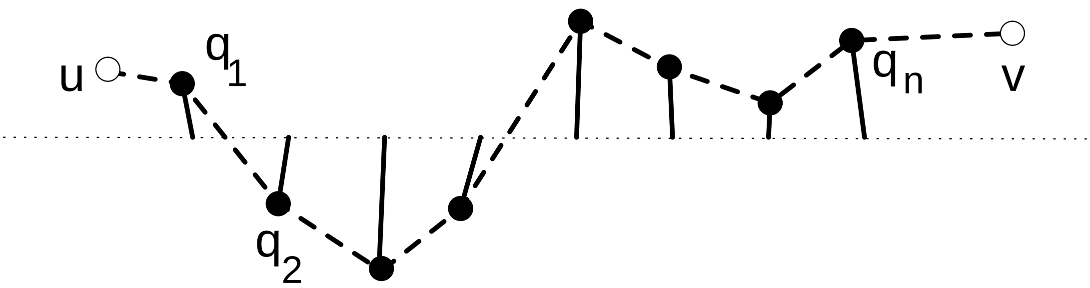
- Select a function q satisfying the conditioning, and such that

  $$q^{(\alpha+2)} = \frac{d^\alpha}{dt^\alpha}\left(f(q) - u - v\right)$$

  at $t = 0$ and $t = \tau$.
- Set $v = f(q) - \ddot{q} - u$.

Boundary control of the chain

$$
\begin{aligned}
\ddot{q}_1 &= f_1(q_1) - u - q_2,\\
\ddot{q}_2 &= f_2(q_2) - q_1 - q_3,\\
&\vdots\\
\ddot{q}_{n-1} &= f_{n-1}(q_{n-1}) - q_{n-2} - q_n,\\
\ddot{q}_n &= f_n(q_n) - q_{n-1} - v,
\end{aligned}
$$



Conditioning:

- $q(0), \dot{q}(0), q(\tau), \dot{q}(\tau)$ are prescribed.
- $u\colon [0,\tau] \to \mathbb{R}^d$ is prescribed.
- $v^{(\alpha)}(0), v^{(\alpha)}(\tau)$ are prescribed for $\alpha \le M$.

Induction hypothesis:

- This can be done for a chain of $n-1$ oscillators, and arbitrary M.

Induction step:

- The last equation $\ddot{q}_n = f_n(q_n) - q_{n-1} - v$ can be used to prescribe $q_n^{(\alpha)}(0), q_n^{(\alpha)}(\tau)$ for $\alpha \leq M+2$:
  - ▷ $q_n^{(3)} = F_3(q_n, \dot{q}_n, q_{n-1}, \dot{q}_{n-1}, v, \dot{v}; u)$
  - ▷ $q_n^{(4)} = F_4(q_n, \dot{q}_n, q_{n-1}, \dot{q}_{n-1}, q_{n-2}, v, \dot{v}, \ddot{v}; u)$
  - ▷ $\cdots$
  - ▷ $q_n^{(2j)} = F_{2j}(q_n, \dot{q}_n, \cdots, q_{n-j}, v, \cdots, v^{(2j-2)}; u)$
  - ▷ $q_n^{(2j+1)} = F_{2j+1}(q_n, \dot{q}_n, \cdots, \dot{q}_{n-j}, v, \cdots, v^{(2j-1)}; u)$
  - ▷ ...

- By the induction hypothesis, we can find a con trol q_n which solves the problem for the first $n-1$ oscillators.

- By construction, $v \equiv f_n(q_n) - \ddot{q}_n - q_{n-1}$ solves the problem for n oscillators.

Energy fluxes

Infinitesimal generator of the diffusion process:

$$\begin{aligned} L &\equiv \nabla_s \cdot T \nabla_s + G_s \cdot \nabla_s \\ &+ (G_p \cdot \nabla_q - G_q \cdot \nabla_p) + (F G_s \cdot \nabla_p - G_p \cdot F \nabla_s) \end{aligned}$$

where $G \equiv p^2/2 + V(q) + s \cdot \Gamma s/2$ is an effective energy.

- Mean energy of the chain: $e^{Lt} H_S$.
- Energy flux: $\partial_t e^{Lt} H_S = e^{Lt} L H_S \equiv e^{Lt} \Phi$, whith $\Phi \equiv L H_S = F G_s \cdot \nabla_p H_S = p \cdot F \Gamma s$.
- By the structure of the coupling: $\Phi = \Phi_L + \Phi_R$, where

  $$\begin{aligned} \Phi_L &= p_1 \cdot F_L \Gamma_L s_L, \\ \Phi_R &= p_n \cdot F_R \Gamma_R s_R, \end{aligned}$$

  are energy fluxes through the two ends of the chain.
- In the stationary state μ on has: $\langle \Phi \rangle_\mu = \langle \mu | L H_S \rangle = \left\langle L^\dagger \mu | H_S \right\rangle = 0$, i.e. $\langle \Phi_L \rangle_\mu = - \langle \Phi_R \rangle_\mu$.

Entropy production

The rate of production of thermodynamic entropy is therefore

$$\sigma \equiv \frac{\Phi_L}{T_L} + \frac{\Phi_R}{T_R} = p \cdot F T^{-1} \Gamma s.$$

Relation to timereversal:

- Time reversal map: $(Jf)(s, q, p) = f(s, q, -p)$.
- Density of the stationary state: $\rho = J e^{-R} e^{-\varphi}$ with $R \equiv s \cdot \Gamma T^{-1} s/2$.
- $L_\lambda \equiv L + \lambda\sigma$, and L_λ^* the adjoint of L_λ in the space $L^2(X, d\mu)$.

Theorem. The following operator identity holds for $\lambda \in \mathbb{R}$

$$e^{-\varphi} J L_\lambda^* J e^{\varphi} = L_{1-\lambda}.$$

The proof is a simple calculation.

Corollary. The following identities between functions hold

$$\begin{aligned} L\varphi &= \sigma + |T^{1/2}\nabla_s\varphi|^2, \\ L^*J\varphi &= -\sigma - |T^{1/2}\nabla_s J\varphi|^2. \end{aligned}$$

Corollary. In the stationary state μ, the entropy production satisfies

$$\langle\sigma\rangle_\mu = -\left\langle |T^{1/2}\nabla_s\varphi|^2 \right\rangle_\mu = -\left\langle |T^{1/2}\nabla_s\varphi|^2 \right\rangle_\mu \leq 0.$$

Theorem. In the stationary state μ, the entropy production satisfies

$$\langle\sigma\rangle_\mu = 0,$$

if and only if $T_L = T_R$.

Idea of the proof: If $\langle\sigma\rangle_\mu = 0$ then, by the second Corollary, φ is independent of s. By the first Corollary, $L\varphi = \sigma$. A careful investigation of this equation shows that it can not hold unless $T_L = T_R$.

The equation $L\varphi = \sigma$

Since φ is independent of s, we have

$$0 = (p \cdot \nabla_q \varphi - (\nabla V) \cdot \nabla_p \varphi) + F\Gamma s \cdot \left(\nabla_p \varphi - T^{-1} p\right).$$

Again, since φ is independent of s we must have

$$\begin{aligned} \{H_S, \varphi\} &= 0, \\ \nabla_{p_1} \varphi &= T_L^{-1} p_1, \\ \nabla_{p_n} \varphi &= T_R^{-1} p_n. \end{aligned}$$

- The first two equations have the solution

$$\varphi = H_S / T_L + Const.$$

- The first and the last equation have the solution

$$\varphi = H_S / T_R + Const.$$

To prove the Theorem, it suffices to show that these two couples of equations have a unique solu tion, up to constants.

We show that the homogeneous system

$$\begin{aligned} \{H_S, \varphi\} &= 0, \\ \nabla_{p_1}\varphi &= 0, \end{aligned}$$

has no nonconstant solution.

- φ independent of p_1 implies

$$0 = \{H_S, \varphi\} = p_1 \cdot \nabla_{q_1}\varphi + p_1 - \text{independent}$$

  and thus φ is also independent of q_1.

- φ independent of q_1, p_1 implies

$$\begin{aligned} 0 = \{H_S, \varphi\} &= -(\nabla U_2^{(1)})(q_1 - q_2) \cdot \nabla_{p_2}\varphi \\ &+ q_1 - \text{independent}, \end{aligned}$$

  which, in view of Hypothesis (H2), shows that φ is independent of p_2.

- Iterating the procedure leads to the desired con clusion.

Gibbs vs. Boltzmann entropy

If ν_0 is a probability measure on X, its time evolu tion

$$\nu_t(dx) \equiv \int \nu(dx_0) P^t(x_0, dx),$$

has a smooth density f_t. The Gibbs entropy of ν_0 at time t is

$$S(\nu_t) = - \left\langle \log(f_t) \right\rangle_{\nu_t} .$$

Theorem. The following formula holds

$$\partial_t S(\nu_t) - \langle \sigma \rangle_{\nu_t} = \left\langle |T^{1/2} \nabla_s J \varphi|^2 \right\rangle_{\nu_t} + \partial_t \langle R \rangle_{\nu_t} .$$

The proof is a tedious calculation. The physical content of this relation is still unclear.