Entropy Production and Fluctuations in (Classical) Statistical Mechanics

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joint work with

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mostly based on works by

Cohen, Evans, Gallavotti, Kurchan, Lebowitz, Morriss, Searles, Spohn, . . .

History...

- Seminal works by Evans–Cohen–Morriss [93] and Evans–Searles [94]: Numerical investigations and theoretical analysis of microscopic violation of the 2nd Law in steady shear flows $\to$ Transient Fluctuation Theorem
- Gallavotti–Cohen [95]: Chaotic hypothesis and nonequilibrium steady state ensembles (à la Ruelle) $\to$ Steady State Fluctuation Theorem
- Kurchan [98] + Lebowitz–Spohn [99]: Extension to stochastic dynamics and Markovian processes
- Maes [99]: Fluctuation Theorems as a Gibbs property
- ..... a lot more, see reviews by Rondoni–Mejia-Monasterio [07], and Marconi et al. [08]

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... and Motivations

- Similar results for thermostated, open, stochastic, Markovian, ... systems, but no unified description
- No universal rationale to define an entropy production observable
- What about quantum mechanics ?

Overview

- Classical framework
- Entropy production
- Finite time Evans-Searles identity/symmetry
- Finite time Generalized Evans-Searles identity/symmetry
- Finite time linear response
- Nonequilibrium Steady States (NESS)
- Linear response: The large time limit
- The Central Limit Theorem – Fluctuation-Dissipation
- The Evans-Searles fluctuation theorem
- The Gallavotti-Cohen fluctuation theorem
- The principle of regular entropic fluctuations
- Further Examples

0. Classical Framework

Measurable dynamical system with decent metric properties $(M, \mathcal{F}, \phi^t, \mu)$

- Phase space $(M, \mathcal{F})$: complete separable metric space with Borel σ-field
- Dynamics $(\phi^t)_{t\in\mathcal{T}}$: $\mathcal{T} = \mathbb{Z}$ or $\mathbb{R}$ (continuous) group of homeomorphisms of M
- Reference state μ: $\mu \in \mathcal{P}$, the space of Borel probability measures on $(M, \mathcal{F})$
- Observables f : $f \in \mathcal{B}$, the space of bounded measurable real functions on M
- Time-reversal: ϑ continuous involution of M s.t. $\phi^t \circ \vartheta = \vartheta \circ \phi^{-t}$

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Notation: For $\mu \in \mathcal{P}$, $f \in \mathcal{B}$ and $t \in \mathcal{T}$

$$\mu(f) = \int_M f d\mu$$

$$f_t = f \circ \phi^t, \qquad \mu_t(f) = \mu(f_t)$$

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Notation:

$$\mathcal{P}_I = \{\mu \in \mathcal{P} \,|\, \forall t \in \mathcal{T} : \mu_t = \mu\} \qquad \text{(steady states)}$$

$$\mathcal{P}_\mu = \{\nu \in \mathcal{P} \,|\, \nu \ll \mu\} \qquad \text{(μ-normal states)}$$

$$\mu \sim \nu \iff \mu \ll \nu \text{ and } \nu \ll \mu \qquad \text{(equivalent states)}$$

$$\text{For } \nu \in \mathcal{P}_\mu : \Delta_{\nu|\mu} = \frac{d\nu}{d\mu}, \qquad \ell_{\nu|\mu} = \log \Delta_{\nu|\mu}$$

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Relative entropy: For $\mu, \nu \in \mathcal{P}$

$$0 \geq \mathrm{Ent}(\nu|\mu) = -\sup_{\mathrm{f}\in\mathcal{B}} \Big(\nu(\mathrm{f}) - \log \mu(\mathrm{e}^{\mathrm{f}})\Big) = \begin{cases} -\nu(\ell_{\nu|\mu}) & \text{if } \nu \in \mathcal{P}_\mu \\ -\infty & \text{otherwise} \end{cases}$$

Note: $\mathrm{Ent}(\nu|\mu) = 0 \iff \nu = \mu$.

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Rényi relative α-entropy: For $\mu, \nu \in \mathcal{P}$ and $\alpha \in \mathbb{R}$

$$\mathrm{Ent}_\alpha(\nu|\mu) = \begin{cases} \log \mu(\Delta^\alpha_{\nu|\mu}) & \text{if } \nu \in \mathcal{P}_\mu \\ -\infty & \text{otherwise} \end{cases}$$

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Basic assumptions:

$$\text{(REG)} \qquad \boxed{\forall t \in \mathcal{T} : \quad \mu_t \sim \mu}$$

$$\text{(TRI)} \qquad \boxed{\forall f \in \mathcal{B} : \quad \mu(f \circ \vartheta) = \mu(f)}$$

We do not assume the reference state μ to be invariant!

1. Mean entropy production rate

Proposition.

1. (REG) $\Rightarrow \forall s,t\in\mathcal{T}:\quad \ell_{\mu_{t+s}|\mu}=\ell_{\mu_t|\mu}+\ell_{\mu_s|\mu}\circ\phi^{-t}$ (cocycle property)

2. (REG)+(TRI) $\Rightarrow \forall t\in\mathcal{T}:\quad \ell_{\mu_t|\mu}\circ\vartheta=\ell_{\mu_{-t}|\mu}$

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2. (REG)+(TRI) $\Rightarrow \forall t \in \mathcal{T}: \quad \ell_{\mu_t|\mu} \circ \vartheta = \ell_{\mu_{-t}|\mu}$

The entropy balance equation

$$0 \leq -\frac{1}{t}\left(\mathrm{Ent}(\mu_t|\mu) - \mathrm{Ent}(\mu|\mu)\right) = \mu\left(\frac{\ell_{\mu_t|\mu} \circ \phi^t}{t}\right)$$

suggests

Definition. Mean entropy production rate over the time interval $[0,t]$: $\Sigma^t = t^{-1}\,\ell_{\mu_t|\mu} \circ \phi^t$

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Corollary.

1. $\Rightarrow \forall t \in \mathcal{T}: \quad \Sigma^t = -t^{-1}\ell_{\mu_{-t}|\mu} = \Sigma^{-t} \circ \phi^t$

2. $\Rightarrow \forall t \in \mathcal{T}: \quad \Sigma^t \circ \vartheta = -t^{-1}\ell_{\mu_t|\mu} = -\Sigma^{-t}$

2. Entropic fluctuations: The Evans–Searles identity

$$P^t(f) = \mu(f(\Sigma^t)) \qquad \overline{P}^t(f) = \mu(f(-\Sigma^t))$$ (distributions of Σ^t and $-\Sigma^t$)

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Theorem. (Finite time Evans–Searles [94] or Transient Fluctuation Theorem)

Under Assumptions (REG)+(TRI) negative values of Σ^t become exponentially rare as $t \to \infty$ (microscopic form of 2nd law !)

$$\frac{d\overline{P}^t}{dP^t}(s) = e^{-ts}$$

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Proof. Use our Corollary: $t^{-1}\ell_{\mu_{-t}|\mu} = -\Sigma^t = \Sigma^{-t} \circ \vartheta = \Sigma^t \circ \phi^{-t} \circ \vartheta$

$$\mu\left(f\left(-\Sigma^t\right)\right) = \mu\left(f\left(\Sigma^t \circ \phi^{-t} \circ \vartheta\right)\right) = \mu\left(f\left(\Sigma^t \circ \phi^{-t}\right)\right) = \mu_{-t}\left(f\left(\Sigma^t\right)\right)$$

$$= \mu\left(f\left(\Sigma^t\right) e^{\ell_{\mu_{-t}|\mu}}\right) = \mu\left(f\left(\Sigma^t\right) e^{-t\Sigma^t}\right)$$

$\square$

3. Entropic fluctuations: The Evans–Searles symmetry

$$e_t(\alpha) = \mathrm{Ent}_\alpha(\mu_t|\mu) = \log \mu\left(e^{\alpha t \Sigma^{-t}}\right)$$

(finite time ES-function)

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Proposition. Properties of the finite time ES-function: $\mathbb{R} \ni \alpha \mapsto e_t(\alpha)$

1. It is is convex.
2. $e_t(0) = e_t(1) = 0$.
3. It is real analytic on the intervall $]0,1[$.
4. $e_t(1-\alpha) = e_{-t}(\alpha)$.
5. (TRI) $\Rightarrow e_{-t}(\alpha) = e_t(\alpha)$.

Proof. 1. Hölder inequality.

2. $e_t(0) = \log \mu(1) = 0$ and $e_t(1) = \log \mu\left(e^{\ell_{\mu_t|\mu}}\right) = \log \mu_t(1) = 0$.

3. $\alpha \mapsto \mu\left(e^{\alpha t \Sigma^{-t}}\right) = \int e^{\alpha t s} dP^{-t}(s)$ is analytic in the strip $0 < \mathrm{Re}\,\alpha < 1$.

4. $e_t(1-\alpha) = \log \mu\left(e^{\ell_{\mu_t|\mu}} e^{-\alpha t \Sigma^{-t}}\right) = \log \mu\left(e^{-\alpha t \Sigma^{-t} \circ \phi^t}\right) = \log \mu\left(e^{-\alpha t \Sigma^t}\right) = e_{-t}(\alpha)$

5. $e_t(\alpha) = \log \mu\left(e^{\alpha t \Sigma^{-t}}\right) = \log \mu\left(e^{-\alpha t \Sigma^t \circ \vartheta}\right) = \log \mu\left(e^{-\alpha t \Sigma^t}\right) = e_{-t}(\alpha)$.

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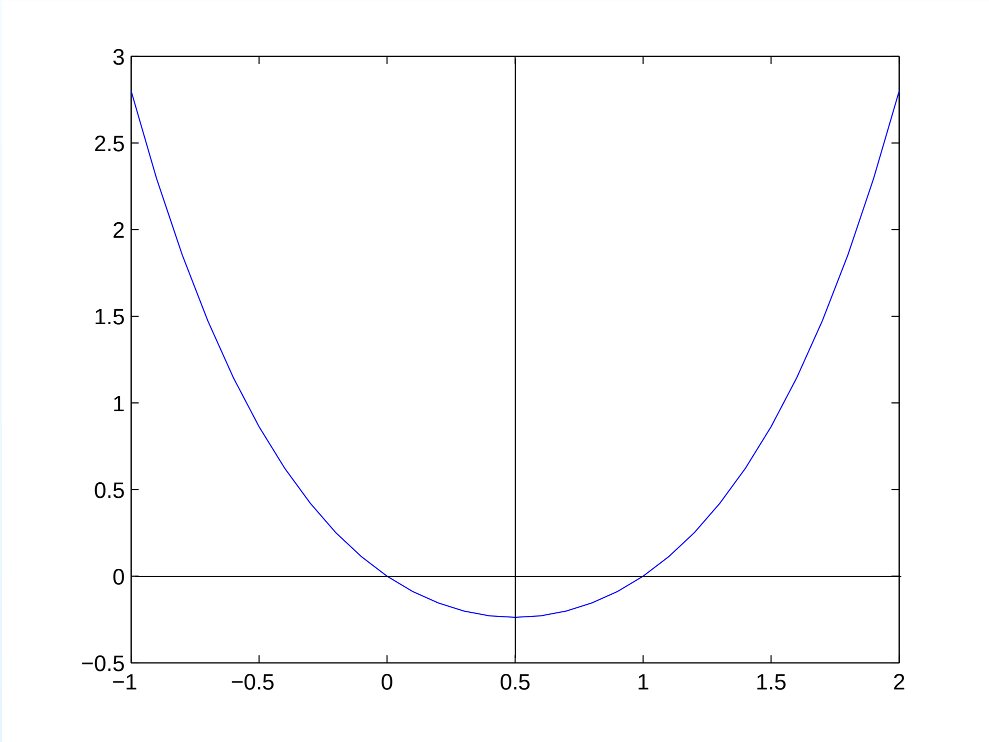

Alternative formulation of the finite time ES theorem: the finite time ES symmetry

$$\boxed{e_t(1-\alpha) = e_t(\alpha)}$$

4. Entropy production observable – Discrete time

$$\ell_{\mu_{t+1}|\mu} = \ell_{\mu_t|\mu} + \ell_{\mu_1|\mu} \circ \phi^{-t} \implies \ell_{\mu_t|\mu} = \sum_{s=0}^{t-1} \ell_{\mu_1|\mu} \circ \phi^{-s}$$

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$$\Sigma^t = \frac{1}{t} \ell_{\mu_t|\mu} \circ \phi^t = \frac{1}{t} \sum_{s=0}^{t-1} \sigma \circ \phi^s,$$

$$\boxed{\sigma = \ell_{\mu_1|\mu} \circ \phi^1 \qquad (\text{Entropy production observable})}$$

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$\sigma = \ell_{\mu_1|\mu} \circ \phi^1$ (Entropy production observable)

Proposition.
1. $\mu(\sigma) \geq 0$ and $\mu(\sigma_{-1}) \leq 0$.
2. (TRI) $\Rightarrow$ $\sigma \circ \vartheta = -\sigma_{-1}$.

Proof. 1. $\mu(\sigma) = \mu_1(\ell_{\mu_1|\mu}) = -\mathrm{Ent}(\mu_1|\mu) \geq 0$.

Jensen $\Rightarrow$ $e^{\mu_{-1}(\sigma)} \leq \mu_{-1}(e^\sigma) = \mu(e^{\ell_{\mu_1|\mu}}) = \mu_1(1) = 1$.

2. $\sigma \circ \vartheta = \ell_{\mu_1|\mu} \circ \phi \circ \vartheta = \ell_{\mu_1|\mu} \circ \vartheta \circ \phi^{-1} = \ell_{\mu_{-1}|\mu} \circ \phi^{-1} = -\ell_{\mu_1|\mu} \circ \phi^{-2} = -\sigma \circ \phi^{-1}$.

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$$\boxed{\sigma = \ell_{\mu_1|\mu} \circ \phi^1 \qquad \text{(Entropy production observable)}}$$

$$-\mathrm{Ent}(\mu_t|\mu) = \sum_{s=0}^{t-1} \mu(\sigma_s)$$

$$e_t(\alpha) = \log \mu \left(e^{\alpha \sum_{s=0}^{t-1} \sigma_{-s}} \right)$$

$$\text{(TRI)} \Rightarrow e_t(\alpha) = \log \mu \left(e^{-\alpha \sum_{s=0}^{t-1} \sigma_s} \right)$$

4. Entropy production observable – Continuous time

At the current level of generality, it is not possible to define entropy production for continuous time dynamical systems. Hence, we shall assume:

$\mathbb{R} \ni t \mapsto \Delta_{\mu_t|\mu} \in L^1(M,\mu)$ is strongly C^1 and

$$\sigma = \frac{d}{dt}\Delta_{\mu_t|\mu}\Big|_{t=0} \qquad \text{(Entropy production observable)}$$

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Cocycle property

$\Downarrow$

$$\Sigma^t = \frac{1}{t}\int_0^t \sigma_s ds$$

$\Downarrow$

$$-\mathrm{Ent}(\mu_t|\mu) = \int_0^t \mu(\sigma_s)ds \qquad e_t(\alpha) = \log\mu\left(e^{\alpha\int_0^t \sigma_{-s}ds}\right) \qquad \mu(\sigma) = 0$$

$\Downarrow$(TRI)$\Downarrow$

$$\sigma\circ\vartheta = -\sigma \qquad e_t(\alpha) = \log\mu\left(e^{-\alpha\int_0^t \sigma_s ds}\right)$$

5. Example: A thermostated ideal gas

Flow ϕ^t on $\mathbb{R}^N \times \mathbb{T}^N$:

$$\dot{L}_j = F - \lambda L_j, \qquad \dot{\theta}_j = L_j, \qquad (j = 1, \dots, N)$$

$$\lambda = F\frac{l}{u}, \qquad l = \frac{1}{N}\sum_j L_j, \qquad u = \frac{1}{N}\sum_j L_j^2$$

preserves mean kinetic energy u (iso-kinetic thermostat) + exactly solvable

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$$\sigma = \sum_j \frac{\partial}{\partial L_j}\left(F - \lambda L_j\right)\bigg|_M = (N-1)\frac{F}{\sqrt{\epsilon}}\tanh\xi, \qquad \xi = -\frac{1}{2}\log\frac{\sqrt{u}-l}{\sqrt{u}+l},$$

where the motion of ξ is governed by $\dot{\xi} = \epsilon^{-1/2}F$.

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It easily follows that

$$e_t(\alpha) = \log\left(\frac{\Gamma(N/2)}{\sqrt{\pi}\Gamma((N-1)/2)}\int_{-\infty}^{\infty}(\cosh\xi)^{-(N-1)(1-\alpha)}(\cosh(\xi + F\epsilon^{-1/2}t))^{-(N-1)\alpha}d\xi\right)$$

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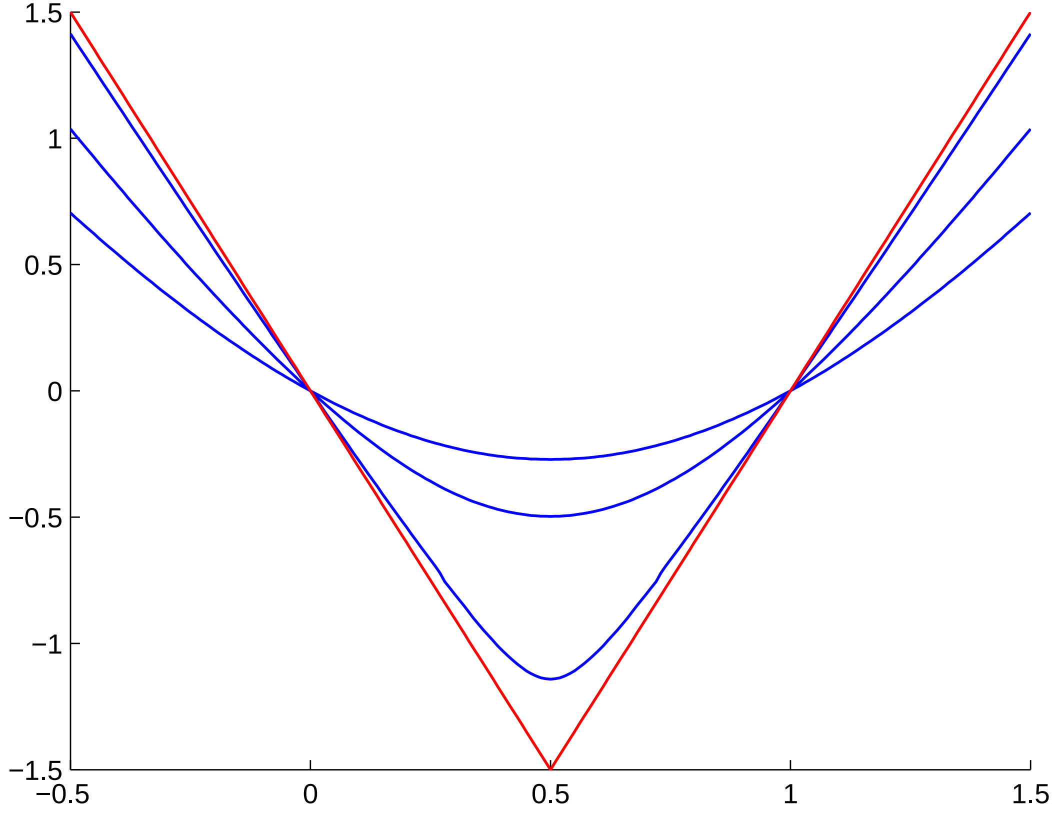

$$\frac{1}{t} e_t(\alpha) \text{ for various values of } t > 0$$

6. Thermodynamics: Forces & fluxes

Assume we have some control of our dynamical system

$$\mathbb{R}^n \ni X \mapsto (M, \phi_X^t, \mu_X)$$

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- $X = (X_1, \ldots, X_n)$ are mechanical or thermodynamical forces (affinities).
- $\boxed{\mu_0 \text{ is } \phi_0^t\text{-invariant}}$ i.e., $X = 0$ is equilibrium $\Rightarrow \sigma_{X=0} = 0$.
- $$\boxed{\sigma_X = X \cdot \mathbf{\Phi}_X = \sum_{j=1}^{n} X_j \Phi_X^{(j)}.}$$
- $\Phi_X^{(j)}$ is the flux (current) associated to X_j.
- For simplicity ϑ is idependant of X and (M, ϕ_X^t, μ_X) is TRI

$$\boxed{\mathbf{\Phi}_X \circ \vartheta = -\mathbf{\Phi}_X} \quad \Rightarrow \quad \mu_X(\mathbf{\Phi}_X) = 0.$$

7. Generalized ES–identity/symmetry

$$P_X^t(f) = \mu_X\left(f\left(\frac{1}{t}\int_0^t \mathbf{\Phi}_{X_s}\, ds\right)\right) \qquad \overline{P}_X^t(f) = \mu_X\left(f\left(-\frac{1}{t}\int_0^t \mathbf{\Phi}_{X_s}\, ds\right)\right)$$

7. Generalized ES–identity/symmetry

$$P_X^t(f) = \mu_X \left(f \left(\frac{1}{t} \int_0^t \boldsymbol{\Phi}_{X\,s} \, ds \right) \right) \qquad \overline{P}_X^t(f) = \mu_X \left(f \left(-\frac{1}{t} \int_0^t \boldsymbol{\Phi}_{X\,s} \, ds \right) \right)$$

Theorem. (Finite time Generalized ES fluctuation theorem) Under our assumptions, as $t \to \infty$, the averaged current $\boldsymbol{\Phi}$ likes to flow s.t. $X \cdot \boldsymbol{\Phi} > 0$:

$$\frac{d\overline{P}_X^t}{dP_X^t}(\boldsymbol{\Phi}) = \exp\left(-tX \cdot \boldsymbol{\Phi}\right)$$

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Equivalently the generalized ES function

$$g_t(X, Y) = \log \mu_X\left(e^{-Y \cdot \int_0^t \Phi_{X_s}\, ds}\right)$$

satisfies the generalized ES symmetry

$$\boxed{g_t(X, X - Y) = g_t(X, Y)}$$

7. Generalized ES–identity/symmetry

$$P_X^t(f) = \mu_X\left(f\left(\frac{1}{t}\int_0^t \mathbf{\Phi}_{X\,s}\,ds\right)\right) \qquad \overline{P}_X^t(f) = \mu_X\left(f\left(-\frac{1}{t}\int_0^t \mathbf{\Phi}_{X\,s}\,ds\right)\right)$$

Theorem. (Finite time Generalized ES fluctuation theorem) Under our assumptions, as $t \to \infty$, the averaged current $\mathbf{\Phi}$ likes to flow s.t. $X \cdot \mathbf{\Phi} > 0$:

$$\frac{d\overline{P}_X^t}{dP_X^t}(\mathbf{\Phi}) = \exp\left(-tX \cdot \mathbf{\Phi}\right)$$

Equivalently the generalized ES function

$$g_t(X,Y) = \log \mu_X\left(e^{-Y\cdot\int_0^t \Phi_{X\,s}\,ds}\right)$$

satisfies the generalized ES symmetry

$$\boxed{g_t(X, X-Y) = g_t(X,Y)}$$

Proof. $-(X-Y)\cdot \mathbf{\Phi}_{X\,s} \circ \vartheta = \sigma_{X\,-s} - Y \cdot \mathbf{\Phi}_{X\,-s}$.

8. Finite time linear response

If

$$X \mapsto \langle \Phi_X \rangle_t = \frac{1}{t} \int_0^t \mu_X(\Phi_{X\,s})\, ds$$

is differentiable at $X = 0$ we set

$$L^t_{jk} = \partial_{X_k} \langle \Phi^{(j)}_X \rangle_t \Big|_{X=0} \qquad \text{(finite time transport matrix)}$$

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$$L_{jk}^t = \partial_{X_k} \langle \Phi_X^{(j)} \rangle_t \Big|_{X=0}$$ (finite time transport matrix)

Theorem. (Finite time Green-Kubo formula and Onsager reciprocity relations)
Assume that $(X,Y) \mapsto g_t(X,Y)$ is C^2 near $(0,0)$. Then

$$L_{jk}^t = \frac{1}{2} \int_{-t}^t \mu_0 \left(\Phi_0^{(k)} \Phi_{0s}^{(j)} \right) \left(1 - \frac{|s|}{t} \right) ds = \frac{1}{t} \int_0^t \left[\frac{1}{2} \int_{-s}^s \mu_0 \left(\Phi_0^{(k)} \Phi_{0u}^{(j)} \right) du \right] ds$$

where $\Phi_{0s}^{(j)} = \Phi_0^{(j)} \circ \phi_0^s$. In particular the finite time transport matrix is symmetric.

8. Finite time linear response

Remark. The following shows that the transport matrix is non-negative

$$0 \leq \langle \sigma_X \rangle_t = \sum_{j=1}^{n} X_j \langle \Phi_X^{(j)} \rangle_t = \sum_{j,k=1}^{n} L_{jk}^t X_j X_k + o(|X|^2).$$

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Proof of the theorem. One has

$$\langle \Phi_X^{(j)} \rangle_t = -\frac{1}{t} \partial_{Y_j} g_t(X,Y)\Big|_{Y=0} \Rightarrow L_{jk}^t = \partial_{X_k} \langle \Phi_X^{(j)} \rangle_t \Big|_{X=0} = -\frac{1}{t}\, \partial_{X_k} \partial_{Y_j} g_t(X,Y)\Big|_{X=Y=0}$$

As a consequence of the generalized ES symmetry one also has

$$-\partial_{X_k} \partial_{Y_j} g_t(X,Y)\Big|_{X=Y=0} = \frac{1}{2}\, \partial_{Y_k} \partial_{Y_j} g_t(X,Y)\Big|_{X=Y=0}$$

(note that the symmetry of L^t already follows from this formula!) Thus we can write

$$L_{jk}^t = \frac{1}{2t} \int_0^t \int_0^t \mu_0 \left(\Phi_{0 s_1}^{(k)} \Phi_{0 s_2}^{(j)} \right) ds_1 ds_2 = \frac{1}{2t} \int_0^t \int_0^t \mu_0 \left(\Phi_0^{(k)} \Phi_{0 (s_2 - s_1)}^{(j)} \right) ds_1 ds_2$$

and the result follows from change of integration variables and integration by parts.

9. Example: Thermally driven open system

Hamiltonian description:

- Small system S: $H_S(p_S, q_S)$ on M_S.
- Large reservoirs R_j: $H_j(p_j, q_j)$ on M_j ($j = 1, \ldots, N$).
- Decoupled joint system: $H_0(p, q) = H_S(p_S, q_S) + \sum_j H_j(p_j, q_j)$.
- Coupling: $V(p, q) = \sum_j V_j(p_S, q_S, p_j, q_j)$.
- Coupled system: $H(p, q) = H_0(p, q) + V(p, q)$.
- Hamiltonian flow: ϕ^t on $M = M_S \times M_1 \times \cdots M_N$.
- TRI holds with $\vartheta(p, q) = (-p, q)$ provided $H \circ \vartheta = H$.

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- Reference state: $\dfrac{1}{Z} e^{-\beta H_S - \sum_j \beta_j H_j} dp\, dq$.
- Thermodynamic forces: $X_j = \beta - \beta_j \Rightarrow \nu_X = \dfrac{1}{Z} e^{-\beta H_0 + \sum_j X_j H_j} dp\, dq$.

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Problem: μ_0 is not ϕ^t invariant (recall our assumption!)

Cure: If V is well localized, $\mu_X = \frac{1}{Z} e^{-\beta H + \sum_j X_j H_j} dp\, dq$ describes the same thermodynamics as $\nu_X \to (M, \phi^t, \mu_X)$

9. Example: Thermally driven open system

Energy conservation + Liouville theorem $\Rightarrow \mu_{Xt} = \dfrac{1}{Z} e^{-\beta H + \sum_j X_j H_j \circ \phi^{-t}} dp\, dq$

$$\Downarrow$$

$$\Delta_{\mu_{Xt}|\mu_X} = e^{\sum_j X_j (H_j \circ \phi^{-t} - H_j)}$$

$$\Downarrow$$

$$\sigma_X = \frac{d}{dt} \Delta_{\mu_{Xt}|\mu_X} \Big|_{t=0} = -\sum_j X_j \{H, H_j\} = \sum_j X_j \{H_j, V_j\} = \sum_j X_j \Phi^{(j)}$$

$$\Downarrow$$

Fluxes $\Phi^{(j)} = -\{H, H_j\} = \{H_j, V\} = \{H_j, V_j\}$ are independant of X

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Fluxes $\Phi^{(j)} = -\{H, H_j\} = \{H_j, V\} = \{H_j, V_j\}$ are independant of X

[Assume $H_j \circ \vartheta = H_j \Rightarrow \Phi^{(j)} \circ \vartheta = -\Phi^{(j)}$]

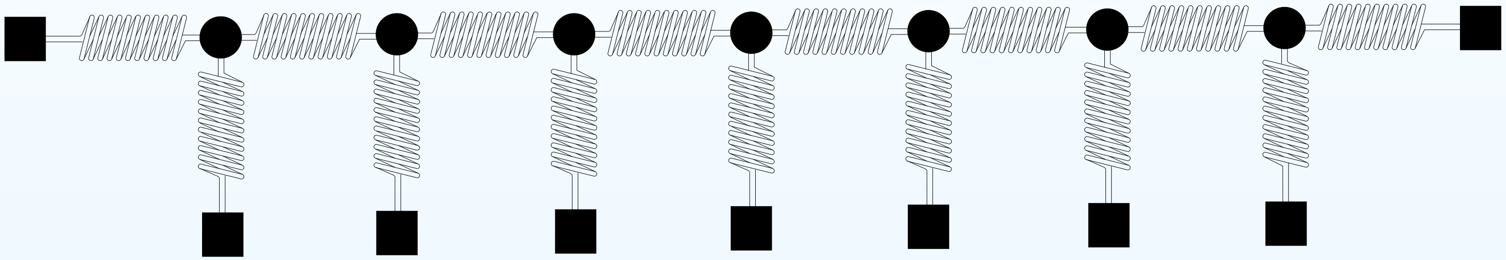
$$H_j \circ \phi^t - H_j = -\int_0^t \Phi_s^{(j)} ds$$

$$\Downarrow$$

$\Phi^{(j)}$ is the energy flux out of reservoir R_j

9. Example: Open harmonic chain

$$H_S(p_S, q_S) = \sum_{|x|\le m} \frac{p_x^2 + q_x^2}{2} + \sum_{x=-m}^{m+1} \frac{(q_x - q_{x-1})^2}{2}\Bigg|_{q_{-m-1}=q_{m+1}=0}$$



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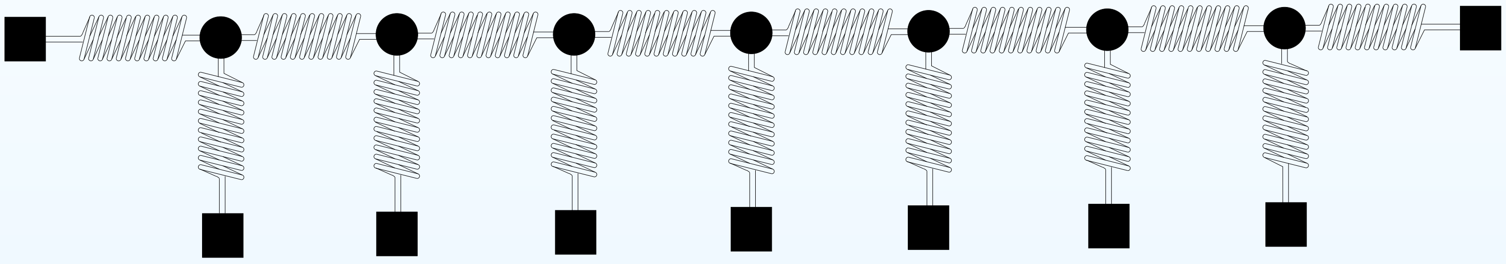

The two reservoirs R_L and R_R are similar but much longer chains ($n \gg m$)

$$H_L(p_L, q_L) = \sum_{x=-n}^{-m-1} \frac{p_x^2 + q_x^2}{2} + \sum_{x=-n}^{-m} \frac{(q_x - q_{x-1})^2}{2} \Bigg|_{q_{-n-1}=q_{-m}=0}$$

$$H_R(p_R, q_R) = \sum_{x=m+1}^{n} \frac{p_x^2 + q_x^2}{2} + \sum_{x=m+1}^{n+1} \frac{(q_x - q_{x-1})^2}{2} \Bigg|_{q_m=q_{n+1}=0}$$

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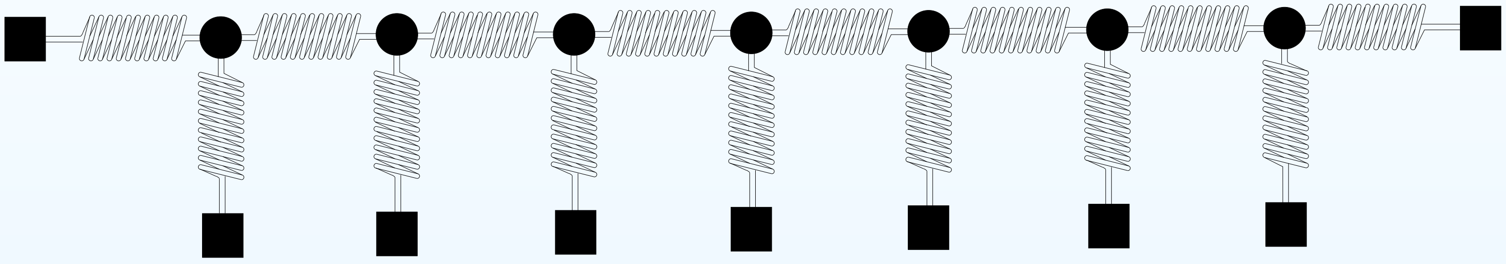
$$H_S(p_S, q_S) = \sum_{|x| \le m} \frac{p_x^2 + q_x^2}{2} + \sum_{x=-m}^{m+1} \frac{(q_x - q_{x-1})^2}{2} \Bigg|_{q_{-m-1}=q_{m+1}=0}$$



Fully coupled chain

$$H(p, q) = \sum_{x=-n}^{n} \frac{p_x^2 + q_x^2}{2} + \sum_{x=-n}^{n+1} \frac{(q_x - q_{x-1})^2}{2} \Bigg|_{q_{-n-1}=q_{n+1}=0}$$

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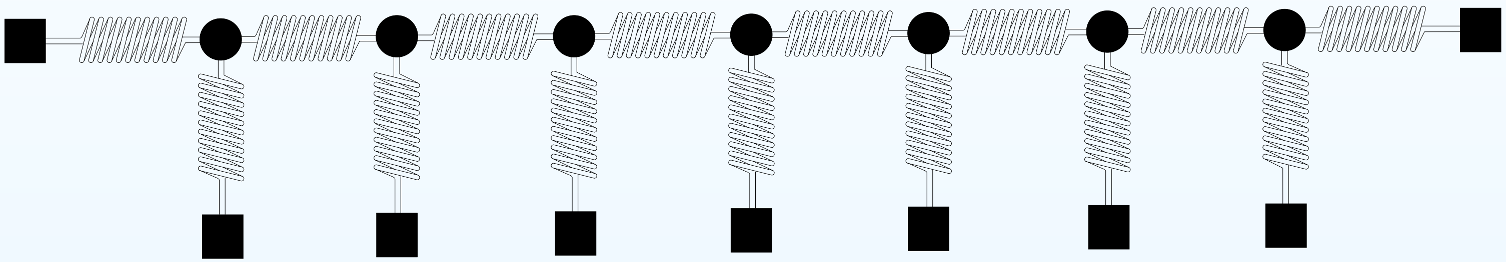
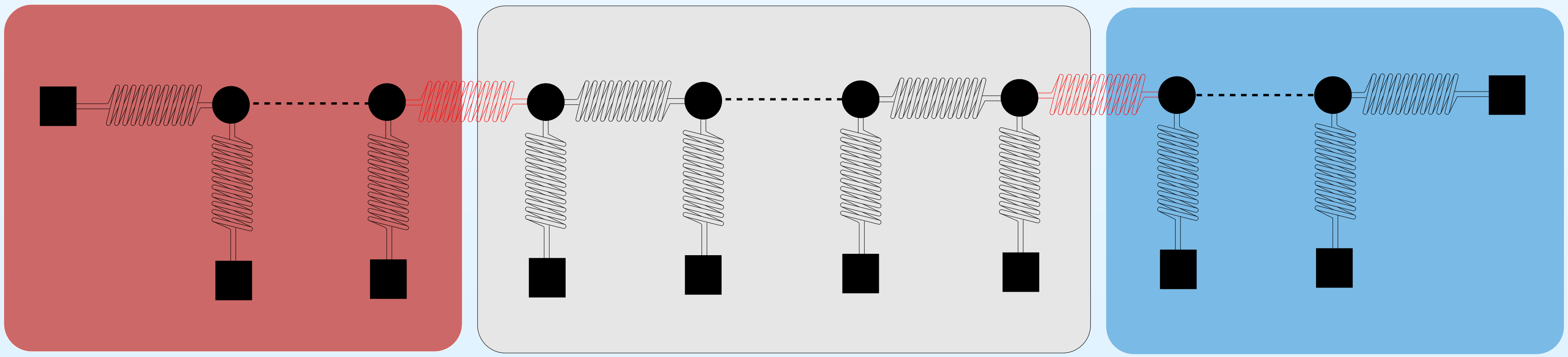
$$H_S(p_S, q_S) = \sum_{|x|\leq m} \frac{p_x^2 + q_x^2}{2} + \sum_{x=-m}^{m+1} \frac{(q_x - q_{x-1})^2}{2} \Bigg|_{q_{-m-1}=q_{m+1}=0}$$



Coupling

$$V = H - H_0 = H - (H_L + H_S + H_R) = -q_{-m-1}q_{-m} - q_m q_{m+1}$$



9. Example: Open harmonic chain

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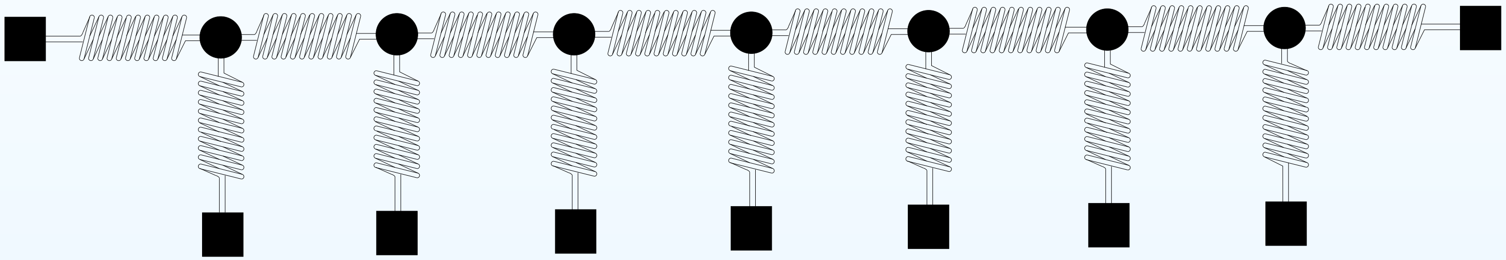
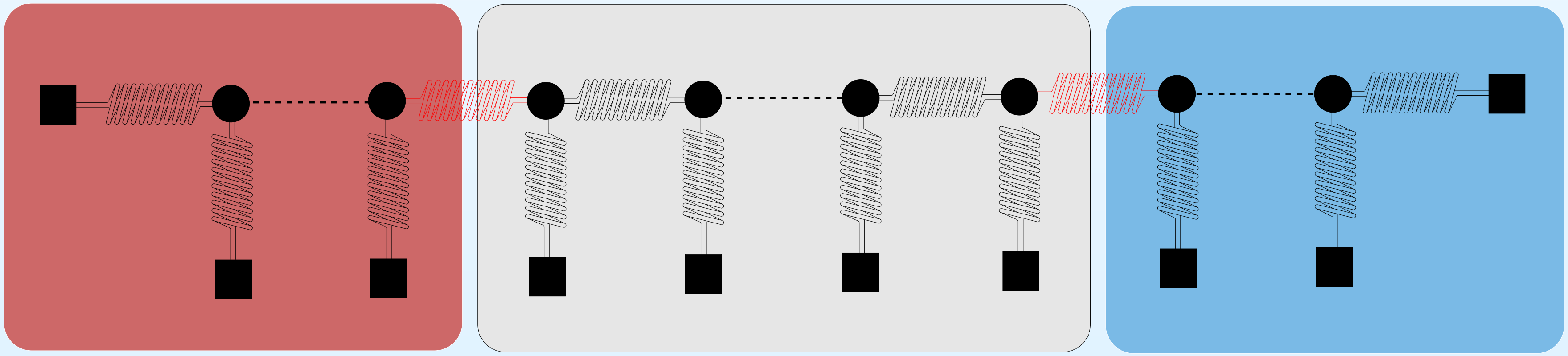


Fluxes

$$\Phi^{(L)} = \{H_L, V\} = -p_{-m-1}q_{-m} \qquad \Phi^{(R)} = \{H_R, V\} = -p_{m+1}q_m$$



9. Example: Open harmonic chain

Linear equations of motion $\longleftrightarrow$ Linear Hamiltonian flow $\phi^t = e^{t\mathcal{L}}$

Quadratic forms $2H$, $2H_L$, $2H_R \longleftrightarrow$ Symmetric matrices h ,h_L, h_R

$$k(X) = X_L h_L \oplus X_R h_R$$

Reference state		Gaussian with covariance
$\mu_X = \frac{1}{Z} e^{-\beta H + X_L H_L + X_R H_R} dp\, dq$	$\longleftrightarrow$	$D_X = (\beta h - k(X))^{-1}$

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Generalized ES-function reduces to a Gaussian integral

$$g_t(X, Y) = -\frac{1}{2} \log\det\left(I - D_X\left(e^{t\mathcal{L}^*} k(Y) e^{t\mathcal{L}} - k(Y)\right)\right)$$

In particular

$$e_t(\alpha) = g_t(X, \alpha X) = -\frac{1}{2} \log\det\left(I - \alpha D_X\left(e^{t\mathcal{L}^*} k(X) e^{t\mathcal{L}} - k(X)\right)\right)$$

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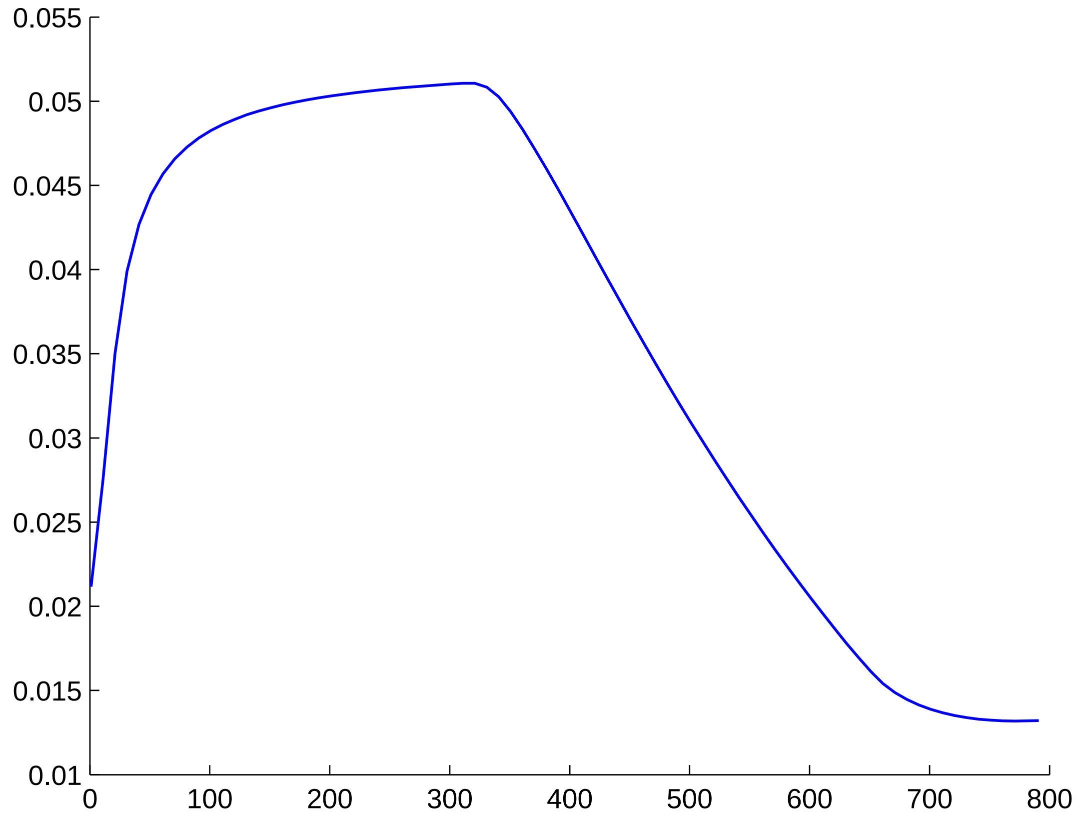

Mean entropy production rate $\mu(\Sigma^t) = -\left.\frac{d}{d\alpha} e_t(\alpha)\right|_{\alpha=0}$

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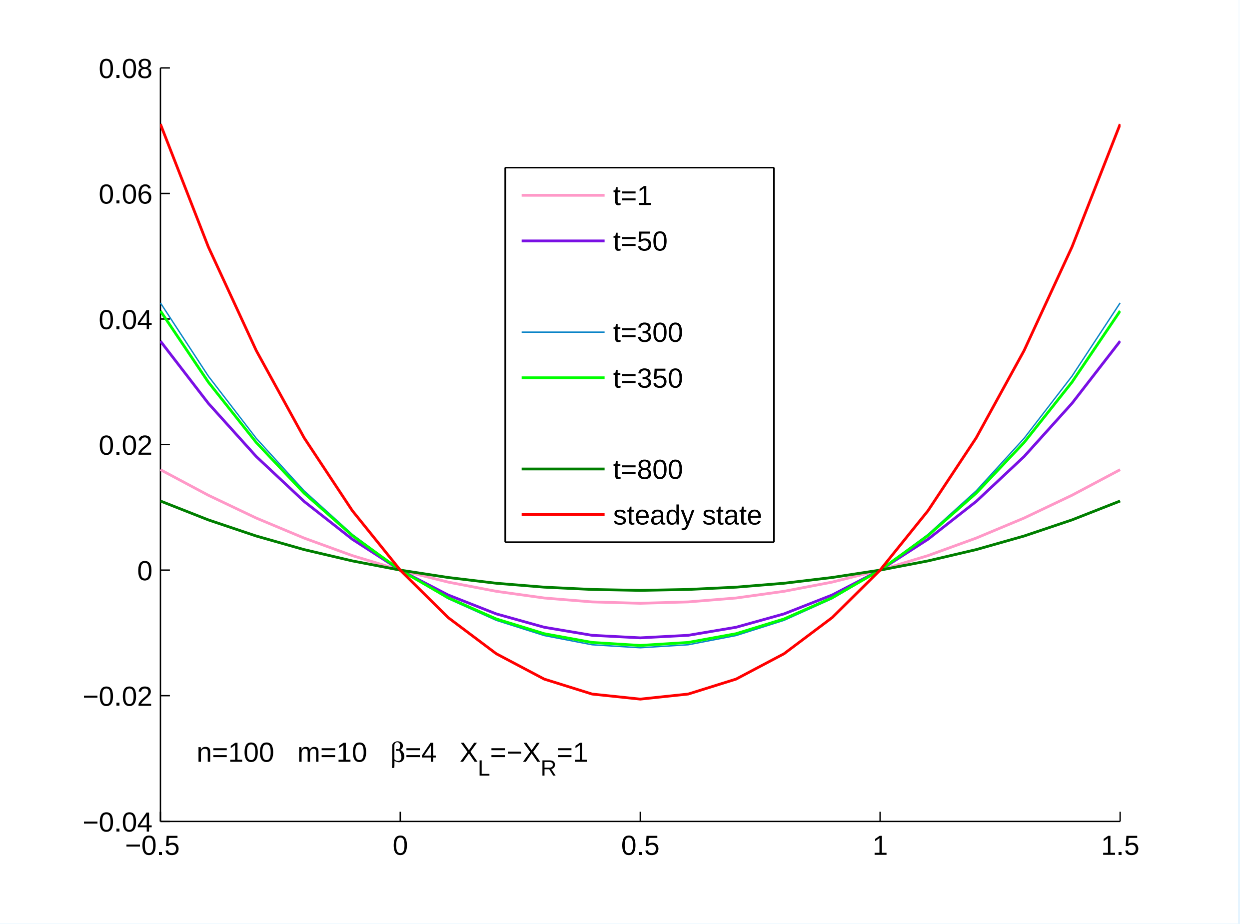

$$\frac{1}{t} e_t(\alpha) \text{ for various values of } t > 0$$

10. Nonequilibrium Steady States

Definition. $\mu_+ \in \mathcal{P}_I$ is the NESS of (M, ϕ^t, μ) if

$$\lim_{t\to\infty} \frac{1}{t} \int_0^t \mu_s(f)\, ds = \mu_+(f)$$

for all bounded continuous f. μ_+ is entropy producing if $\mu_+(\sigma) > 0$.

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Quasi-Theorem. The NESS μ_+ of (M, ϕ^t, μ) is entropy producing if and only if $\mu_+ \notin \mathcal{P}_\mu$, i.e., μ_+ is singular w.r.t. μ.

$$\boxed{\text{Entropy production is the signature of non-equilibrium}}$$

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Theorem.
1. If $\nu \in \mathcal{P}_I \cap \mathcal{P}_\mu$ then $\nu(\sigma) = 0$.
2. If $\mu_t(\sigma) - \mu_+(\sigma) = O(t^{-1})$ then $\mu_+(\sigma) = 0$ implies $\mu_+ \in \mathcal{P}_I \cap \mathcal{P}_\mu$.

11. Linear response: The large time limit

Assume that for small $X \in \mathbb{R}^n$ the controlled system (M, ϕ_X^t, μ_X) has a NESS μ_{X+}

$$\langle \mathbf{\Phi}_X \rangle_+ = \lim_{t \to \infty} \langle \mathbf{\Phi}_X \rangle_t = \mu_{X+}(\mathbf{\Phi}_X) \qquad \text{(steady currents in the NESS } \mu_{X+}\text{)}$$

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Finally assume that the equilibrium current-current correlation function satisfies

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Theorem. The Green-Kubo Formula

$$L_{jk} = \frac{1}{2} \int_{-\infty}^{\infty} \mu_0 \left(\Phi_0^{(k)} \Phi_{0s}^{(j)} \right) \, ds \left[:= \lim_{T\to\infty} \frac{1}{2} \int_T^T \mu_0 \left(\Phi_0^{(k)} \Phi_{0s}^{(j)} \right) \, ds \right]$$

holds if and only if $L_{jk} = \lim_{t\to\infty} L_{jk}^t$.

11. Linear response: The large time limit

Remarks. 1. The 3 assumptions are delicate dynamical problems that can only be checked in specific models.

2. If the GK-Formula holds, so do the Onsager Reciprocity Relations $L_{jk} = L_{kj}$.

3. The condition $L_{jk} = \lim_{t\to\infty} L_{jk}^t$ means that the limit and derivative can be exchanged in the following expression

$$\partial_{X_k}\left[\lim_{t\to\infty}\langle\Phi_X^{(j)}\rangle_t\right]\Big|_{X=0} = \lim_{t\to\infty}\left[\partial_{X_k}\langle\Phi_X^{(j)}\rangle_t\Big|_{X=0}\right]$$

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3. The condition $L_{jk} = \lim_{t\to\infty} L^t_{jk}$ means that the limit and derivative can be exchanged in the following expression

$$\partial_{X_k} \left[\lim_{t\to\infty} \langle \Phi_X^{(j)} \rangle_t \right] \Big|_{X=0} = \lim_{t\to\infty} \left[\partial_{X_k} \langle \Phi_X^{(j)} \rangle_t \Big|_{X=0} \right]$$

This is also a delicate dynamical problem.

Proof. Recall that

$$L^t_{jk} = \frac{1}{t} \int_0^t F(s) ds, \qquad F(s) = \frac{1}{2} \int_{-s}^{s} \mu_0 \left(\Phi_0^{(k)} \Phi_{0u}^{(j)} \right) du$$

If the GK-Formula holds, then $F(t) \to L_{jk}$ and the fundamental property of the Cesàro mean implies that $L^t_{jk} \to L_{jk}$. Invoking Hardy-Littlewood's Tauberian theorem one gets the reverse implication.

12. Central Limit Theorem – Fluctuation-Dissipation

The Central Limit Theorem (CLT) holds for the current $\mathbf{\Phi}_0$ if there is a positive semi-definite matrix D s.t., for all bounded continuous function $f : \mathbb{R}^n \to \mathbb{R}$,

$$\lim_{t\to\infty} \mu_0 \left(f \left(\frac{1}{\sqrt{t}} \int_0^t \mathbf{\Phi}_{0s} \, ds \right) \right) = m_D(f)$$

where m_D is the centered Gaussian measure of covariance D on $\mathbb{R}^n$.

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The following well known result of Bryc is often useful to establish the validity of the CLT.
We set $I_\epsilon = \{X \in \mathbb{R}^n \,|\, |X| < \epsilon\}$ and $D_\epsilon = \{X \in \mathbb{C}^n \,|\, |X| < \epsilon\}$.

Theorem. Suppose that for some $\epsilon > 0$ the function $g_t(0,Y) = \log \mu_0 \left(e^{Y \cdot \int_0^t \mathbf{\Phi}_{0s} ds} \right)$ is analytic in D_ϵ, satisfies

$$\sup_{Y \in D_\epsilon, t>1} \frac{1}{t} |g_t(0,Y)| < \infty$$

and $\lim_{t\to\infty} \frac{1}{t} g_t(0,Y)$ exists for all $Y \in I_\epsilon$. Then the CLT holds for $\mathbf{\Phi}_0$ with covariance matrix

$$D_{jk} = \lim_{t\to\infty} \int_{-t}^{t} \mu_0 \left(\Phi_0^{(k)} \Phi_{0s}^{(j)} \right) \left(1 - \frac{|s|}{t} \right) ds$$

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where m_D is the centered Gaussian measure of covariance D on $\mathbb{R}^n$.

We say that the Fluctuation-Dissipation Theorem holds for the system (M, ϕ_X^t, μ_X) if:

- The Green-Kubo Formula

$$L_{jk} = \frac{1}{2} \int_{-\infty}^{\infty} \mu_0 \left(\Phi_0^{(k)} \Phi_{0s}^{(j)} \right) \, ds$$

  (and therefore the Onsager Reciprocity Relations $L_{jk} = L_{kj}$) hold.
- The CLT holds for $\mathbf{\Phi}_0$ with a covariance matrix $[D_{jk}]$ satisfying Einstein's Relation

$$D_{jk} = 2L_{jk}$$

12. Central Limit Theorem – Fluctuation-Dissipation

Remark. Both, the exchange of $\lim_{t\to\infty}$ and ∂_{X_k} and Bryc's theorem can often be justified by the following multi-variable version of Vitali's convergence theorem.

Theorem. Suppose that the function $F_t : D_\epsilon \to \mathbb{C}$ is analytic for all $t > 0$ and satisfies

$$\sup_{X\in D_\epsilon, t>1} |F_t(X)| < \infty.$$

If $\lim_{t\to\infty} F_t(X)$ exists for $X \in I_\epsilon$ then it exists for all $X \in D_\epsilon$ and defines an anaytic function F. Moreover, the derivatives of F_t converge to the corresponding derivatives of F uniformly on compact subsets of D_ϵ.

13. Large deviations

A vector valued observable $\mathbf{f} = (f^{(1)}, \ldots, f^{(n)})$ satisfies a Large Deviation Principle (LDP) w.r.t. (M, ϕ, μ) if there exists a upper-semicontinuous function

$$I : \mathbb{R}^n \to [-\infty, 0]$$

with compact level sets such that, for all Borel sets $G \subset \mathbb{R}^n$

$$\begin{aligned}
\sup_{Z \in \mathring{G}} I(Z) \quad &\leq \quad \liminf_{t\to\infty} \frac{1}{t} \log \mu\left(\left\{x \in M \;\middle|\; \frac{1}{t}\int_0^t \mathbf{f}_s(x)ds \in G\right\}\right) \\
&\leq \quad \limsup_{t\to\infty} \frac{1}{t} \log \mu\left(\left\{x \in M \;\middle|\; \frac{1}{t}\int_0^t \mathbf{f}_s(x)ds \in G\right\}\right) \quad \leq \quad \sup_{Z \in \bar{G}} I(Z).
\end{aligned}$$

where $\mathring{G}$ denotes the interior of G and $\bar{G}$ its closure. I is called the rate function.

14. The Gärtner-Ellis theorem

Assume that the limit

$$h(Y) = \lim_{t\to\infty} \frac{1}{t} \log \mu(e^{-\int_0^t Y\cdot \mathbf{f_s} ds})$$

exists in $[-\infty, +\infty]$ for all $Y \in \mathbb{R}^n$ and is finite for Y in some open neighborhood of 0.

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1. Suppose that $h(Y)$ is differentiable at $Y = 0$. Then, the limit

$$\langle \mathbf{f} \rangle_+ = \lim_{t\to\infty} \frac{1}{t} \int_0^t \mu(\mathbf{f}_s) ds$$

exists and $\langle \mathbf{f} \rangle_+ = -\nabla h(0)$.

For any regular sequence t_n one has

$$\lim_{n\to\infty} \frac{1}{t_n} \int_0^{t_n} \mathbf{f}_s(x) ds = \langle \mathbf{f} \rangle_+$$

for μ-a.e. $x \in M$.

[t_n is regular if $\sum_n e^{-at_n} < \infty$ for all $a > 0$]

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2. Suppose that $h(Y)$ is a lower semicontinuous function on $\mathbb{R}^n$ which is differentiable on the interior of the set $\mathcal{D} = \{Y \in \mathbb{R}^n \,|\, h(Y) < \infty\}$ and satisfies

$$\lim_{\mathring{\mathcal{D}} \ni Y \to Y_0} |\nabla h(Y)| = \infty$$

for all $Y_0 \in \partial\mathcal{D}$. Then the Large Deviation Principle holds for $\mathbf{f}$ w.r.t. (M, ϕ, μ) with the rate function

$$I(Z) = \inf_{Y\in\mathbb{R}^n} (Y \cdot Z + h(Y))$$

$[\ -I(Z)$ is the Legendre transform of $h(-Y)$, in particular $I(Z)$ is concave $]$

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exists in $[-\infty, +\infty]$ for all $Y \in \mathbb{R}^n$ and is finite for Y in some open neighborhood of 0.

Remarks. 1. The conclusion of Part 2 holds in particular if $h(Y)$ is differentiable on $\mathbb{R}^n$.

2. There are other (local) versions of the Gärtner-Ellis theorem that are useful in applications. Suppose, for example, that the function $h(Y)$ is finite, strictly convex and continuously differentiable in some open neighborhood $B \subset \mathbb{R}^n$ of the origin. Then Part 1 holds as well as a weaker version of Part 2:

> The large deviation principle holds provided the set G is contained in a sufficiently small neighborhood of $\langle \mathbf{f} \rangle_+$.

15. The Evans–Searles fluctuation theorem

Recall that the finite time ES-function $e_t(\alpha) = \mu\left(e^{-\alpha \int_0^t \sigma_s\, ds}\right)$

satisfies the ES-symmetry $e_t(1-\alpha) = e_t(\alpha)$ and $e_t(0) = e_t(1) = 0$ for all t

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Assume that the ES-function $e(\alpha) = \lim_{t\to\infty} \frac{1}{t} \log e_t(\alpha) \in [-\infty, \infty]$ exists for all $\alpha \in \mathbb{R}$

$$\Downarrow$$

$e(\alpha)$ is a convex function satisfying the ES-symmetry $e(1-\alpha) = e(\alpha)$ and
$e(0) = e(1) = 0$

15. The Evans–Searles fluctuation theorem

Theorem.

If $e(\alpha)$ is differentiable at $\alpha = 0$ then:

1. $\mu_+(\sigma) = -e'(0) = e'(1)$. In particular, the system is entropy producing ($\mu_+(\sigma) > 0$) iff $e(\alpha)$ is not identically zero on $[0, 1]$.

2. (Strong law of large numbers) For all regular sequences t_n

$$\frac{1}{t_n}\int_0^{t_n} \sigma_s(x)\, ds \to \mu_+(\sigma)$$

for μ-a.e. $x \in M$.

3. If $e(\alpha)$ is differentiable on $\mathbb{R}$, then σ satisfies a LDP w.r.t. (M, ϕ, μ) with the rate function $I(s) = \inf_{\alpha\in\mathbb{R}}(\alpha s + e(\alpha))$. Moreover,

$$I(-s) = I(s) - s$$

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Proof. $I(-s) = \inf_{\alpha\in\mathbb{R}}(-\alpha s + e(\alpha)) = \inf_{\alpha\in\mathbb{R}}(-\alpha s + e(1-\alpha))$
$= \inf_{\alpha\in\mathbb{R}}(-(1-\alpha)s + e(\alpha)) = -s + I(s)$

15. The Evans–Searles fluctuation theorem

Similar conclusions hold for currents $\Phi_X^{(j)}$ if one assumes that the GES function

$$g(X,Y) = \lim_{t\to\infty} \frac{1}{t} \log g_t(X,Y) = \lim_{t\to\infty} \frac{1}{t} \log \mu_X \left(e^{-Y\cdot\int_0^t \mathbf{\Phi}_{X\,s}\, ds} \right)$$

exists. It automatically satisfies the GES-symmetry $g(X, X-Y) = g(X,Y)$.

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exists. It automatically satisfies the GES-symmetry $g(X, X-Y) = g(X,Y)$.

Theorem.

1. If $Y \mapsto g(X,Y)$ is differentiable at $Y=0$ then

$$\langle \mathbf{\Phi}_X \rangle_+ = \mu_{X+}(\mathbf{\Phi}_X) = -\nabla_Y g(X,Y)|_{Y=0}$$

and for any regular sequence t_n

$$\frac{1}{t_n} \int_0^{t_n} \mathbf{\Phi}_{X\,s}(x)\, ds \to \mu_{X+}(\mathbf{\Phi}_X)$$

for μ_X-a.e. $x \in M$.

Proof. Gärtner-Ellis.

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exists. It automatically satisfies the GES-symmetry $g(X,X-Y)=g(X,Y)$.

2. If $g(X,Y)$ is C^2 near $(X,Y)=(0,0)$ then the transport matrix $[L_{jk}]$ is well defined and satisfies the Onsager reciprocity relations.

3. If in addition $\mu_0(\Phi_0^{(k)}\Phi_{0t}^{(j)})=O(t^{-1})$ and, for some $\epsilon>0$,

$$\sup_{Y\in D_\epsilon,t>1}\frac{1}{t}\,|g_t(0,Y)|<\infty$$

then the Fluctuation-Dissipation Theorem holds.

Proof. 2. Since $\langle\Phi_X^{(j)}\rangle_+=\partial_{Y_j}g(X,Y)\big|_{Y=0}$, the GES-symmetry yields

$$L_{jk}=\partial_{X_k}\partial_{Y_j}g(X,Y)\big|_{X=Y=0}=-\frac{1}{2}\partial_{Y_j}\partial_{Y_k}g(X,Y)\big|_{X=Y=0}\Rightarrow L_{jk}=L_{kj}$$

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Similar conclusions hold for currents $\Phi_X^{(j)}$ if one assumes that the GES function

$$g(X,Y) = \lim_{t\to\infty} \frac{1}{t} \log g_t(X,Y) = \lim_{t\to\infty} \frac{1}{t} \log \mu_X \left(e^{-Y\cdot\int_0^t \mathbf{\Phi}_{X\,s}\,ds} \right)$$

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$$\sup_{Y\in D_\epsilon, t>1} \frac{1}{t} |g_t(0,Y)| < \infty$$

then the Fluctuation-Dissipation Theorem holds.

Proof. 3. By our general result the GK-Formula holds iff one can interchange $\lim\limits_{t\to\infty}$ and $\partial_{Y_J}\partial_{Y_k}$. This is ensured by Vitali's theorem. The CLT follows from Bryc's theorem.

15. The Evans–Searles fluctuation theorem

Similar conclusions hold for currents $\Phi_X^{(j)}$ if one assumes that the GES function

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exists. It automatically satisfies the GES-symmetry $g(X, X-Y) = g(X,Y)$.

4. If $Y \mapsto g(X,Y)$ is differentiable on $\mathbb{R}^n$ then the LDP holds for $\mathbf{\Phi}_X$ with the rate function $I_X(s) = \inf_{Y\in\mathbb{R}^n}(Y\cdot s + g(X,Y))$. Moreover,

$$I_X(-s) = I_X(s) - X\cdot s$$

Proof. Again Gärtner-Ellis.

16. The Gallavotti-Cohen fluctuation theorem

Let μ_+ be a NESS of (M, ϕ^t, μ) and assume that the Gallavotti-Cohen function

$$e_+(\alpha) = \lim_{t\to\infty} \frac{1}{t} \log \mu_+ \left(e^{-\alpha \int_0^t \sigma_s \, ds} \right)$$

exists.

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exists.

Remark. In general, unlike the ES-function $e_t(\alpha)$, the finite time GC-function

$$e_{+t}(\alpha) = \log \mu_+ \left(e^{-\alpha \int_0^t \sigma_s \, ds} \right)$$

does not satisfy "the symmetry", i.e. $e_{+t}(1-\alpha) \neq e_{+t}(\alpha)$.

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Definition. The GC symmetry holds if, for all $\alpha \in \mathbb{R}$, $e^+(1-\alpha) = e^+(\alpha)$.

16. The Gallavotti-Cohen fluctuation theorem

Theorem.

If the GC-symmetry holds and $e_+(\alpha)$ is differentiable at $\alpha = 0$ then:

1. $\mu_+(\sigma) = -e'_+(0) = e'_+(1)$. In particular, the system is entropy producing ($\mu_+(\sigma) > 0$) iff $e_+(\alpha)$ is not identically zero on $[0, 1]$.

2. (Strong law of large numbers) For all regular sequences t_n

$$\frac{1}{t_n} \int_0^{t_n} \sigma_s(x)\, ds \to \mu_+(\sigma)$$

for μ_+-a.e. $x \in M$.

3. If $e_+(\alpha)$ is differentiable on $\mathbb{R}$, then σ satisfies a LDP w.r.t. (M, ϕ, μ_+) with the rate function $I_+(s) = \inf_{\alpha\in\mathbb{R}}(\alpha s + e_+(\alpha))$. Moreover,

$$I_+(-s) = I_+(s) - s$$

16. The Gallavotti-Cohen fluctuation theorem

In a similar way, assuming the existence of the GGC-function

$$g_+(X,Y) = \lim_{t\to\infty} \frac{1}{t} \log \mu_+ \left(e^{-Y\cdot \int_0^t \mathbf{\Phi}_{X\,s}\, ds} \right)$$

and the GGC-symmetry $g_+(X, X-Y) = g_+(X,Y)$ yields the fluctuation-dissipation theorem if $g_+(X,Y)$ is C^2.

17. Example: A thermostated ideal gas

Recall that $\sigma = (N-1)\epsilon^{-1/2}F\tanh\xi$ with $\dot{\xi} = \epsilon^{-1/2}F$. If $F \neq 0$, it follows that

$$\lim_{t\to\infty} \sigma_t(L,\theta) = (N-1)\frac{|F|}{\sqrt{\epsilon}},$$

for (Lebesgue)-a.e. (L,θ). In particular $\langle\sigma\rangle_+ = (N-1)\frac{|F|}{\sqrt{\epsilon}} > 0$: The system is entropy producing. Explicit solution of the equations of motion show that the NESS is given by

$$d\mu_+ = \prod_j \delta(L_j - \frac{|F|}{F}\sqrt{\epsilon})\frac{dL_j\, d\theta_j}{2\pi}.$$

Note that it is singular w.r.t. Lebesgue!
It is also easy to show that the ES-function exists and is given by

$$e(\alpha) = \lim_{t\to\infty}\frac{1}{t}e_t(\alpha) = -\langle\sigma\rangle_+\left(\frac{1}{2} - \left|\alpha - \frac{1}{2}\right|\right).$$

It is differentiable near $\alpha = 0$. The ES Fluctuation Theorem yields $e'(0) = -\langle\sigma\rangle_+$ (!), the strong law of large number (much more is true!) and a (local) LDP for σ.

17. Example: A thermostated ideal gas

σ does not fluctuate in the NESS μ_+, and one has

$$e_{+t}(\alpha) = \log \mu_+ \left(e^{-\alpha \int_0^t \sigma_s \, ds} \right) = -\alpha t \langle \sigma \rangle_+$$

The GC-function also exists

$$e_+(\alpha) = \lim_{t \to \infty} \frac{1}{t} e_{+t}(\alpha) = -\alpha \langle \sigma \rangle_+$$

but does not satisfy the symmetry $e_+(1-\alpha) \neq e_+(\alpha)$: The GC Fluctuation Theorem fails!
With F as a control parameter we get $\sigma_F = F\Phi$ with $\Phi = (N-1)\epsilon^{-1/2} \tanh \xi$. The GES-function

$$g(F,Y) = \lim_{t \to \infty} \frac{1}{t} e_t(Y/F) = e(Y/F) = -\frac{N-1}{F\sqrt{\epsilon}} \left(\frac{F}{2} - \left| Y - \frac{F}{2} \right| \right)$$

is not C^2 near $(0,0)$. The ES Fluctuation Theorem does not provide the Fluctuation-Dissipation Theorem.

17. Example: A thermostated ideal gas

In fact, the finite time transport matrix

$$L^t = \partial_F \langle \Phi \rangle_t |_{F=0} = \frac{1}{2} \int_{-t}^{t} \mu(\Phi \Phi_s) \left(1 - \frac{|s|}{t} \right) ds = \frac{t}{2} \mu(\Phi^2) = \frac{(N-1)^2}{N} \frac{t}{2\epsilon} \to \infty$$

diverges as $t \to \infty$.

This does not come as a surprise since

$$\langle \Phi \rangle_+ = \mu_+(\Phi) = \frac{(N-1)}{\sqrt{\epsilon}} \frac{|F|}{F}$$

is not differentiable at $F = 0$.

18. Example: Open harmonic chain

With finite reservoirs, the large time limit

$$\langle \Phi^{(L/R)} \rangle_+ = \lim_{t\to\infty} \frac{1}{t} \int_0^t \mu_X \left(\Phi_s^{(L/R)} \right) ds = \lim_{t\to\infty} \frac{1}{2t} \mathrm{tr} \left(D_X (h_{L/R} - e^{t\mathcal{L}^*} h_{L/R} e^{t\mathcal{L}}) \right) = 0$$

is trivial. To get entropy production we need to take the thermodynamic limit of the reservoir: $n \to \infty$, m fixed.
As $n \to \infty$ the matrices h, h_L, h_R (naturally imbedded in $\mathcal{B}(\ell^2(\mathbb{Z}) \oplus \ell^2(\mathbb{Z}))$) have strong limits. For example

$$h \to \left(\begin{array}{cc} I & 0 \\ 0 & I - \Delta \end{array} \right),$$

where Δ is the finite difference Laplacian on $\ell^2(\mathbb{Z})$. In the same way the generators $\mathcal{L}$, $\mathcal{L}_0$ of the Hamiltonian flow and of the decoupled flow have strong limits and the corresponding groups $e^{t\mathcal{L}}$, $e^{t\mathcal{L}_0}$ converge strongly and uniformly on compact time intervals.

$$\Downarrow$$

$$g_t(X, Y) = -\frac{1}{2} \log\det \left(I + \int_0^t D_X e^{s\mathcal{L}^*} \phi(Y) e^{s\mathcal{L}} ds \right)$$

18. Example: Open harmonic chain

To perform the $t \to \infty$ limit, we note that the wave operators

$$W_\pm = \lim_{t \to \pm\infty} h^{1/2} e^{-t\mathcal{L}} e^{t\mathcal{L}_0} h_0^{-1/2} (p_L + p_R)$$

exist and are complete (Kato-Birman). Explicit calculation of the scattering matrix $S = W_+^* W_-$ then leads to

$$g(X,Y) = \lim_{t \to \infty} g_t(X,Y) = -\frac{1}{\pi} \log \left(\frac{[(\beta - X_L) - (Y_R - Y_L)][(\beta - X_R) - (Y_R - Y_L)]}{(\beta - X_L)(\beta - X_R)} \right)$$

which is real analytic in $\{Y \in \mathbb{R}^2 \mid -(\beta - X_R) < Y_R - Y_L < \beta - X_L\}$. One can show

$$\sup_{Y \in D_\epsilon, t > 1} \frac{1}{t} |g_t(0,Y)| < \infty$$

for small anough ϵ. Finally from local decay estimate for the lattice Klein-Gordon equation

$$|(\delta_x, e^{-it\sqrt{I-\Delta}} \delta_y)| \leq C_{x,y} |t|^{-1/2} \quad \Rightarrow \quad \mu_0(\Phi_0^{(j)} \Phi_{0t}^{(k)}) = O(t^{-1})$$

18. Example: Open harmonic chain

Thus, all conclusions of the ES Fluctuation Theorem hold.

The state μ_{Xt} is Gaussian with covariance $D_{Xt} = e^{t\mathcal{L}} D_X e^{t\mathcal{L}^*}$. Since

$$D_{Xt} \to D_{X+} = h^{-1/2} W_-(\beta - X_L p_L - X_R p_R)^{-1} W_-^* h^{-1/2} \quad \text{(strongly)}$$

the NESS μ_{X+} exists and is Gaussian with covariance D_{X+}.
The GGC-function is thus

$$g_{+t}(X,Y) = -\frac{1}{2} \log\det\left(I + \int_0^t D_{X+} e^{s\mathcal{L}^*} \phi(Y) e^{s\mathcal{L}} ds \right)$$

and one shows

$$g_+(X,Y) = \lim_{t\to\infty} g_{+t}(X,Y) = g(X,Y).$$

It follows that all the conclusions of the GC Fluctuation Theorem also hold.

Remark. The difference $D_X - D_{X+}$ is not trace class, therefore the NESS μ_{X+} is singular w.r.t. the reference state μ_X.

19. The principle of regular entropic fluctuations

Remark. Since, for entropy producing systems, μ and μ_+ are mutually singular, the ES-symmetry and the GC-symmetry are two very different statements. The ES symmetry is a mathematical triviality (even though it has deep consequences) while the GC-symmetry is a true mathematical finesse containing a lot of interesting information about the NESS μ_+.

19. The principle of regular entropic fluctuations

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Cohen-Gallavotti: *Note on two theorems in nonequilibrium statistical mechanics.* J. Stat. Phys. 96, 1343–1349 (1999)

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Consequently one expects the two functions $e(\alpha)$ and $e_+(\alpha)$ as well as the two generalized functions $g(X,Y)$ and $g_+(X,Y)$ to be quite different.

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Consequently one expects the two functions $e(\alpha)$ and $e_+(\alpha)$ as well as the two generalized functions $g(X,Y)$ and $g_+(X,Y)$ to be quite different.

Our main contribution to the subject (as far as classical systems are concerned) is the following

Principle of regular entropic fluctuations. In all systems known to exhibit the GC-symmetry, respectively the GGC-symmetry, one has

$$e_+(\alpha) = e(\alpha), \qquad \text{respectively} \qquad g_+(X,Y) = g(X,Y),$$

which is equivalent to

$$\lim_{t\to\infty}\lim_{s\to\infty}\frac{1}{t}\log\mu_s\left(e^{-\alpha\int_0^t \sigma_\tau\, d\tau}\right) = \lim_{s\to\infty}\lim_{t\to\infty}\frac{1}{t}\log\mu_s\left(e^{-\alpha\int_0^t \sigma_\tau\, d\tau}\right)$$

20. Further examples

- A shift. The left shift on the sequences $x = (x_i)_{i\in\mathbb{Z}} \in \mathbb{R}^{\mathbb{Z}}$ with the measure

$$d\mu(x) = \left(\prod_{i\le 0} F(-x_i)dx_i\right)\left(\prod_{i>0} F(x_i)dx_i\right)$$

  Time revesal is $\vartheta(x)_i = -x_{-i}$ and $d\mu^+(x) = \prod_{i\in\mathbb{Z}} F(x_i)dx_i$. A simple calculation yields

$$e(\alpha) = e^+(\alpha) = \log \int F(x)^\alpha F(-x)^{(1-\alpha)}dx$$

  and one immediately checks that $e(1-\alpha) = e(\alpha)$.
- Linear dynamics of Gaussian random fields
- Markov chains
- Chaotic Homeomorphisms of compact metric spaces
- Anosov diffeomorphisms