Nonequilibrium Statistical Mechanics of Harmonic Networks

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Joint work with
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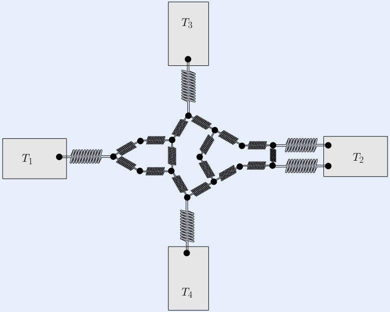
- Experimental verifications [Ciliberto et al., ’05 – ’13, ...]
- Reviews [Rondoni–Mejia-Monasterio ’07, Seifert ’12]
- ”Entropic regularity” [Jakšić–P–Rey-Bellet ’11]

Heat transfers through dynamical networks



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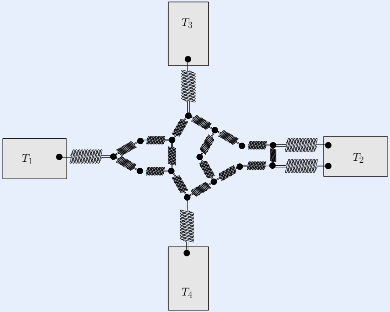

"Thermodynamic Entropy Balance"

Entropy S_{system} is **not** a conserved quantity

$$\frac{\mathrm{d}S_{\text{system}}}{\mathrm{d}t} = -\sum_i \frac{\Phi_i(t)}{T_i} + \sigma(t), \qquad \left\{ \begin{array}{lcl} \Phi_i & = & \text{energy flux to } i^{\text{th}} \text{ reservoir} \\ \sigma & = & \text{entropy production rate} \end{array} \right.$$

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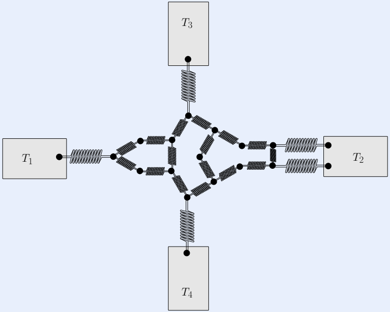


Out of thermal equilibium

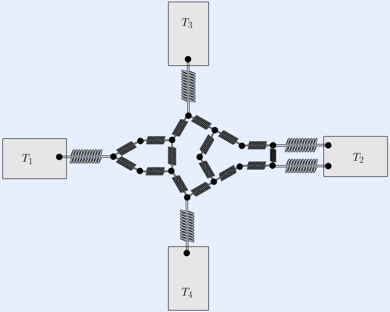
Thermodynamic (Clausius) entropy S_{system} is **not even defined**

But in many cases of interest (Hamiltonian systems, Langevin stochastic dynamics) a microscopic entropy balance equation holds

$$S_{\text{system}} = \text{Gibbs-Shannon entropy},$$

is a state dependent quantity.

Heat transfers through dynamical networks



"1 st and 2nd Law" for steady states

$$\sum_i \langle \Phi_i(t) \rangle_{\text{steady state}} = 0, \qquad \langle \sigma(t) \rangle_{\text{steady state}} = \sum_i \frac{\langle \Phi_i(t) \rangle_{\text{steady state}}}{T_i} \geq 0,$$

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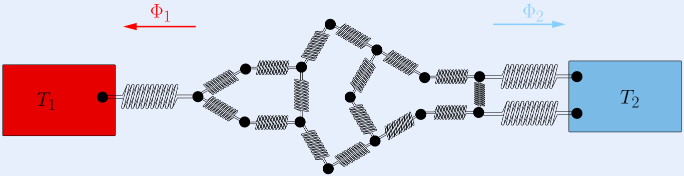
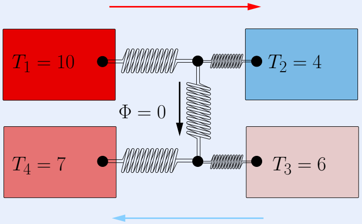


Steady state with $T_1 > T_2$

$$\langle\Phi_1\rangle + \langle\Phi_2\rangle = 0, \quad \frac{\langle\Phi_1\rangle}{T_1} + \frac{\langle\Phi_2\rangle}{T_2} \geq 0 \quad \Rightarrow \langle\Phi_2\rangle = -\langle\Phi_1\rangle \geq 0$$

Heat transfers through dynamical networks



Strange heat fluxes [Eckmann-Zabey '04]

$$\sum_{i=1}^{4} \frac{\langle \Phi_i \rangle}{T_i} \geq 0, \quad \text{but} \quad \frac{\langle \Phi_3 \rangle}{T_3} + \frac{\langle \Phi_4 \rangle}{T_4} < 0$$

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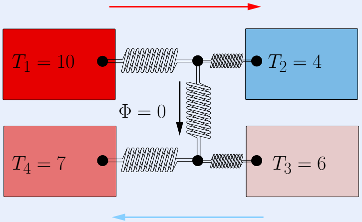

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Understanding the statistics of entropy production is fundamental for heat pump engineering, and much more ($\rightarrow$ next talk by Tristan Benoist)!

Fluctuation "Theorems"

No matter how the entropy production rate σ is defined, the fact that $\langle\sigma(t)\rangle \geq 0$ does not preclude the entropy production $\mathfrak{S}_t = \int_0^t \sigma(s)\mathrm{d}s$ to become negative.

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Fluctuation theorems give **universal** quantitative information on the probability of such violations of the 2$^{\mathrm{nd}}$ law. Roughly stated, $\mathfrak{S}_t$ satisfies a FT whenever

$$\frac{\mathbb{P}[\mathfrak{S}_t = st]}{\mathbb{P}[\mathfrak{S}_t = -st]} \simeq \mathrm{e}^{st}, \qquad (s \in \mathbb{R}, t \to \infty)$$

i.e., Negative values of $\mathfrak{S}_t$ are exponentially suppressed as $t \to \infty$.

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As stressed by [Gallavotti-Cohen ’95], the physically interesting and mathematically non-trivial aspects of FT can be formulated in terms of **large deviations**.

Fluctuation "Theorems"

A functional $\mathfrak{S}_t$ of a dynamical/stochastic process satisfies a FT if:

$$\lim_{t\to\infty}\frac{1}{t}\log\mathbb{P}\left[\frac{1}{t}\mathfrak{S}_t\in\mathcal{O}\right]=-\inf_{s\in\mathcal{O}}I(s) \qquad (1)$$

for all open sets $\mathcal{O}\subset\mathbb{R}$ with a rate function satisfying

$$I(-s)-I(s)=s, \qquad (s\in\mathbb{R}) \qquad (2)$$

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$$I(-s) - I(s) = s, \qquad (s \in \mathbb{R}) \qquad (2)$$

Gärtner-Ellis theorem relates $I(s)$ to the CGF of $\mathfrak{S}_t$

$$I(s) = \sup_{\alpha}(\alpha s - e(-\alpha)), \qquad e(\alpha) \equiv \lim_{t\to\infty} \frac{1}{t} \log \mathbb{E}_\mu[\mathrm{e}^{-\alpha \mathfrak{S}_t}]$$

FT (2) translates into *Gallavotti-Cohen symmetry*

$$e(1-\alpha) = e(\alpha), \qquad (\alpha \in \mathbb{R}) \qquad (3)$$

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(a) steady state/transient FT $\leftrightarrow$ stationary/non-stationary process

(b) local FT $\leftrightarrow$ (1) only holds for $\mathcal{O}\subset]s_-,s_+[$

(c) a given system may have several, distinct functionals satisfying a FT

Positive Results

- [Gallavotti–Cohen '95, Ruelle '99] *Global steady-state FT* for the phase-space contraction of strongly chaotic dynamical systems.

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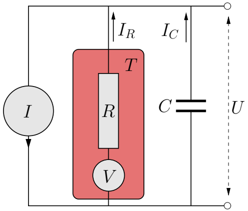
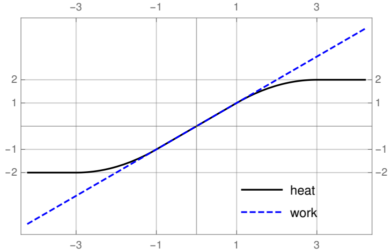
- [Rey-Bellet–Thomas '02] For transient quasi-Markovian anharmonic chains the GC symmetry holds for the entropy flux $\mathfrak{S}_t = \int_0^t (\frac{\Phi_1(s)}{T_1} + \frac{\Phi_2(s)}{T_2})\mathrm{d}s$ on $]-\delta, 1+\delta[$ for some $\delta > 0$. This yields a *local transient FT*.
- [Jakšić–P–Shirikyan '15] For regular enough transient Gaussian dynamical systems the GC symmetry holds on some open interval $]-\delta, 1+\delta[$ and yields a *global transient FT* for some natural entropy production functional.

Negative Results

- [Farago, '02, van Zon-Cohen '03, Visco '06,...] In some *linear* stochastic models one observes a breakdown of the symmetry leading to the concept of *extended fluctuation relations* $I(-s) - I(s) = \mathfrak{s}(s)$.





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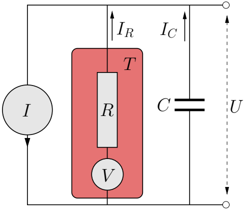

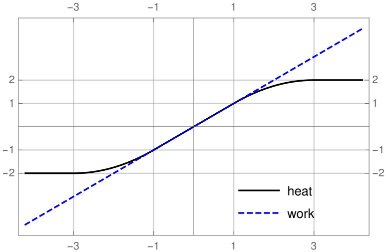

- [Jakšić-P-Shirikyan '15] For stationary Gaussian dynamical systems the symmetry only holds on some open interval $]-\delta, \delta[$ ($\delta > 0$). One can cook up simple examples where $\delta < 1/2$ and where $e(\alpha) = +\infty$ for $|\alpha| > \delta$.

The Folklore

Let $\mathfrak{S}_t$ be a putative entropy production for a process with state variable x_t

- The CGF $e(\alpha)$ of $\mathfrak{S}_t$ can be $+\infty$ outside an interval $[\alpha_-, \alpha_+] \ni 0$.
- If $\frac{1}{2} \in]\alpha_-, \alpha_+[$ then for $|\alpha - \frac{1}{2}| < \min(\alpha_+ - \frac{1}{2}, \frac{1}{2} - \alpha_-)$

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- For systems with compact phase space, adding a boundary term $f(x_t) - g(x_0)$ to $\mathfrak{S}_t$ does not affect its CGF. This is not so for non-compact phase space: $[\alpha_-, \alpha_+]$ may depend on f and g.

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Our main interest in harmonic networks is to substantiate this folklore on a well defined, simple but non trivial class of nonequilibrium dynamical systems.

Model

$$\mathbb{R}^{\mathcal{I}} \oplus \mathbb{R}^{\mathcal{I}} \ni (p, q) \mapsto H(p, q) = \frac{1}{2}|p|^2 + \frac{1}{2} q \cdot \omega^2 q, \qquad \omega > 0$$

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$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}$$

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$$\partial\mathcal{I} \subset \mathcal{I}, \qquad \sigma : \mathbb{R}^{\partial\mathcal{I}} \to \mathbb{R}^{\mathcal{I}}, \qquad T : \mathbb{R}^{\partial\mathcal{I}} \to \mathbb{R}^{\partial\mathcal{I}}$$

$$(\sigma u)_i = \begin{cases} \sqrt{2\gamma_i} u_i & i \in \partial\mathcal{I} \\ 0 & i \in \mathcal{I} \setminus \partial\mathcal{I} \end{cases} \qquad (Tu)_i = T_i u_i$$

$$\mathbb{E}[\dot{w}_i(t)] = 0, \qquad \mathbb{E}[\dot{w}_i(s)\dot{w}_j(t)] = \delta_{ij}\delta(t-s) \qquad (i,j \in \partial\mathcal{I})$$

Time reversal $\theta : (p,q) \mapsto (-p,q)$

Fokker-Planck operator

$$x = \begin{bmatrix} p \\ \omega q \end{bmatrix}, \quad Q = \begin{bmatrix} \sigma T^{1/2} \\ 0 \end{bmatrix}, \quad \Omega = \begin{bmatrix} 0 & -\omega \\ \omega & 0 \end{bmatrix},$$

$$\Gamma = Q T^{-1} Q^*, \qquad B = QQ^*, \qquad A = \Omega - \frac{1}{2}\Gamma$$

$$\mathrm{d}x_t = Ax_t \mathrm{d}t + B\mathrm{d}w_t \quad \Rightarrow L = \frac{1}{2}\nabla \cdot B\nabla - Ax \cdot \nabla$$

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Kalman Condition: (A, Q) is controllable

$$\bigvee_n \mathrm{Ran}(A^n Q) = \mathbb{R}^{\mathcal{I}} \oplus \mathbb{R}^{\mathcal{I}}$$

$$\Downarrow$$

L is hypoelliptic with unique ”ground state”

The process has an ergodic (even mixing) invariant measure μ with a smooth and strictly positive density (a Gaussian!)

Entropy (heat) dissipation

Work of Langevin forces

$$\mathrm{d}H = LH\mathrm{d}t + Q^T x \cdot \mathrm{d}w = \sum_{i \in \partial \mathcal{I}} \mathrm{d}\phi_i$$

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Dissipated entropy

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Entropy flux is a “natural” functional from physical perspective

$$\mathfrak{S}_t = \int_0^t \mathrm{d}\mathfrak{S} = -\int_0^t \left(T^{-1}Q^*x \cdot \mathrm{d}w - \frac{1}{2}|T^{-1}Q^*x|^2\mathrm{d}t - \tfrac{1}{2}\mathrm{tr}(QT^{-1}Q^*)\mathrm{d}t \right)$$

The Mother of GC-symmetry

The “Traditional” approach to FT

Choose your favorite physically relevant quantity (work performed on the system, heat dissipated in the reservoirs, phase space contraction rate,...) compute its CGF and show by some clever tricks that it satisfies/does not satisfy the symmetry.

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Example. In our model, $\mathfrak{S}_t$ has a CGF

$$e_{\mathfrak{S}}(\alpha) = \lim_{t\to\infty} \frac{1}{t} \log \mathbb{E}\left[\mathrm{e}^{-\alpha\mathfrak{S}_t}\right]$$

which is finite on $]-\delta, 1[$ for some $\delta > 0$ and infinite on the complement of $[-\delta, 1]$. It satisfies the GC symmetry on $]0, 1[$

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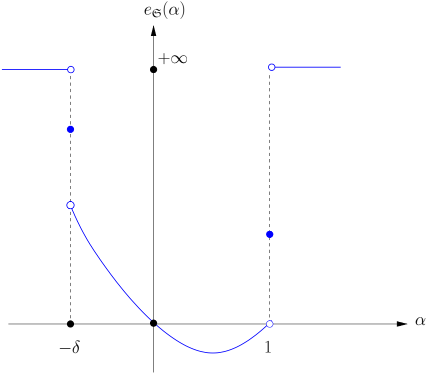

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A canonical construction [Jakšić–P–Rey-Bellet ’11]

Radically different philosophy: define a canonical entropy production functional Ep_t which **by construction** satisfies the symmetry. Whether or not a given physical quantity also satisfies the symmetry depends on how it is related to Ep_t.

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- θ measurable involution of Ω s.t. $\widetilde{\mathbb{P}} = \mathbb{P} \circ \theta \sim \mathbb{P}$
- Canonical entropy production

$$\mathrm{Ep} = \log \frac{\mathrm{d}\mathbb{P}}{\mathrm{d}\widetilde{\mathbb{P}}} = -\mathrm{Ep} \circ \theta$$

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- Expected value = Relative entropy

$$\int \mathrm{Ep} \, \mathrm{d}\mathbb{P} = \mathrm{Ent}(\mathbb{P}|\widetilde{\mathbb{P}}) \geq 0$$

with equality iff $\widetilde{\mathbb{P}} = \mathbb{P}$

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- If the symmetry θ is broken $\widetilde{\mathbb{P}} \neq \mathbb{P}$ then $\mathbb{P}$ favors positive values of Ep
- The CGF of Ep is Rényi's relative α-entropy

$$e(\alpha) = \log \int \mathrm{e}^{-\alpha \mathrm{Ep}} \mathrm{d}\mathbb{P} = \mathrm{Ent}_\alpha(\widetilde{\mathbb{P}}|\mathbb{P})$$

The Mother of GC-symmetry

Rényi relative α-entropy of two equivalent measures $\mu \sim \nu$ is defined by

$$\mathrm{Ent}_\alpha(\nu|\mu) = \log \int \left(\frac{\mathrm{d}\nu}{\mathrm{d}\mu}\right)^\alpha \mathrm{d}\mu.$$

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- convex function of α
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- non-positive for $\alpha \in]0, 1[$
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- trivially satisfies

$$\mathrm{Ent}_{1-\alpha}(\nu|\mu) = \mathrm{Ent}_\alpha(\mu|\nu)$$

- vanishes identically iff $\mu = \nu$

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- The laws P and $\tilde{P}$ of Ep and $-\mathrm{Ep}$ satisfy the FT

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- In applications to dynamical processes, $\mathbb{P}$ is the path-space measure for a finite time interval $[0, t]$ and θ is time-reversal

Martingales

Path-space: $C([0,\tau], \mathbb{R}^{\mathcal{I}} \oplus \mathbb{R}^{\mathcal{I}})$
Path-space measure: $\mathbb{P}_{\mu}^{\tau}$ (stationary Markov process)
Time-reversal: $\Theta^{\tau}(x)_t = \theta x_{\tau - t}$
Time-reversed path-space measure: $\widetilde{\mathbb{P}}_{\mu}^{\tau} = \mathbb{P}_{\mu}^{\tau} \circ \Theta^{\tau}$

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Theorem I

(i) Canonical entropy production is a modification of the entropy flux by boundary terms

$$\widetilde{\mathbb{P}}_\mu^\tau \sim \mathbb{P}_\mu^\tau \quad \text{and} \quad \mathrm{Ep}_\tau = \log\frac{\mathrm{d}\mathbb{P}_\mu^\tau}{\mathrm{d}\widetilde{\mathbb{P}}_\mu^\tau} = \mathfrak{S}_\tau - \log\frac{\mathrm{d}\mu}{\mathrm{d}x}(\theta x_\tau) + \log\frac{\mathrm{d}\mu}{\mathrm{d}x}(x_0)$$

(ii) The limit

$$e(\alpha) = \lim_{\tau\to\infty}\frac{1}{\tau}\log\int \mathrm{e}^{-\alpha\mathrm{Ep}_\tau}\mathrm{d}\mathbb{P}_\mu^\tau$$

exists for all $\alpha\in\mathbb{R}$

The maximal CGF

Let $\beta \in L(\mathbb{R}^{\mathcal{I}} \oplus \mathbb{R}^{\mathcal{I}})$ be such that

$$\theta\beta = \beta\theta, \qquad \beta Q = QT^{-1}$$

and set

$$\mathrm{d}\mu_\beta(x) = \mathrm{e}^{-\frac{1}{2}x\cdot\beta x}\mathrm{d}x, \qquad \sigma_\beta(x) = \frac{1}{2}x \cdot \Sigma_\beta x, \qquad \Sigma_\beta = [\Omega, \beta]$$

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Theorem II

- $\mathrm{Ep}_t = \int_0^t \sigma_\beta(x_s)\mathrm{d}s - \log\frac{\mathrm{d}\mu}{\mathrm{d}\mu_\beta}(\theta x_\tau) + \log\frac{\mathrm{d}\mu}{\mathrm{d}\mu_\beta}(x_0)$
- $E(\nu) = Q^*(A^* - \mathrm{i}\nu)^{-1}\Sigma_\beta(A + \mathrm{i}\nu)^{-1}Q$ is independent of the choice of β

$$\varepsilon_- = \min_{\nu\in\mathbb{R}} \operatorname{minspec}(E(\nu)) \leq 0, \quad 0 \leq \varepsilon_+ = \max_{\nu\in\mathbb{R}} \operatorname{maxspec}(E(\nu)) < 1$$

$$\kappa_c = \frac{1}{\varepsilon_+} - \frac{1}{2} \geq \frac{1}{2}\frac{\vartheta_{\max}+\vartheta_{\min}}{\vartheta_{\max}-\vartheta_{\min}} > \frac{1}{2}$$

- $$e(\alpha) = \begin{cases} \int_{-\infty}^{\infty} \log\det(I - \alpha E(\nu))\frac{\mathrm{d}\nu}{4\pi} & |\alpha - \frac{1}{2}| \leq \kappa_c \\ +\infty & |\alpha - \frac{1}{2}| > \kappa_c \end{cases}$$

The maximal CGF

Let

$$K_\alpha = \begin{bmatrix} -A_\alpha & B \\ C_\alpha & A_\alpha^* \end{bmatrix}, \qquad A_\alpha = (1-\alpha)A + \alpha\theta A\theta, \qquad C_\alpha = \alpha(1-\alpha)QT^{-2}Q^*$$

Corollary

- $e(\alpha)$ is continuous on $\bar{\mathfrak{I}}_c = [\frac{1}{2} - \kappa_c, \frac{1}{2} + \kappa_c]$ and has an analytic continuation to the cut plane $(\mathbb{C} \setminus \mathbb{R}) \cup]\frac{1}{2} - \kappa_c, \frac{1}{2} + \kappa_c[$.
- Either $\kappa_c = \infty$ and $e(\alpha) \equiv 0$, or $\kappa_c < \infty$ and $e(\alpha)$is strictly convex on $\bar{\mathfrak{I}}_c$

$$\begin{cases} e(\alpha) \le 0 & |\alpha - \frac{1}{2}| \le \frac{1}{2} \\ e(\alpha) \ge 0 & |\alpha - \frac{1}{2}| \ge \frac{1}{2} \end{cases}$$

- If $\kappa_c < \infty$ then $e'(1) = -e'(0) = \mathrm{ep} > 0$ and

$$\lim_{\alpha \downarrow \frac{1}{2} - \kappa_c} e'(\alpha) = -\infty, \qquad \lim_{\alpha \uparrow \frac{1}{2} + \kappa_c} e'(\alpha) = +\infty$$

-

$$e(\alpha) = \frac{1}{4}\mathrm{tr}(QT^{-1}Q^*) - \frac{1}{4} \sum_{k \in \mathrm{spec}(K_\alpha)} |\mathrm{Re}\, k| m_k$$

Global LDP for the canonical entropy production

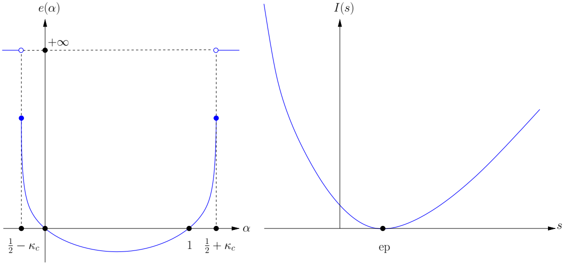
Theorem III

$$\liminf_{t\to\infty} \frac{1}{t}\log \mathbb{P}_\mu\left[\frac{\mathrm{Ep}_t}{t}\in C\right] \geq -\inf_{s\in C} I(s)$$

$$\limsup_{t\to\infty} \frac{1}{t}\log \mathbb{P}_\mu\left[\frac{\mathrm{Ep}_t}{t}\in O\right] \leq -\inf_{s\in O} I(s)$$

$$I(s) = \sup_\alpha(\alpha s - e(-\alpha))$$

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



The Algebraic Riccati Equation

Theorem IV

For $\alpha \in \bar{\mathfrak{I}}_c$ the matrix equation

$$XBX - XA_\alpha - A_\alpha^* X - C_\alpha = 0 \tag{3}$$

has a maximal symmetric solution X_α, a real-analytic concave function of α such that

$$X_\alpha \begin{cases} < 0 & \text{for} \quad \alpha \in]\frac{1}{2} - \kappa_c, 0[; \\ = 0 & \text{for} \quad \alpha = 0; \\ > 0 & \text{for} \quad \alpha \in]0, \frac{1}{2} + \kappa_c[; \end{cases}$$

(3) is an algebraic Riccati equation whose solutions are closely related to some invariant subspaces of K_α. It appears in many problems of linear control/filtering. Efficient numerical algorithms are available to compute the maximal solution.

Perturbations of Ep_t by boundary terms

Consider the CGF

$$g_t(\alpha) = \frac{1}{t}\log\int \mathrm{e}^{\mathrm{Ep}_t + \Phi(x_t) - \Psi(x_0)}\mathrm{d}\mathbb{P}_\nu^t, \qquad \Phi(x) = \tfrac{1}{2}x\cdot Fx, \quad \Psi(x) = \tfrac{1}{2}x\cdot Gx$$

where ν is Gaussian with covariance N. Denote by $\widehat{N}$ the Moore-Penrose inverse of N and P_ν the projection on $\mathrm{Ran}N$.

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where ν is Gaussian with covariance N. Denote by $\widehat{N}$ the Moore-Penrose inverse of N and P_ν the projection on $\mathrm{Ran}N$.

Theorem V

- $g_t(\alpha)$ is finite on some interval $]\alpha_-(t),\alpha_+(t)[$ and infinite on the closure of its complement.
  - Either $\alpha_-(t)=-\infty$ or $\lim_{\alpha\downarrow\alpha_-(t)} g_t'(\alpha)=-\infty$
  - Either $\alpha_+(t)=+\infty$ or $\lim_{\alpha\uparrow\alpha_+(t)} g_t'(\alpha)=+\infty$
- Let $\mathfrak{I}_\infty=\mathfrak{I}_-\cap\mathfrak{I}_+$ where

$$\mathfrak{I}_- = \{\alpha\in\bar{\mathfrak{I}}_c \,|\, \theta X_{1-\alpha}\theta+\alpha(X_1+F)>0\}$$

$$\mathfrak{I}_+ = \{\alpha\in\bar{\mathfrak{I}}_c \,|\, \widehat{N}+P_\nu(X_\alpha-\alpha(G+\theta X_1\theta))|_{\mathrm{Ran}N}>0\}$$

  then $\lim_{t\to\infty} g_t(\alpha)=e(\alpha)$ for $\alpha\in\mathfrak{I}_\infty$.
- Let $\alpha_- = \inf\mathfrak{I}_\infty$, $\alpha_+=\sup\mathfrak{I}_\infty$. Then

$$\lim_{t\to\infty}\alpha_\pm(t)=\alpha_\pm, \qquad \lim_{t\to\infty} g_t(\alpha)=+\infty,\ \text{for } \alpha\notin[\alpha_-,\alpha_+]$$

LDP for perturbations of Ep_t

Set

$$\eta_- = \begin{cases} -\infty & \text{if } \alpha_+ = \frac{1}{2} + \kappa_c \\ e'(\alpha_+) & \text{if } \alpha_+ < \frac{1}{2} + \kappa_c \end{cases} \qquad \eta_+ = \begin{cases} +\infty & \text{if } \alpha_- = \frac{1}{2} - \kappa_c \\ e'(\alpha_+ = -) & \text{if } \alpha_- > \frac{1}{2} - \kappa_c \end{cases}$$

Theorem VI

- Under the law $\mathbb{P}_\nu$ the functional $S_t = \mathrm{Ep}_t + \Phi(x_t) - \Psi(x_0)$ satisfies a **global LDP** with rate function

$$J(s) = \begin{cases} -s\alpha_+ - e(\alpha_+) & \text{if } s < \eta_- \\ I(s) & \text{if } \eta_- \le s \le \eta_+ \\ -s\alpha_- - e(\alpha_-) & \text{if } s > \eta_+ \end{cases}$$

- $J(-s) - J(s) < s$ for $s > \max(-\eta_-, \eta_+)$, i.e., S_t satisfies an extended FT.

LDP for perturbations of Ep_t

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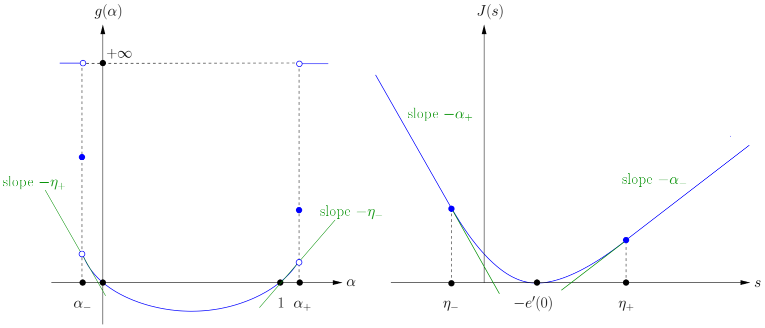
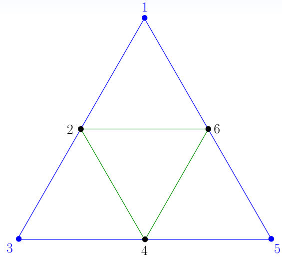
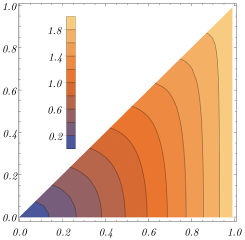
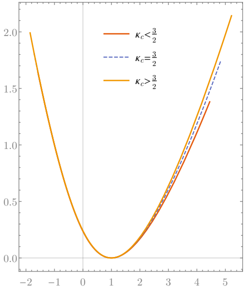
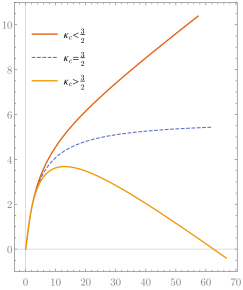


Example: a triangular network

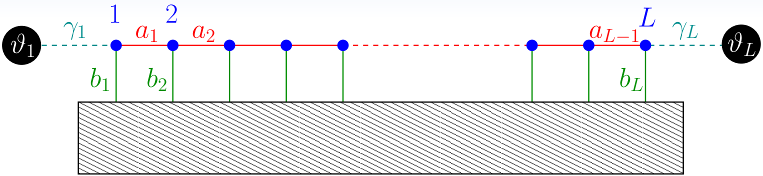








Example: Jacobi chains



$$\frac{1}{2}|\omega q|^2 = \frac{1}{2}\sum_{i=1}^{L} b_i q_i^2 + \sum_{i=1}^{L-1} a_i q_i q_{i+1}$$

Theorem VII

- Assuming $\omega > 0$ and $a_1 \cdots a_{L-1} \neq 0$, the chain is controllable.
- If $\vartheta_1 \neq \vartheta_L$, then $\mathrm{ep} > 0$.
- If the chain is symmetric, then

$$\kappa_c = \kappa_0 := \frac{1}{2}\frac{\vartheta_{\max}+\vartheta_{\min}}{\vartheta_{\max}-\vartheta_{\min}}$$

otherwise $\kappa_c > \kappa_0$.

Open Problems

- External forcing (work statistics)
- LDP for fluctuations of individual fluxes
- Get sharper estimates on κ_c in terms of the topology of the network and its symmetries
- Martingale approach to anharmonic networks