Nonequilibrium Statistical Mechanics of Harmonic Networks

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Joint work with
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Background

LDP for entropy production
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- Reviews [Rondoni–Mejia-Monasterio '07, Seifert '12]
- "Entropic regularity" [Jakšić–P–Rey-Bellet '11]

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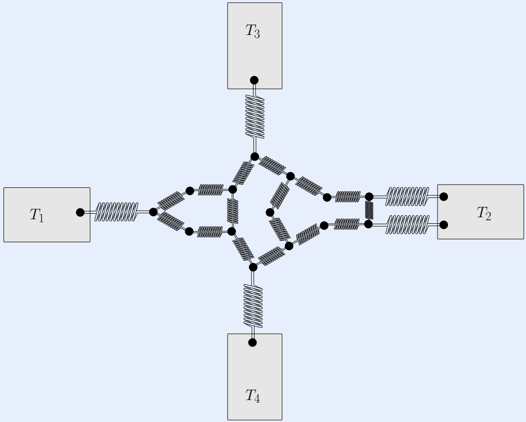

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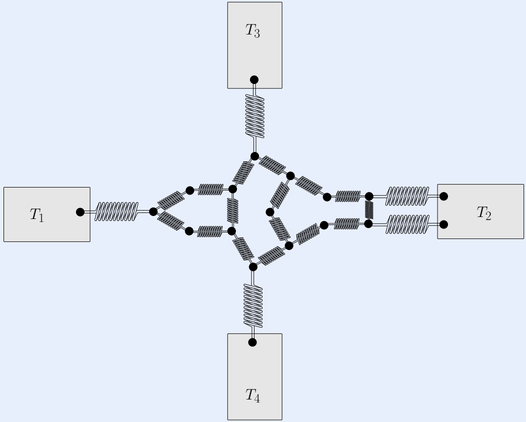

"Entropy Production"

$$\dot{S}_t = \sum_i \frac{\Phi_i(t)}{T_i}, \qquad \Phi_i = \text{Energy flux from system to } i^{\text{th}} \text{ reservoir}$$

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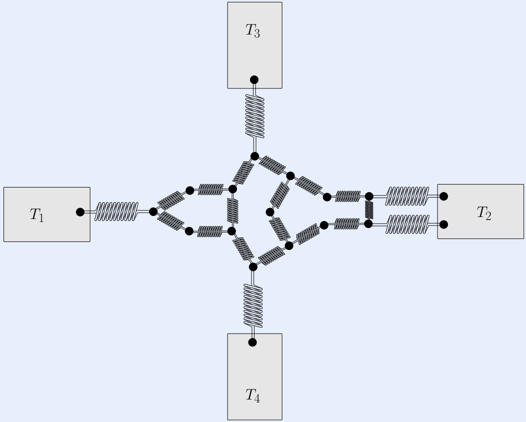

"1st and 2nd Law"

$$\sum_i \langle \Phi_i \rangle_{\text{steady state}} = 0, \qquad \left\langle \frac{S_t}{t} \right\rangle_{\text{steady state}} = \sum_i \frac{\langle \Phi_i \rangle_{\text{steady state}}}{T_i} \geq 0,$$

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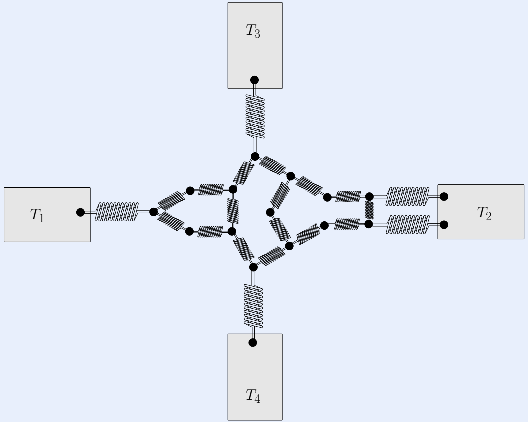

Strange heat fluxes [Eckmann-Zabey '04]

$$\frac{\langle \Phi_1 \rangle_{\text{steady state}}}{T_1} + \frac{\langle \Phi_2 \rangle_{\text{steady state}}}{T_2} < 0$$

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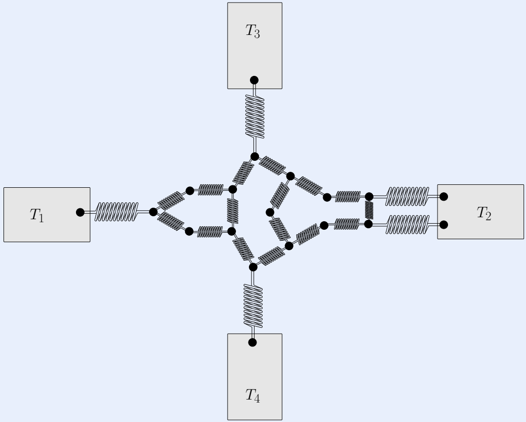

Instantaneous fluctuations can violate the 2nd Law

$\mathrm{Prob}[S_t < 0] \neq 0$ (but expected to be small for large t)

Fluctuation "Theorems"

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

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

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

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

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

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(a) steady state/transient FT $\leftrightarrow$ stationary/non-stationary process
(b) Local FT $\leftrightarrow$ (1) only holds for $\mathcal{O} \subset]s_-, s_+[$

Positive Results

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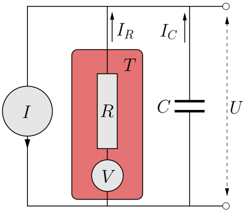
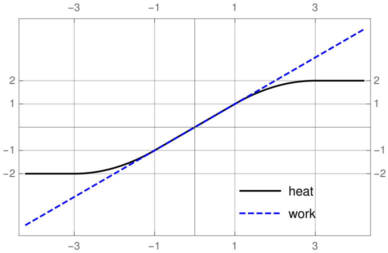
- [Rey-Bellet–Thomas '02] For transient quasi-Markovian anharmonic chains the symmetry holds on $]-\delta, 1+\delta[$ for some $\delta > 0$. This yields a *local transient FT*.
- [Jakšić–P–Shirikyan '15] For regular enough transient Gaussian dynamical systems the symmetry holds on some open interval $]-\delta, 1+\delta[$ 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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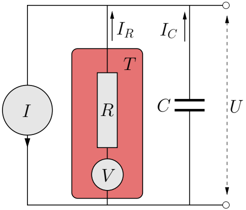

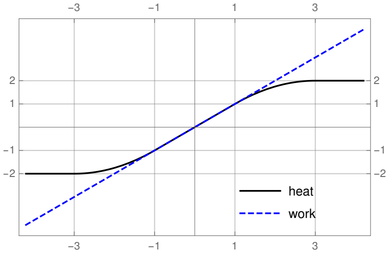

- [Jakšić-P-Shirikyan '15] For stationary Gaussian dynamical systems the symmetry only holds on some open interval $]-\delta, \delta[$ ($\delta > 0$). One can cook up simple examples where $\delta < 1/2$ and where $e(\alpha) = +\infty$ for $|\alpha| > \delta$.

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- There should be a simple modification of the entropy production functional S_t (a cocycle) which yields the **maximal** interval of finiteness of its CGF.
- The Gärtner-Ellis theorem only yields a **global** LDP if the maximal CGF is steep, i.e., as $\alpha \to \alpha_\pm$ either $e(\alpha)$ or $e'(\alpha)$ diverges.

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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$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i} - \frac{1}{2}(\sigma\sigma^* p)_i + (\sigma T^{1/2} \dot{w})_i$$

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

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

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

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

Non-selfadjoint ☺ Fokker-Planck operator

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

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

$$L = \frac{1}{2}\nabla \cdot B\nabla - Ax \cdot \nabla$$

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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 with a smooth strictly positive density μ

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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Entropy production (in NESS)

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

A formal Girsanov formula

$$\mathrm{d}(\mathrm{e}^{-\alpha\mathfrak{S}_t} f(x_t)) = \mathrm{e}^{-\alpha\mathfrak{S}_t}\big[(L_\alpha f)(x_t)\mathrm{d}t$$
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But "the Devil hides in the details", unboundedness of the phase space raises difficulties to:

- justify Girsanov formula (martingale problem)
- control the "prefactor" $\langle \mu | \Phi_\alpha \rangle \langle \Psi_\alpha | 1 \rangle$
- What can we say about $e(\alpha)$?

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

Radically different philosophy: any system has 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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- Probability space $(\Omega, \mathbb{P}, \mathcal{P})$
- θ measurable involution of Ω s.t. $\widetilde{\mathbb{P}} = \mathbb{P} \circ \theta \sim \mathbb{P}$
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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

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

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

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- trivially satisfies
$$\mathrm{Ent}_{1-\alpha}(\nu|\mu) = \mathrm{Ent}_\alpha(\mu|\nu)$$
- vanishes identically iff $\mu = \nu$

The Mother of GC-symmetry

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

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

- convex function of α
- vanishing for $\alpha \in \{0, 1\}$
- non-positive for $\alpha \in]0, 1[$
- non-negative for $\alpha \notin [0, 1]$
- real-analytic on some interval $I \supset]0, 1[$ and infinite on the complement of its closure
- trivially satisfies

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

- vanishes identically iff $\mu = \nu$

CGF of Ep satisfies GC symmetry

$$e(\alpha) = \mathrm{Ent}_\alpha(\widetilde{\mathbb{P}}|\mathbb{P}) = \mathrm{Ent}_{1-\alpha}(\mathbb{P}|\widetilde{\mathbb{P}}) = \mathrm{Ent}_{1-\alpha}(\widetilde{\mathbb{P}}|\mathbb{P}) = e(1-\alpha)$$

The Mother of GC-symmetry

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

$$\frac{\mathrm{d}P}{\mathrm{d}\tilde{P}}(s) = e^{s}$$

The Mother of GC-symmetry

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$$\frac{\mathrm{d}P}{\mathrm{d}\tilde{P}}(s) = e^s$$

- 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: $\mathbb{P}_\mu$
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)

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

(ii) The limit

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

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

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

$$\varepsilon_- = \min_{\nu\in\mathbb{R}} \mathrm{spec}(E(\nu)) \le 0, \quad 0 \le \varepsilon_+ = \max_{\nu\in\mathbb{R}} \mathrm{spec}(E(\nu)) < 1$$

$$\kappa_c = \frac{1}{\varepsilon_+} - \frac{1}{2} > \frac{1}{2}$$

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

The maximal CGF

Let

$$K_\alpha = \begin{bmatrix} -A_\alpha & B \\ C_\alpha & A_\alpha^* \end{bmatrix}$$

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 $\bar{\mathfrak{I}}_c$

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

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

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

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

LDP for the canonical entropy production S_t

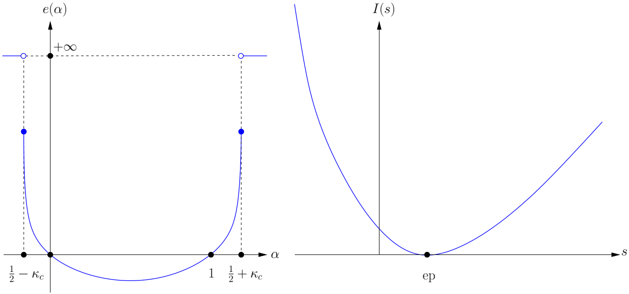
Theorem III

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

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

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

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



The Algebraic Riccati Equation

Theorem IV

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

$$XBX - XA_\alpha - A_\alpha^* X - C_\alpha = 0$$

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

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

Cocycle perturbations of S_t

Consider the CGF

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

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 cocycle perturbations of S_t

Set

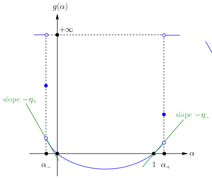
$$\eta_- = \begin{cases} -\infty & \text{if } \alpha_+ = \frac{1}{2} + \kappa_c \\ e'(\alpha_+) & \text{if } \alpha_+ < \frac{1}{2} + \kappa_c \end{cases} \qquad \eta_+ = \begin{cases} +\infty & \text{if } \alpha_- = \frac{1}{2} - \kappa_c \\ e'(\alpha_+ = -) & \text{if } \alpha_- > \frac{1}{2} - \kappa_c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

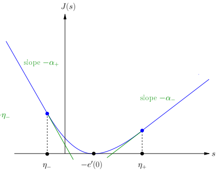
Theorem VI

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

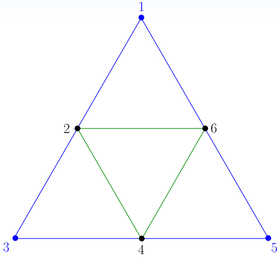
$$J(s) = \begin{cases} -s\alpha_+ - e(\alpha_+) & \text{if } s < \eta_- \\ I(s) & \text{if } \eta_- \le s \le \eta_+ \\ -s\alpha_- - e(\alpha_-) & \text{if } s > \eta_+ \end{cases}$$

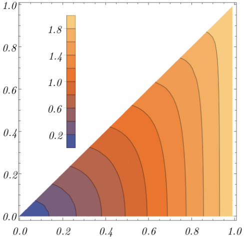
- $J(-s) - J(s) < s$ for $s > \max(-\eta_-, \eta_+)$

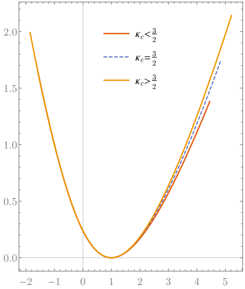


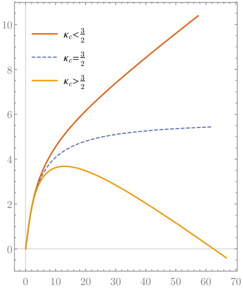


Example


1
2
6
3
4
5


1.8
1.4
1.0
0.6
0.2
0.0 0.2 0.4 0.6 0.8 1.0


$\kappa_c<\frac{3}{2}$
$\kappa_c=\frac{3}{2}$
$\kappa_c>\frac{3}{2}$
0.0 0.5 1.0 1.5 2.0
−2 −1 0 1 2 3 4 5


$\kappa_c<\frac{3}{2}$
$\kappa_c=\frac{3}{2}$
$\kappa_c>\frac{3}{2}$
0 2 4 6 8 10
0 10 20 30 40 50 60 70

Open Problems

- External forcing
- LDP for fluctuations of individual fluxes
- Develop the martingale approach to anharmonic networks