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 → Transient Fluctuation Theorem

- Gallavotti–Cohen [95]: Chaotic hypothesis and nonequilibrium steady state ensembles (à la Ruelle) → 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 \(\sigma\)-field
- Dynamics \((\phi^t)_{t \in T}\): \(T = \mathbb{Z}\) or \(\mathbb{R}\) (continuous) group of homeomorphisms of \(M\)
- Reference state \(\mu\): \(\mu \in \mathcal{P}\), 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: \(\vartheta\) 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 $t \in \mathcal{T}$

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

$$f_t = f \circ \phi^t, \quad \mu_t(f) = \mu(f_t)$$
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Notation:

\[
P_I = \{\mu \in \mathcal{P} | \forall t \in \mathcal{T} : \mu_t = \mu\} \quad \text{(steady states)}
\]

\[
P_\mu = \{\nu \in \mathcal{P} | \nu \ll \mu\} \quad \text{\((\mu\)-normal states)}
\]

\[
\mu \sim \nu \iff \mu \ll \nu \text{ and } \nu \ll \mu \quad \text{(equivalent states)}
\]

For \(\nu \in \mathcal{P}_\mu\):

\[
\Delta_{\nu|\mu} = \frac{d\nu}{d\mu}, \quad \ell_{\nu|\mu} = \log \Delta_{\nu|\mu}
\]
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Relative entropy: For \(\mu, \nu \in \mathcal{P}\)

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

Note: \(\text{Ent}(\nu|\mu) = 0 \iff \nu = \mu\).
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Rényi relative \(\alpha\)-entropy: For \(\mu, \nu \in \mathcal{P}\) and \(\alpha \in \mathbb{R}\)

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

\[(\text{REG}) \quad \forall t \in \mathcal{T} : \mu_t \sim \mu\]

\[(\text{TRI}) \quad \forall f \in \mathcal{B} : \mu(f \circ \vartheta) = \mu(f)\]

We do not assume the reference state \(\mu\) to be invariant!
1. Mean entropy production rate

Proposition.

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

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

The entropy balance equation

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

suggests

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

**Proposition.**
1. (REG) ⇒ ∀s, t ∈ T : \( \ell_{\mu_{t+s}} | \mu = \ell_{\mu_t} | \mu + \ell_{\mu_s} | \mu \circ \phi^{-t} \) (cocycle property)
2. (REG)+(TRI) ⇒ ∀t ∈ T : \( \ell_{\mu_t} | \mu \circ \vartheta = \ell_{\mu_{-t}} | \mu \)

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suggests

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

**Corollary.**
1. ⇒ ∀t ∈ T : \( \Sigma^t = -t^{-1} \ell_{\mu_{-t}} | \mu = \Sigma^{-t} \circ \phi^t \)
2. ⇒ ∀t ∈ T : \( \Sigma^t \circ \vartheta = -t^{-1} \ell_{\mu_t} | \mu = -\Sigma^{-t} \)
2. Entropic fluctuations: The Evans–Searles identity

\[ P^t(f) = \mu(f(\Sigma^t)) \quad \overline{P}^t(f) = \mu(f(-\Sigma^t)) \quad \text{(distributions of } \Sigma^t \text{ and } -\Sigma^t) \]
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**Theorem.** (Finite time Evans–Searles [94] or Transient Fluctuation Theorem)

Under Assumptions (REG)+(TRI) negative values of \( \Sigma^t \) 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: \( t^{-1} \ell_{\mu-t|\mu} = -\Sigma^t = \Sigma^{-t} \circ \vartheta = \Sigma^t \circ \phi^{-t} \circ \vartheta \)

\[ \begin{align*}
\mu(f(-\Sigma^t)) &= \mu(f(\Sigma^t \circ \phi^{-t} \circ \vartheta)) = \mu(f(\Sigma^t \circ \phi^{-t})) = \mu_t(f(\Sigma^t)) \\
&= \mu(f(\Sigma^t) e^{\ell_{\mu-t|\mu}}) = \mu(f(\Sigma^t) e^{-t\Sigma^t})
\end{align*} \]
3. Entropic fluctuations: The Evans–Searles symmetry

\[ e_t(\alpha) = \text{Ent}_\alpha(\mu_t|\mu) = \log \mu \left( e^{\alpha t \Sigma^{-t}} \right) \]  
(finite time ES-function)
3. Entropic fluctuations: The Evans–Searles symmetry

\[ e_t(\alpha) = \text{Ent}_\alpha(\mu_t | \mu) = \log \mu \left( e^{\alpha t \Sigma^{-t}} \right) \] (finite time ES-function)

**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 interval \( ]0, 1[. \)
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 \( 0 < \text{Re} \alpha < 1. \)
4. \( e_t(1 - \alpha) = \log \mu \left( e^{\ell \mu_t | \mu} e^{-\alpha t \Sigma^{-t}} \right) = \log \mu \left( e^{-\alpha t \Sigma^{-t} \circ \vartheta} \right) = \log \mu \left( e^{-\alpha t \Sigma^t} \right) = e_{-t}(\alpha) \)
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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\( \text{(finite time ES-function)} \)

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

\[ e_t(1 - \alpha) = e_t(\alpha) \]
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,
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**Proposition.**

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

**Proof.**

1. \( \mu(\sigma) = \mu_1(\ell_{\mu_1|\mu}) = -\text{Ent}(\mu_1|\mu) \geq 0 \).
   
   Jensen \( \Rightarrow e^{\mu-1(\sigma)} \leq \mu_{-1}(e^{\sigma}) = \mu(\ell_{\mu_1|\mu}) = \mu_1(1) = 1 \).

2. \( \sigma \circ \vartheta = \ell_{\mu_1|\mu} \circ \vartheta \circ \phi = \ell_{\mu_1|\mu} \circ \vartheta \circ \phi^{-1} = \ell_{\mu_{-1}|\mu} \circ \phi^{-1} = -\ell_{\mu_1|\mu} \circ \phi^{-2} = -\sigma \circ \phi^{-1} \).
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\[ \Sigma^t = \frac{1}{t} \ell_{\mu_t|\mu} \circ \phi^t = \frac{1}{t} \sum_{s=0}^{t-1} \sigma \circ \phi^s, \]

\[ \sigma = \ell_{\mu_1|\mu} \circ \phi^1 \quad \text{(Entropy production observable)} \]

\[ -\text{Ent}(\mu_t|\mu) = \sum_{s=0}^{t-1} \mu(\sigma_s) \]

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

(TRI) \implies 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:

\[ \mathbb{R} \ni t \mapsto \Delta_{\mu_t} \in L^1(M, \mu) \]

is strongly \( C^1 \) and

\[ \sigma = \frac{d}{dt} \Delta_{\mu_t} \bigg|_{t=0} \]

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Cocycle property

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

\[ -\Ent(\mu_t|\mu) = \int_0^t \mu(\sigma_s) ds \]

\[ e_t(\alpha) = \log \mu \left( e^{\alpha \int_0^t \sigma - s ds} \right) \quad \mu(\sigma) = 0 \]

\[ \sigma \circ \vartheta = -\sigma \]

\[ e_t(\alpha) = \log \mu \left( e^{-\alpha \int_0^t \sigma_s ds} \right) \]
5. Example: A thermostated ideal gas

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

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

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

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

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

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

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

It easily follows that

$$e_t(\alpha) = \log \left( \frac{\Gamma(N/2)}{\sqrt{\pi} \Gamma((N - 1)/2)} \int_{-\infty}^{\infty} (\cosh \xi)^{-(N-1)(1-\alpha)} (\cosh(\xi + F \epsilon^{-1/2} t))^{-(N-1)\alpha} d\xi \right)$$
5. Example: A thermostated ideal gas

\[ \frac{1}{t} e_{t}(\alpha) \] for various values of \( t > 0 \)
6. Thermodynamics: Forces & fluxes

Assume we have some control of our dynamical system

\[ \mathbb{R}^n \ni X \mapsto (M, \phi^t_X, \mu_X) \]
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\[ \mathbb{R}^n \ni X \mapsto (M, \phi^t_X, \mu_X) \]

- \( X = (X_1, \ldots, X_n) \) are mechanical or thermodynamical forces (affinities).
- \( \mu_0 \) is \( \phi^t_0 \)-invariant i.e., \( X = 0 \) is equilibrium \( \Rightarrow \sigma_X = 0 \).
- \( \sigma_X = X \cdot \Phi_X = \sum_{j=1}^n X_j \Phi_X^{(j)} \).
- \( \Phi^{(j)}_X \) is the flux (current) associated to \( X_j \).
- For simplicity \( \vartheta \) is independant of \( X \) and \( (M, \phi^t_X, \mu_X) \) is TRI

\[ \Phi_X \circ \vartheta = -\Phi_X \quad \Rightarrow \quad \mu_X(\Phi_X) = 0. \]

\[ P_X^t(f) = \mu_X \left( f \left( \frac{1}{t} \int_0^t \Phi_{X_s} \, ds \right) \right) \]

\[ \overline{P}_X^t(f) = \mu_X \left( f \left( -\frac{1}{t} \int_0^t \Phi_{X_s} \, ds \right) \right) \]

\[ P^t_X(f) = \mu_X \left( f \left( \frac{1}{t} \int_0^t \Phi_{X_s} \, ds \right) \right) \quad \overline{P}^t_X(f) = \mu_X \left( f \left( -\frac{1}{t} \int_0^t \Phi_{X_s} \, ds \right) \right) \]

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

\[ \frac{d\overline{P}^t_X}{dP^t_X}(\Phi) = \exp \left( -tX \cdot \Phi \right) \]

\[ P^t_X(f) = \mu_X \left( f \left( \frac{1}{t} \int_0^t \Phi_X s \, ds \right) \right) \quad \overline{P}^t_X(f) = \mu_X \left( f \left( -\frac{1}{t} \int_0^t \Phi_X s \, ds \right) \right) \]

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\[ \frac{d\overline{P}^t_X}{dP^t_X}(\Phi) = \exp (-t X \cdot \Phi) \]

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**

\[ g_t(X, X - Y) = g_t(X, Y) \]

\[ P^t_X(f) = \mu X \left( f \left( \frac{1}{t} \int_0^t \Phi_X s \, ds \right) \right) \]
\[ \bar{P}^t_X(f) = \mu X \left( f \left( -\frac{1}{t} \int_0^t \Phi_X s \, ds \right) \right) \]

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

\[ \frac{d\bar{P}^t_X}{dP^t_X}(\Phi) = \exp \left( -tX \cdot \Phi \right) \]

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

\[ g_t(X, X - Y) = g_t(X, Y) \]

**Proof.** \(- (X - Y) \cdot \Phi_X \circ \vartheta = \sigma_{X - s} - Y \cdot \Phi_{X - s} \).
8. Finite time linear response

If

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

is differentiable at \( X = 0 \) we set

\[ L_{jk}^t = \left. \frac{\partial X_k}{\partial X_j} \langle \Phi_X^{(j)} \rangle_t \right|_{X=0} \]  

(finite time transport matrix)
8. Finite time linear response

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

is differentiable at \( X = 0 \) we set

\[ L^t_{jk} = \partial \langle \Phi^{(j)}_X \rangle_t \bigg|_{X=0} \] (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

\[ L^t_{jk} = \frac{1}{2} \int_{-t}^t \mu_0 \left( \Phi^{(k)}_0 \Phi^{(j)}_{0s} \right) \left( 1 - \frac{|s|}{t} \right) \, ds = \frac{1}{t} \int_0^t \left[ \frac{1}{2} \int_{-s}^s \mu_0 \left( \Phi^{(k)}_0 \Phi^{(j)}_{0u} \right) \, du \right] \, ds \]

where \( \Phi^{(j)}_{0s} = \Phi^{(j)}_0 \circ \phi^{s}_0 \). 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

\[ 0 \leq \langle \sigma X \rangle_t = \sum_{j=1}^{n} X_j \langle \Phi^{(j)}_X \rangle_t = \sum_{j,k=1}^{n} L_{jk}^t X_j X_k + o(|X|^2). \]
8. Finite time linear response

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Proof of the theorem. One has

\[ \langle \Phi_X^{(j)} \rangle_t = -\frac{1}{t} \partial_{Y_j} g_t(X, Y) \bigg|_{Y=0} \Rightarrow L^t_{jk} = \partial_{X_k} \langle \Phi_X^{(j)} \rangle_t \bigg|_{X=0} = -\frac{1}{t} \partial_{X_k} \partial_{Y_j} g_t(X, Y) \bigg|_{X=Y=0} \]

As a consequence of the generalized ES symmetry one also has

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

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

\[ L^t_{jk} = \frac{1}{2t} \int_0^t \int_0^t \mu_0 \left( \Phi_{0s_1}^{(k)} \Phi_{0s_2}^{(j)} \right) ds_1 ds_2 = \frac{1}{2t} \int_0^t \int_0^t \mu_0 \left( \Phi_{0s_1}^{(k)} \Phi_{0(s_2-s_1)}^{(j)} \right) ds_1 ds_2 \]

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: $\phi^t$ 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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- TRI holds with $\vartheta(p, q) = (-p, q)$ provided $H \circ \vartheta = H$.
- Reference state: $\frac{1}{Z} e^{-\beta H_S - \sum_j \beta_j H_j} dp \, dq$.
- Thermodynamic forces: $X_j = \beta - \beta_j \Rightarrow \nu_X = \frac{1}{Z} e^{-\beta H_0 + \sum_j X_j H_j} dp \, dq$. 
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- Small system $S$: $H_S(p_S, q_S)$ on $M_S$.
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Problem: $\mu_0$ is not $\phi^t$ 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 $\nu_X \rightarrow (M, \phi^t, \mu_X)$
9. Example: Thermally driven open system

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

\[ \Delta \mu_{Xt} |_{\mu_X} = e^{\sum_j X_j (H_j \circ \phi^{-t} - H_j)} \]

\[ \sigma_X = \frac{d}{dt} \Delta \mu_{Xt} |_{\mu_X} \bigg|_{t=0} = -\sum_j X_j \{H, H_j\} = \sum_j X_j \{H_j, V_j\} = \sum_j X_j \Phi^{(j)} \]

Fluxes \( \Phi^{(j)} = -\{H, H_j\} = \{H_j, V\} = \{H_j, V_j\} \) are independent of \( X \)
9. Example: Thermally driven open system

Energy conservation + Liouville theorem \( \Rightarrow \mu_X t = \frac{1}{Z} e^{-\beta H + \sum_j X_j H_j \circ \phi^{-t}} dp dq \)

\[ \downarrow \]

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

\[ \downarrow \]

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\[ \downarrow \]

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

\[ \left[ \begin{align*}
    \text{Assume } H_j \circ \vartheta &= H_j \Rightarrow \Phi^{(j)} \circ \vartheta &= -\Phi^{(j)} \\
    H_j \circ \phi^t - H_j &= -\int_0^t \Phi^{(j)}_s ds
\end{align*} \right] \]

\[ \downarrow \]

\( \Phi^{(j)} \) is the energy flux out of reservoir \( R_j \)
9. Example: Open harmonic chain

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

\[ q_{m+1} = 0 \]
9. Example: Open harmonic chain

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

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

\[ H_L(p_L, q_L) = \sum_{x = -n}^{-m-1} \frac{p_x^2 + q_x^2}{2} + \sum_{x = -n}^{-m} \frac{(q_x - q_{x-1})^2}{2} \]

\[ H_R(p_R, q_R) = \sum_{x = m+1}^{n} \frac{p_x^2 + q_x^2}{2} + \sum_{x = m+1}^{n+1} \frac{(q_x - q_{x-1})^2}{2} \]
9. Example: Open harmonic chain

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\[ q_{m-1} = q_{m+1} = 0 \]

Fully coupled chain

\[ H(p, q) = \sum_{x = -n}^{n} \frac{p_x^2 + q_x^2}{2} + \sum_{x = -n}^{n+1} \frac{(q_x - q_x - 1)^2}{2} \]

\[ q_{n-1} = q_{n+1} = 0 \]
9. Example: Open harmonic chain

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

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

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

Fluxes

\[ \Phi^{(L)} = \{ H_L, V \} = -p_{m-1} q_m \]
\[ \Phi^{(R)} = \{ H_R, V \} = -p_{m+1} q_m \]
9. Example: Open harmonic chain

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

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

$$\mu_X = \frac{1}{Z} e^{-\beta H + X_L H_L + X_R H_R} dp \, dq$$

Gaussian with covariance

$$D_X = (\beta h - k(X))^{-1}$$
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Gaussian with covariance

$$D_X = (\beta h - k(X))^{-1}$$

Generalized ES-function reduces to a Gaussian integral

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

In particular

$$e_t(\alpha) = g_t(X, \alpha X) = -\frac{1}{2} \log \det \left( I - \alpha D_X \left( e^{tL^*} k(X) e^{tL} - k(X) \right) \right)$$
Mean entropy production rate $\mu(\Sigma^t) = - \frac{d}{d\alpha} e_t(\alpha) \bigg|_{\alpha=0}$
9. Example: Open harmonic chain

\[ \frac{1}{t} e^{t(\alpha)} \] for various values of \( t > 0 \)

\( n=100 \quad m=10 \quad \beta=4 \quad X_L=-X_R=1 \)

\( t=1 \quad t=50 \quad t=300 \quad t=350 \quad t=800 \)

steady state
10. Nonequilibrium Steady States

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

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

for all bounded continuous $f$. $\mu_+$ is entropy producing if $\mu_+(\sigma) > 0$. 
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Quasi-Theorem. The NESS $\mu_+$ of $(M, \phi^t, \mu)$ is entropy producing if and only if $\mu_+ \not\in \mathcal{P}_\mu$, i.e., $\mu_+$ is singular w.r.t. $\mu$.

Entropy production is the signature of non-equilibrium
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Entropy production is the signature of non-equilibrium

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 \((M, \phi_X^t, \mu_X)\) has a NESS \( \mu_{X^+} \)

\[
\langle \Phi_X \rangle_+ = \lim_{t \to \infty} \langle \Phi_X \rangle t = \mu_{X^+}(\Phi_X) \quad \text{(steady currents in the NESS } \mu_{X^+})
\]
11. Linear response: The large time limit

Assume that for small $X \in \mathbb{R}^n$ the controlled system $(M, \phi_X^t, \mu_X)$ has a NESS $\mu_X$.

$$\langle \Phi_X \rangle_+ = \lim_{t \to \infty} \langle \Phi_X \rangle_t = \mu_X + \langle \Phi_X \rangle$$

(steady currents in the NESS $\mu_X$)

Assume that $X \mapsto \langle \Phi_X \rangle_+$ is differentiable at $X = 0$ and set

$$L_{jk} = \partial_{X_k} \langle \Phi_X^{(j)} \rangle_+ \bigg|_{X=0}$$

(NESS transport matrix)
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(\text{steady currents in the NESS } \mu_X +)
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\[
L_{jk} = \partial_{X_k} \langle \Phi_X^{(j)} \rangle_+ \bigg|_{X=0} \\
(\text{NESS transport matrix})
\]

Finally assume that the \textit{equilibrium current-current correlation function} satisfies

\[
\mu_0 \left( \Phi_0^{(k)} \Phi_0^{(j)} \right) = O(t^{-1}) \quad (t \to \infty)
\]
11. Linear response: The large time limit

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

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Assume that $X \mapsto \langle \Phi_X \rangle_+$ is differentiable at $X = 0$ and set

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Finally assume that the equilibrium current-current correlation function satisfies

$$\mu_0 \left( \Phi_0^{(k)} \Phi_0^{(j)} \right) = O(t^{-1}) \quad (t \to \infty)$$

**Theorem.** The Green-Kubo Formula

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

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

\[
\partial X_k \left[ \lim_{t \to \infty} \langle \Phi^{(j)}_X(t) \rangle \right]_{X=0} = \lim_{t \to \infty} \left[ \partial X_k \langle \Phi^{(j)}_X(t) \rangle \right]_{X=0}
\]

This is also a delicate dynamical problem.
11. Linear response: The large time limit

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

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

This is also a delicate dynamical problem.

Proof. Recall that

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

If the GK-Formula holds, then $F(t) \to L_{jk}$ and the fundamental property of the Cesàro
mean implies that $L_{jk}^t \to L_{jk}$. 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 $\Phi_0$ if there is a positive semi-definite matrix $D$ s.t., for all bounded continuous function $f : \mathbb{R}^n \to \mathbb{R}$,

$$\lim_{t \to \infty} \mu_0 \left( f \left( \frac{1}{\sqrt{t}} \int_0^t \Phi_0 s \, ds \right) \right) = m_D(f)$$

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

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

**Theorem.** Suppose that for some $\epsilon > 0$ the function $g_t(0, Y) = \log \mu_0 \left( e^Y \cdot \int_0^t \Phi_0 s \, ds \right)$ is analytic in $D_\epsilon$, 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 $\Phi_0$ with covariance matrix

$$D_{jk} = \lim_{t \to \infty} \int_{-t}^t \mu_0 \left( \Phi_0^{(k)} \Phi_0^{(j)} \right) \left( 1 - \frac{|s|}{t} \right) \, ds$$
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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 $(M, \phi^t_X, \mu_X)$ if:

- The Green-Kubo Formula

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

(and therefore the Onsager Reciprocity Relations $L_{jk} = L_{kj}$) hold.

- The CLT holds for $\Phi_0$ 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 $\partial X_k$ 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 analytic function $F$. Moreover, the derivatives of $F_t$ converge to the corresponding derivatives of $F$ uniformly on compact subsets of $D_\epsilon$. 
13. Large deviations

A vector valued observable $\mathbf{f} = (f^{(1)}, \ldots, f^{(n)})$ satisfies a Large Deviation Principle (LDP) w.r.t. $(M, \phi, \mu)$ if there exists an upper-semicontinuous function $I : \mathbb{R}^n \to [-\infty, 0]$ with compact level sets such that, for all Borel sets $G \subset \mathbb{R}^n$

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

$$\sup_{Z \in \mathring{G}} I(Z) \leq \liminf_{t \to \infty} \frac{1}{t} \log \mu \left( \left\{ x \in M \mid \frac{1}{t} \int_0^t f_s(x) ds \in G \right\} \right)$$

$$\leq \limsup_{t \to \infty} \frac{1}{t} \log \mu \left( \left\{ x \in M \mid \frac{1}{t} \int_0^t f_s(x) ds \in G \right\} \right) \leq \sup_{Z \in \bar{G}} I(Z).$$

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

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

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

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

\[ \langle f \rangle_+ = \lim_{t \to \infty} \frac{1}{t} \int_0^t \mu(f_s) ds \]

exists and \(\langle f \rangle_+ = -\nabla h(0)\).

For any regular sequence \(t_n\) one has

\[ \lim_{n \to \infty} \frac{1}{t_n} \int_0^{t_n} f_s(x) ds = \langle f \rangle_+ \]

for \(\mu\)-a.e. \(x \in M\).

\([ t_n \text{ is regular if } \sum_n e^{-at_n} < \infty \text{ for all } a > 0 \]
14. The Gärtner-Ellis theorem

Assume that the limit

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

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

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

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

for all $Y_0 \in \partial D$. Then the Large Deviation Principle holds for $f$ w.r.t. $(M, \phi, \mu)$ 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 $]$
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.

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 \( t \).
15. The Evans–Searles fluctuation theorem

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

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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 \( \mu \text{-a.e. } x \in M \).

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

\[
I(-s) = I(s) - s
\]
15. The Evans–Searles fluctuation theorem

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

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\[
I(-s) = I(s) - s
\]

Proof. \( I(-s) = \inf_{\alpha \in \mathbb{R}} (-\alpha s + e(\alpha)) = \inf_{\alpha \in \mathbb{R}} (-\alpha s + e(1 - \alpha)) = \inf_{\alpha \in \mathbb{R}} (-1 + \alpha - \alpha s + e(\alpha)) = -s + I(s) \)
15. The Evans–Searles fluctuation theorem

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

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

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

$$\langle \Phi_X \rangle_+ = \mu_X + (\Phi_X) = -\nabla_Y g(X, Y)|_{Y=0}$$

and for any regular sequence $t_n$

$$\frac{1}{t_n} \int_0^{t_n} \Phi_{X_s}(x) \, ds \to \mu_X + (\Phi_X)$$

for $\mu_X$-a.e. $x \in M$.

**Proof.** Gärtner-Ellis.
15. The Evans–Searles fluctuation theorem

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

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

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 $\mu_0(\Phi_0^{(k)} \Phi_0^{(j)}) = O(t^{-1})$ 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 $\langle \Phi^{(j)}_X \rangle^+ = \partial_{Y_j} g(X, Y) \big|_{Y=0}$, the GES-symmetry yields

$$ L_{jk} = \partial_{X_k} \partial_{Y_j} g(X, Y) \big|_{X=Y=0} = -\frac{1}{2} \partial_{Y_j} \partial_{Y_k} g(X, Y) \big|_{X=Y=0} \Rightarrow L_{jk} = L_{kj} $$
15. The Evans–Searles fluctuation theorem

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

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

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 $\mu_0(\Phi^{(k)}_0 \Phi^{(j)}_0 t) = O(t^{-1})$ 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.** 3. By our general result the GK-Formula holds iff one can interchange $\lim_{t \to \infty}$ 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

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

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 $\Phi_X$ 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.
Let $\mu_+$ be a NESS of $(M, \phi^t, \mu)$ 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.
16. The Gallavotti-Cohen fluctuation theorem

Let $\mu_+$ be a NESS of $(M, \phi^t, \mu)$ 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.

**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. $e_{+t}(1 - \alpha) \neq e_{+t}(\alpha)$.
16. The Gallavotti-Cohen fluctuation theorem

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

**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 \( \mu_+ \)-a.e. \( x \in M \).

3. If \( e_+ (\alpha) \) is differentiable on \( \mathbb{R} \), then \( \sigma \) satisfies a LDP w.r.t. \((M, \phi, \mu_+)\) 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

\[ g_+(X, Y) = \lim_{t \to \infty} \frac{1}{t} \log \mu_+ \left( e^{-Y \cdot \int_0^t \Phi_X \, ds} \right) \]

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. $(L, \theta)$. 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 $\sigma$. 
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 \( \Phi = (N - 1)e^{-1/2} \tanh \xi \). 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

\[ L^t = \partial_F \langle \Phi \rangle_0 \bigg|_{F=0} = \frac{1}{2} \int_{-t}^{t} \mu(\Phi \phi_s) \left( 1 - \frac{|s|}{t} \right) ds = \frac{t}{2} \mu(\phi^2) = \frac{(N-1)^2}{N} \frac{t}{2\varepsilon} \to \infty \]

diverges as \( t \to \infty \).

This does not come as a surprise since

\[ \langle \phi \rangle_+ = \mu_+(\phi) = \frac{(N-1)}{\sqrt{\varepsilon}} \frac{|F|}{F} \]

is not differentiable at \( F = 0 \).
With finite reservoirs, the large time limit

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

is trivial. To get entropy production we need to take the thermodynamic limit of the reservoir: \( n \to \infty, m \text{ fixed} \).

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

\[ h \to \begin{pmatrix} I & 0 \\ 0 & I - \Delta \end{pmatrix}, \]

where \( \Delta \) 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.

\[ g_t(X, Y) = -\frac{1}{2} \log \det \left( I + \int_0^t D_X e^{s\mathcal{L}}^* \phi(Y) e^{s\mathcal{L}} ds \right) \]
18. Example: Open harmonic chain

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

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

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 $\{Y \in \mathbb{R}^2 | - (\beta - X_R) < Y_R - Y_L < \beta - X_L \}$. One can show

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

for small enough $\epsilon$. Finally from local decay estimate for the lattice Klein-Gordon equation

$$|(\delta_x, e^{-it\sqrt{-\Delta}} \delta_y)| \leq C_{x,y} |t|^{-1/2} \quad \Rightarrow \quad \mu_0(\Phi_0^{(j)} \Phi_0^{(k)}) = O(t^{-1})$$
18. Example: Open harmonic chain

Thus, all conclusions of the ES Fluctuation Theorem hold.

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

$$D_{Xt} \rightarrow D_{X+} = h^{-1/2} W_-(\beta - X_{LP} - X_{RP})^{-1} W^*_h h^{-1/2} \text{ (strongly)}$$

the NESS $\mu_{X+}$ 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

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

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 $\mu_{X+}$ is singular w.r.t. the reference state $\mu_X$. 
19. The principle of regular entropic fluctuations

**Remark.** Since, for entropy producing systems, $\mu$ and $\mu_+$ 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 $\mu_+$. 
19. The principle of regular entropic fluctuations

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19. The principle of regular entropic fluctuations

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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

\[
e_+(\alpha) = e(\alpha), \quad \text{respectively} \quad g_+(X, Y) = g(X, Y),
\]

which is equivalent to

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

\[
d\mu(x) = \left( \prod_{i \leq 0} F(-x_i)dx_i \right) \left( \prod_{i > 0} F(x_i)dx_i \right)
\]

Time reversal 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