Entropic Functionals and Liouvillians

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July 15, 2013

These lectures concern set of ideas that can be traced back to the Grenoble summer school "Open Quantum System", June 16-July 4, 2003.

[1] J., Pillet, Rey-Bellet:
"Entropic fluctuations in statistical mechanics I. Classical dynamical systems." Nonlinearity (2011), 699-763.

[2] J., Ogata, Pautrat, Pillet:
"Entropic fluctuations in non-equlibrium quantum statistical mechanics. An Introduction."
In Quantum Theory from Small to Large Scales, Les Houches Proceeding (2012) , 213-410.

[3] J.,Panati, Pillet:
"Entropic fluctuations in statistical mechanics II. Quantum dynamical systems." In prepartion.

CLASSICAL NEQSM

Phase space: $(\mathcal{E}, \mathcal{F})$, where $\mathcal{E}$ is a complete separable metric space and $\mathcal{F}$ is the Borel σ-algebra in $\mathcal{E}$.

Observable: A measurable function $f : \mathcal{E} \to \mathbb{R}$.

States: Probability measures on $(\mathcal{E}, \mathcal{F})$.
Notation: $\rho(f) = \int_{\mathcal{E}} f \, \mathrm{d}\rho$.

Terminology: $\rho \sim \nu$ iff the measures are equivalent (have the same sets of measure zero).

$$\Delta_{\rho|\nu} = \frac{\mathrm{d}\rho}{\mathrm{d}\nu}, \qquad \ell_{\rho|\nu} = \log \Delta_{\rho|\nu}.$$

Relative entropy: (Kullback-Leibler divergence)

$$S(\rho|\nu) = \int_{\mathcal{E}} \log \Delta_{\rho|\nu} \mathrm{d}\rho.$$

It satisfies $S(\rho|\nu) \geq 0$ and $S(\rho|\nu) = 0$ iff $\rho = \nu$,

$$S(\rho|\nu) = \sup_{f \in C_{\mathbb{R}}(M)} (\rho(f) - \log \nu(\mathrm{e}^f)).$$

The Rényi relative entropy of order $\alpha \in \mathbb{R}$ is defined by

$$S_\alpha(\rho|\nu) = \log \int_{\mathcal{E}} \Delta_{\nu|\rho}^{\alpha} \mathrm{d}\rho.$$

$$S_\alpha(\rho|\nu) = S_{1-\alpha}(\nu|\rho)$$

$$S_0(\rho|\nu) = S_1(\rho|\nu) = 0.$$

$$S_\alpha(\rho \circ h | \nu \circ h) = S_\alpha(\rho|\nu)$$

for any homeomorphism h.

The map $\mathbb{R} \ni \alpha \mapsto S_\alpha(\rho|\nu) \in]-\infty, \infty]$ is convex. It is finite and real-analytic on $]0, 1[$.

$$\frac{\mathrm{d}}{\mathrm{d}\alpha} S_\alpha(\rho|\nu)\Big|_{\alpha=0} = -S(\rho|\nu), \qquad \frac{\mathrm{d}}{\mathrm{d}\alpha} S_\alpha(\rho|\nu)\Big|_{\alpha=1} = S(\nu|\rho).$$

Flows: $\mathcal{I}$–index set (time), $\mathcal{I} = \mathbb{Z}$ or $\mathbb{R}$.

$$\phi^t : \mathcal{E} \to \mathcal{E}, \qquad t \in \mathcal{I},$$

is a group of homeomorphisms of $\mathcal{E}$ describing the dynamics. In the continuous case, $\mathcal{I} = \mathbb{R}$, we assume that the map $(t, \zeta) \mapsto \phi^t(\zeta)$ is continuous.

$$f_t(\zeta) = f(\phi^t(\zeta)) \text{ and } \rho_t(A) = \rho(\phi^{-t}(A))$$

are the induced flows on observables and states.

$$\rho_t(f) = \rho(f_t).$$

Time-reversal: A homeomorphism $\theta : \mathcal{E} \to \mathcal{E}$ such that

$$\theta \circ \theta = \text{id}, \qquad \theta \circ \phi^t = \phi^{-t} \circ \vartheta.$$

A state ρ is TRI if $\rho \circ \vartheta = \rho$.

STARTING POINT: Classical dynamical system

$$(\mathcal{E}, \phi^t, \omega_0)$$

where ϕ^t is the given flow and ω_0 (supp$\omega_0 = \mathcal{E}$) is the given reference state.

Assumption: $\omega_t \sim \omega_0$ for all t.

Cocycle relation: For all $s, t \in \mathcal{I}$, one has

$$\Delta_{\omega_{t+s}|\omega_0}(\zeta) = \Delta_{\omega_t|\omega_0}(\zeta)\Delta_{\omega_s|\omega_0}(\phi^{-t}(\zeta))$$

for ω_0-almost all $\zeta \in \mathcal{E}$.

Proof: Chain rule for the Radon-Nikodym derivative.

Consequence: $\ell_{\omega_t|\omega_0} = \log \Delta_{\omega_t|\omega_0}$.

$$\ell_{\omega_{t+s}|\omega_0} = \ell_{\omega_t|\omega_0} + \ell_{\omega_s|\omega_0} \circ \phi^{-t}.$$

For discrete time dynamical systems we set

$$\sigma(\zeta) = \ell_{\omega_1|\omega}(\zeta)$$

and call σ the entropy production observable of $(\mathcal{E}, \phi^t, \omega_0)$.

$$\ell_{\omega_t|\omega_0} = \sum_{s=0}^{t-1} \sigma_{-s}.$$

Regularity assumption (for simplicity): σ is continuous.

In the continuous case ($\mathcal{I} = \mathbb{R}$) we assume that the function

$$t \mapsto \ell_{\omega_t | \omega_0}(\zeta)$$

is differentiable for all ζ and that

$$\sigma(\zeta) = \frac{\mathrm{d}}{\mathrm{d}t} \ell_{\omega_t | \omega_0}(\zeta) \Big|_{t=0}$$

is continuous. Then

$$\ell_{\omega_t | \omega_0}(\zeta) = \int_0^t \sigma_{-s}(\zeta) \mathrm{d}s.$$

The entropy production observable = the phase space contraction rate.

The definition of relative entropy gives the entropy balance equation:

$$S(\omega_t|\omega_0) = \omega_t(\ell_{\omega_t|\omega_0}) = \int_0^t \omega_0(\sigma_s)\mathrm{d}s.$$

The mean entropy production rate over the interval $[0, t]$ is

$$\frac{S(\omega_t|\omega_0)}{t} = \frac{1}{t}\int_0^t \omega_0(\sigma_s)\mathrm{d}s \geq 0.$$

This is finite time second law of thermodynamics.

Rényi's relative entropy allows for the refinement of the second law.

The function

$$\Sigma^t(\zeta) \equiv \frac{1}{t} \int_0^t \sigma_s(\zeta) \mathrm{d}s$$

is interpreted as the mean entropy production rate observable for the time interval $[0, t]$.

We denote by p^t the probability distribution of Σ^t w.r.t. ω_0. p^t is the Borel probability measure on $\mathbb{R}$ and for any bounded Borel function f on $\mathbb{R}$,

$$\int_{\mathbb{R}} f(\lambda) \mathrm{d}p^t(\lambda) = \int_{\mathcal{E}} f(\Sigma^t(\zeta)) \mathrm{d}\omega_0(\zeta).$$

Back to Rényi's entropy.

$$\int_{\mathcal{E}} \triangle^{\alpha}_{\omega_0|\omega_t} \mathrm{d}\omega_t = \int_{\mathcal{E}} \triangle^{-\alpha}_{\omega_t|\omega_0} \mathrm{d}\omega_t = \int_{\mathcal{E}} \mathrm{e}^{-\alpha \int_0^t \sigma_{-s}\mathrm{d}s} \mathrm{d}\omega_t$$

$$= \int_{\mathcal{E}} \mathrm{e}^{-\alpha t \Sigma^t} \mathrm{d}\omega_0$$

$$S_{\alpha}(\omega_t|\omega) = \log \int_{\mathcal{E}} \mathrm{e}^{-\alpha t \Sigma^t} \mathrm{d}\omega_0 = \log \int_{\mathbb{R}} \mathrm{e}^{-\alpha t \lambda} \mathrm{d}p^t(\lambda).$$

Physical meaning of Rényi's relative entropy: The cumulant generating function of Σ^t w.r.t. ω_0.

General property:

$$S_{\alpha}(\omega_t|\omega_0) = S_{\alpha}(\omega_0|\omega_{-t}) = S_{1-\alpha}(\omega_{-t}|\omega).$$

TRI implies

$$S_{1-\alpha}(\omega_{-t}|\omega) = S_{1-\alpha}(\omega_{-t} \circ \theta|\omega_0 \circ \theta) = S_\alpha(\omega_t|\omega).$$

Hence

$$S_\alpha(\omega_t|\omega) = S_{1-\alpha}(\omega_t|\omega).$$

This is Evans-Searles Fluctuation Relation in (essentially) full generality!

The ES-FR is equivalent to

$$\int_{\mathbb{R}} e^{-(1-\alpha)t\lambda} dp^t(\lambda) = \int_{\mathbb{R}} e^{-\alpha t\lambda} dp^t(\lambda),$$

or,

$$\int_{\mathbb{R}} e^{-\alpha t\lambda} e^{\lambda t} dp^t(-\lambda) = \int_{\mathbb{R}} e^{-\alpha t\lambda} dp^t(\lambda).$$

Hence, ES-FR is equivalent to

$$\mathrm{d}p^t(-\lambda) = \mathrm{e}^{-\lambda t}\mathrm{d}p^t(\lambda).$$

This relation implies the second law

$$\omega_0(\Sigma^t) = \int_{\mathbb{R}} \lambda \mathrm{d}p^t(\lambda) = \int_{\lambda \geq 0} \lambda(1 - \mathrm{e}^{-t\lambda})\mathrm{d}p^t(\lambda) \geq 0,$$

and is saying much more:

The negative values of the mean entropy production rate are exponentially suppressed in a universal manner.

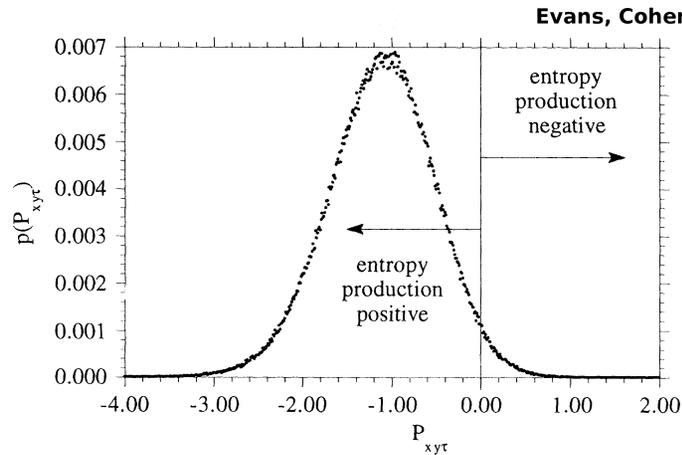# Evans-Cohen-Morris: Probability of second law violations in shearing steady states, PRL (1993).

FIG. 1. The probability distribution of segment averages, $\langle P_{xy,i}\rangle_\tau$, of the xy element of the pressure tensor for 56 WCA disks at $H_0/N = 1.56032$, $n = 0.8$, a shear rate $\gamma = 0.5$, and a segment time $\tau = 0.1$. For those states where $\langle P_{xy,i}\rangle_\tau = P_{xy\tau}$ is positive the entropy production is negative for a period of time τ, counter to the second law of thermodynamics.
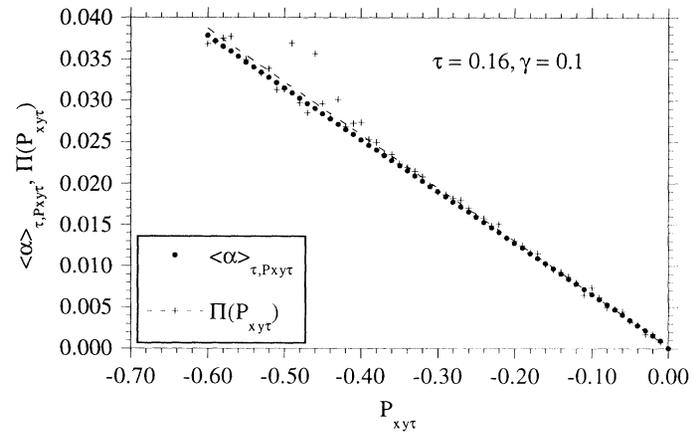
FIG. 2. The logarithmic probability ratio $\Pi(P_{xy\tau})$ and $\langle a \rangle_{\tau, P_{xy\tau}}$ as a function of the segment averaged shear stress $P_{xy\tau} = \langle P_{xy,i}\rangle_\tau$ for $\tau = 0.16$ and $\gamma = 0.1$. As can be seen the two curves are essentially linear [11], with very nearly equal slopes. The agreement between the two slopes becomes progressively better as τ increases. The straight line shows the results of a weighted linear least-squares fit to the logarithmic probability ratio data.

Evans-Searles: Equilibrium microstates which generate second law violating steady states, Physical Review E (1994).

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The basic object is

$$e_t(\alpha) = S_\alpha(\omega_t | \omega_0).$$

Ultimately we wish to study

$$e_+(\alpha) = \lim_{t \to \infty} \frac{1}{t} e_t(\alpha).$$

The Liouvillians shed a light on the mathematical structure of $e_t(\alpha)$ and can help us in the study of this limit.

Liouvillians $\Leftrightarrow$ transfer operators, with long tradition in statistical mechanics (Ruelle).

We assume for simplicity that σ is bounded.

Let $p \in [1, \infty]$. For $f : \mathcal{E} \to \mathbb{R}$ bounded and continuous we set

$$U_p(t)f = f_{-t}e^{-\frac{1}{p}\int_0^t \sigma_s ds}.$$

(1) $U_p(0) = I$, $U_p(t_1 + t_2) = U_p(t_1)U_p(t_2)$.

(2) If $p^{-1} + q^{-1} = 1$ then

$$\omega_0([U_p(t)f][U_q(t)g]) = \omega_0(fg).$$

(3) $\omega_0(|U_p(t)f|^p) = \omega_0(|f|^p)$ and $U_p(t)$ extends to a group of isometries of $L^p(\mathcal{E}, d\omega_0)$.

(4)

$$e_t(\alpha) = \log \|U_{p/\alpha}(t)\mathbf{1}\|_p^p,$$

where $\mathbf{1}(\zeta) = 1$.

Consider the groups $U_p(t)$ on the (complex) Hilbert space $L^2(\mathcal{E}, \mathrm{d}\omega_0)$.

$$\|U_p(t)\| \leq \mathrm{e}^{|t|m_p},$$

where

$$m_p = \sup_{\zeta \in \mathcal{E}} |\sigma(\zeta)||2 - p|/|p|.$$

L^p**-Liouvillean**: L_p, the generator of $U_p(t)$, $U_p(t) = \mathrm{e}^{tL_p}$.

$L_p^* = -L_q$, $\mathrm{sp}L_p \subset \{z : |\mathrm{Re}z| \leq m_p\}$, $\mathrm{Dom}(L_p) = \mathrm{Dom}(L_\infty)$,

$$L_p = L_\infty + \frac{\sigma}{p}$$

If $\alpha = 1/p$,

$$e_t(\alpha) = \log \omega_0(e^{-\alpha \int_0^t \sigma_s ds})$$

$$= \log(1, e^{tL_p}1) = \log \int_{\mathcal{E}} e^{tL_p}1 d\omega_0.$$

This identity yields to a spectral resonance characterization of $e_+(\alpha)$.

Characterization 1.

Suppose that for some $\gamma > 0$ and $c \in \mathbb{R}$,

$$e_t(\alpha) = te_+(\alpha) + c + O(\mathrm{e}^{-\gamma t}),$$

as $t \to \infty$. Then the function

$$z \mapsto (\mathbf{1}, (z - L_p)^{-1}\mathbf{1})$$

has a meromorphic continuation from the half-plane $\operatorname{Re} z > m_p$ to the the half-plane $\operatorname{Re} z > e_+(\alpha) - \gamma$ and its only singularity there is a simple pole at $z = e_+(\alpha)$ with residue e^c. Moreover, for any $\epsilon > 0$ and $j \in \{0, 1\}$,

$$\sup_{x > e_+(\alpha) - \gamma + \epsilon} \int_{|y| > \epsilon} |(\mathbf{1}, (x + \mathrm{i}y - L_p)^{j-2}\mathbf{1})|^{j+1}\mathrm{d}y < \infty.$$

Characterization 2.

Suppose that the function

$$z \mapsto (\mathbf{1}, (z - L_p)^{-1}\mathbf{1})$$

has a meromorphic continuation from the half-plane $\operatorname{Re} z > m_p$ to the half-plane $\operatorname{Re} z > e_+(\alpha) - \gamma$ for some $\gamma > 0$ and that its only singularity there is a simple pole at $z = e_+(\alpha)$. Suppose also that for some $\epsilon > 0$ and any $j \in \{0, 1\}$,
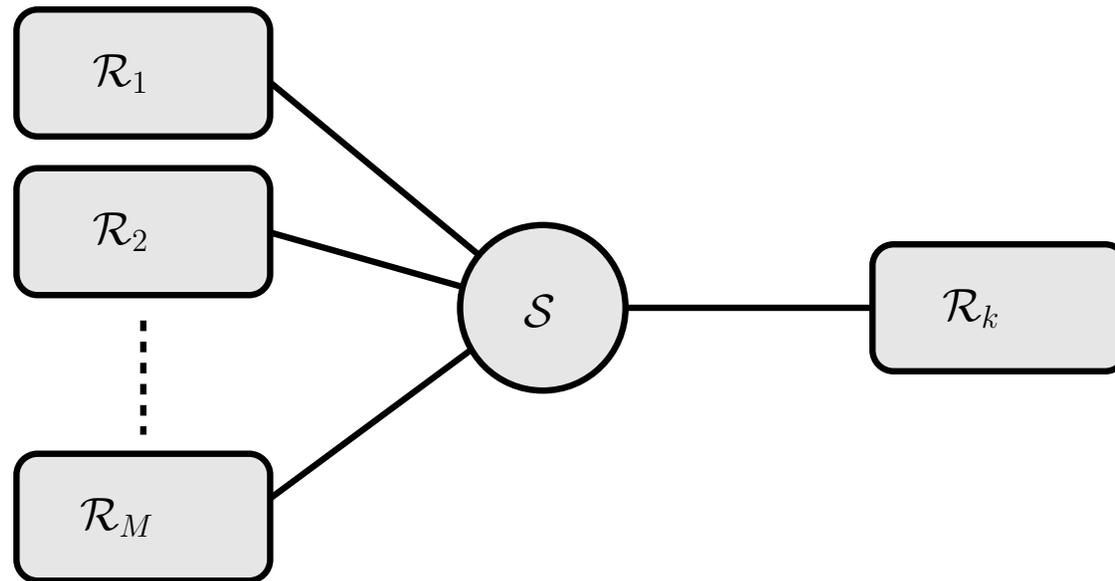
$$\sup_{x > e_+(\alpha) - \gamma} \int_{|y| > \epsilon} |(\mathbf{1}, (x + \mathrm{i}y - L_p)^{j-2}\mathbf{1})|^{j+1} \mathrm{d}y < \infty.$$

Then

$$e_t(\alpha) = t e_+(\alpha) + c + O(\mathrm{e}^{-\gamma t}),$$

as $t \to \infty$.

EXAMPLE: CLASSICAL OPEN SYSTEMS

System S, described by the phase space

$$\Gamma_S = \mathbb{R}^{n_S} \oplus \mathbb{R}^{n_S}$$

and the Hamiltonian $H_S(p_S, q_S)$, coupled to M heat reservoirs $\mathcal{R}_j$.

The phase space and the Hamiltonian of the j-th reservoir are $\Gamma_j = \mathbb{R}^{n_j} \oplus \mathbb{R}^{n_j}$ and $H_j(p_j, q_j)$.

The phase space and the Hamiltonian of the composite system are

$$\Gamma = \Gamma_S \oplus \Gamma_1 \oplus \cdots \oplus \Gamma_M$$

$$H_0(p, q) = H_S(p_S, q_S) + H_1(p_1, q_1) + \cdots + H_M(p_M, q_M).$$

$\mathrm{d}p\mathrm{d}q$ the Lebesgue measure on Γ.

The coupling between the system S and the j-th reservoir is described by the Hamiltonian $V_j(p_S, p_j, q_S, q_j)$.

The full Hamiltonian is

$$H(p, q) = H_0(p, q) + V(p, q) = H_0(p, q) + \sum_{j=1}^{M} V_j(p_S, p_j, q_S, q_j).$$

Dynamics ϕ^t: the induced global Hamiltonian flow on Γ.

For any C^1 observable F, $F_t = F \circ \phi^t$, and

$$\frac{\mathrm{d}F_t}{\mathrm{d}t} = \{H, F\}_t,$$

where $\{\,\cdot\,,\,\cdot\,\}$ denotes the Poisson bracket,

$$\{F, G\} = \nabla_q G \cdot \nabla_p F - \nabla_p G \cdot \nabla_q F.$$

Initial state:

$$\frac{1}{Z}e^{-\beta H_S - \sum_{j=1}^{M}\beta_j H_j}\,\mathrm{d}p\mathrm{d}q.$$

Introducing the control parameters $X_j = \beta - \beta_j$, we can rewrite it as

$$\mathrm{d}\omega_X = \frac{1}{Z}e^{-\beta H_0 + \sum_{j=1}^{M} X_j H_j}\mathrm{d}p\mathrm{d}q$$

A more convenient choice is

$$\mathrm{d}\omega_X = \frac{1}{Z}e^{-\beta(H_S+V) - \sum_{j=1}^{M}\beta_j H_j}\mathrm{d}p\mathrm{d}q$$

$$= \frac{1}{Z}e^{-\beta H + \sum_{j=1}^{M} X_j H_j}\mathrm{d}p\mathrm{d}q.$$

If the reservoirs have a large spatial extension and the coupling Hamiltonians V_j are well localized, the above two states describe the same thermodynamics.

Entropy production observable=phase space contraction rate.

$$\frac{\mathrm{d}\omega_X \circ \phi^{-t}}{\mathrm{d}\omega_X} = \sum_{j=1}^{M} X_j (H_j \circ \phi^{-t} - H_j),$$

$$\sigma_X = \frac{\mathrm{d}}{\mathrm{d}t} \log \frac{\mathrm{d}\omega_X \circ \phi^{-t}}{\mathrm{d}\omega_X}\bigg|_{t=0} = - \sum_{j=1}^{M} X_j \{H, H_j\}.$$

This could be rewritten as

$$\sigma_X = \sum_{j=1}^{M} X_j \{H_j, V_j\}.$$

The equilibrium case corresponds to $X = 0$.

Thermodynamical definition of the entropy production:

$$H_{jt} - H_j = - \int_0^t \Phi_s^{(j)} \mathrm{d}s,$$

where the flux observable

$$\Phi^{(j)} = \{H_j, V_j\}$$

describes the flow of energy out of the j-th reservoir.

$$\sigma_X = \sum_{j=1}^M X_j \Phi^{(j)}.$$

Time reversal: $\theta(p, q) = (-p, q)$, $H \circ \vartheta = H$.

$$\Sigma_X^t = \frac{1}{t} \int_0^t \sigma_{Xs} \mathrm{d}s.$$

$$e_{Xt}(\alpha) = \log \int_\Gamma \mathrm{e}^{-\alpha t \Sigma_X^t} \mathrm{d}\omega_X.$$

TRI implies

$$e_{Xt}(\alpha) = e_{Xt}(1 - \alpha).$$

Evans-Searles with respect to the subsystem structure.

$$\Sigma_X^t = \frac{1}{t} \int_0^t \sigma_{Xs} \mathrm{d}s = \sum_{j=1}^{M} \Sigma_{X_j}^t,$$

$$\Sigma_{X_j}^t = \frac{X_j}{t} \int_0^t \Phi_s^{(j)} \mathrm{d}s.$$

$$e_{Xt}(\alpha_1, \cdots, \alpha_M) = \log \int_\Gamma \mathrm{e}^{-\sum_j \alpha_j t \Sigma_{X_j}^t} \mathrm{d}\omega_X.$$

$$\alpha = (\alpha_1, \cdots, \alpha_M), \qquad 1 - \alpha = (1 - \alpha_1, \cdots, 1 - \alpha_M).$$

TRI implies

$$e_{Xt}(\alpha) = e_{Xt}(1 - \alpha).$$

p_X^t probability distribution of $(\Sigma_{X_1}^t, \cdots, \Sigma_{X_M}^t)$ w.r.t. ω_X.

$$\mathrm{d}p_X^t(-\lambda) = \mathrm{e}^{-t \sum_j \lambda_j} \mathrm{d}p_X^t(\lambda).$$

Change of variable $\alpha_j X_j = Y_j$,

$$G_t(X, Y) = \log \int_\Gamma e^{-\sum_j Y_j \int_0^t \Phi_s^{(j)} ds} d\omega_X.$$

$$G_t(X, Y) = G_t(X, X - Y).$$

The symmetries leads to the finite time linear response theory:

Symmetry lemma:

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

Proof:

$$\partial_{X_k} G_t(X, Y)|_{X=0} = \partial_{X_k} G_t(X, X - Y)|_{X=0}$$
$$= (\partial_{X_k} G_t)(0, -Y) + (\partial_{Y_k} G_t)(0, -Y).$$

which leads to

$$\partial_{Y_j X_k} G_t(X, Y)|_{X=Y=0} = - \partial_{Y_j X_k} G_t(X, Y)|_{X=Y=0}$$
$$- \partial_{Y_j Y_k} G_t(X, Y)|_{X=Y=0}.$$

Consider the time-averaged expectation values

$$\frac{1}{t}\int_0^t \omega_X(\Phi_s^{(j)})\mathrm{d}s = \langle\Phi^{(j)}\rangle_{Xt}$$

$$= -\frac{1}{t}\partial_{Y_j}\int_\Gamma e^{-\sum_k Y_k \int_0^t \Phi_s^{(j)}\mathrm{d}s}\mathrm{d}\omega_X\Big|_{Y=0}$$

$$= -\frac{1}{t}\partial_{Y_j}G_t(X,Y)\Big|_{Y=0}$$

The finite time kinetic transport coefficients are defined by

$$L_{jkt} = \partial_{X_k}\langle\Phi^{(j)}\rangle_{Xt}\Big|_{X=0}.$$

Assuming TRI, one proves that

$$L_{jkt} = \frac{1}{2} \int_{-t}^{t} \omega_0(\Phi^{(k)} \Phi_s^{(j)}) \left(1 - \frac{|s|}{t} \right) ds.$$

This is finite time Green-Kubo formula.

Since ω_0 is ϕ^t-invariant,

$$L_{jkt} = L_{kjt}.$$

These are finite time Onsager reciprocity relations.

Proof:

$$L_{jkt} = \partial_{X_k}\langle\Phi^{(j)}\rangle_{Xt}\Big|_{X=0} = -\frac{1}{t}\partial_{X_kY_j}G_t(X,Y)\Big|_{X=Y=0}$$

$$= \frac{1}{2t}\partial_{Y_kY_j}G_t(X,Y)\Big|_{X=Y=0}$$

$$= \frac{1}{2t}\int_0^t\int_0^t \omega_0(\Phi_{s_1}^{(k)}\Phi_{s_2}^{(j)})\mathrm{d}s_1\mathrm{d}s_2$$

$$= \frac{1}{2}\int_{-t}^t \omega_0(\Phi^{(k)}\Phi_s^{(j)})\left(1 - \frac{|s|}{t}\right)\mathrm{d}s$$

Goal:

$$e_+(\alpha) = \lim_{t \to \infty} \frac{1}{t} \lim_{\text{size of } \mathcal{R}_j \to \infty} e_t(\alpha).$$

$$G_+(X, Y) = \lim_{t \to \infty} \frac{1}{t} \lim_{\text{size of } \mathcal{R}_j \to \infty} G_t(X, Y).$$

What do we learn (assuming enough regularity)?

Symmetries persist:

$$e_+(\alpha) = e_+(1 - \alpha)$$

$$G_+(X, Y) = G_+(X, X - Y),$$

$$G_+(X, Y) = G_+(X, Y + \gamma),$$

$$e_+\left(\alpha + \frac{\gamma}{X}\right) = e_+(\alpha).$$

$$\gamma/X = (\gamma/X_1, \cdots, \gamma/X_M), \gamma = (\gamma, \cdots, \gamma).$$

Steady state heat fluxes:

$$\langle \Phi^{(j)} \rangle_+ = \lim_{t \to \infty} \frac{1}{t} \int_0^t \omega_X(\Phi_s^{(j)}) \mathrm{d}s = \lim_{t \to \infty} -\partial_{Y_j} \frac{1}{t} G_t(X,Y)\Big|_{Y=0}.$$

$$\langle \Phi^{(j)} \rangle_+ = -\partial_{Y_j} G_+(X,Y)\Big|_{Y=0}.$$

The symmetry

$$G_+(X, Y + \gamma) = G_+(X,Y)$$

implies conservation of energy:

$$\sum_{j=1}^M \langle \Phi^{(j)} \rangle_+ = 0.$$

The strict convexity of $\alpha \mapsto e_{X+}(\alpha)$ $(\alpha_1 = \cdots = \alpha_M = \alpha)$,

$$\langle \sigma_X \rangle_+ = -e'_{X+}(0) = \sum_{j=1}^M X_j \langle \Phi^{(j)} \rangle_+ > 0.$$

Linear response theory: Green-Kubo formulas and Onsager relations.

$$L_{jk+} = \partial_{X_k} \langle \Phi^{(j)} \rangle_+ \big|_{X=0} = \partial_{X_k} (\lim_{t\to\infty} \langle \Phi^{(j)} \rangle_{Xt}) \big|_{X=0}$$

$$= \lim_{t\to\infty} \left(\partial_{X_k} \langle \Phi^{(j)} \rangle_{Xt} \big|_{X=0} \right)$$

$$= \lim_{t\to\infty} L_{jkt}$$

$$= \lim_{t\to\infty} \frac{1}{2} \frac{1}{t} \partial_{Y_j Y_k} G_t(X,Y) |_{X=Y=0}$$

$$L_{jk+} = L_{kj+} = \partial_{Y_j Y_k} G_+(X,Y) |_{X=Y=0}.$$

$$L_{jk+} = \lim_{t\to\infty} \frac{1}{2} \int_{-t}^{t} \omega_0(\Phi^{(k)} \Phi_s^{(j)}) \left(1 - \frac{|s|}{t} \right) \mathrm{d}s$$

$$= \frac{1}{2} \int_{-\infty}^{\infty} \omega_0(\Phi^{(k)} \Phi_s^{(j)}) \mathrm{d}s.$$

Central Limit Theorem for measures $\{P^t\}_{t \geq 0}$, where P^t is the probability distribution of vector-valued random variable

$$\mathcal{F}_t = \left(\frac{1}{t} \int_0^t \Phi_s^{(1)} \mathrm{d}s, \cdots, \frac{1}{t} \int_0^t \Phi_s^{(M)} \mathrm{d}s \right).$$

w.r.t. ω_X. P^t is related to old p^t (linked to $e_t(\alpha)$) by scaling.

For any Borel set $B \subset \mathbb{R}^M$,

$$\lim_{t \to \infty} P^t \left(\sqrt{t}(B - \langle \mathcal{F} \rangle_+) \right) = \mu_D(B),$$

where $\mathcal{F} = (\langle \Phi^{(1)} \rangle_+, \cdots, \langle \Phi^{(M)} \rangle_+)$ and μ_D is centered Gaussian measure with variance

$$D(X) = [D_{jk}(X)], \qquad D_{jk}(X) = \partial_{Y_j Y_k} G_+(X, Y)|_{Y=0}.$$

Setting $X = 0$, one derives Einstein relations:

$$D_{jk}(0) = 2L_{jk}.$$

This proves the Fluctuation-Dissipation Theorem!

Large Deviation Principle for $\{P^t\}_{t \geq 0}$ (Gärtner-Ellis theorem). $P^t \to \delta_{\langle \mathcal{F} \rangle_+}$. LDP quantifies the rate of convergence.

$$P^t(B) \simeq \mathrm{e}^{-t \inf_{\varsigma \in B} I(\varsigma)},$$

with the rate function

$$I(\varsigma) = - \inf_{Y \in \mathbb{R}^M} \left(Y \cdot \varsigma + G_+(X, Y) \right).$$

The symmetry $G_+(X, Y) = G_+(X, X - Y)$ implies

$$I(-\varsigma) = X \cdot \varsigma + I(\varsigma).$$

Evans-Searles symmetry.

Generalizations:

An abstract axiomatic dynamical system setting that leads to symmetries

$$e_+(\alpha) = e_+(1 - \alpha), \qquad G_+(X, Y) = G_+(X, X - Y),$$

and all implications without any references to the internal structure of the system.

Open classical system and Anosov diffeomorphisms of compact Riemann manifolds are treated in unified manner.

Important topics that were not discussed: Non-equilibrium steady states, Gallavotti-Cohen fluctuation theorems, Principle of regular entropic fluctuations.

Conclusion:

The fluctuation relations are structural model independent features of classical non-equilibrium statistical mechanics. They can be viewed as a refinement of the second law of thermodynamics with important theoretical, numerical and experimental implications. In the linear regime near equilibrium the fluctuation relations reduce to familiar fluctuation-dissipation formulae (Green-Kubo, Onsager).

During the last decade (starting with works of Kurchan and Tasaki-Matsui) the fluctuation relation have been extended to quantum domain. The extension led to novel entropic functionals (most notable of which is full counting statistics), a novel large deviation theory, and a deep link with modular theory of operator algebras and non-commutative L^p-spaces.

The complete description of quantum theory is beyond the given time limit, but its various aspects have been discussed in talks of Claude-Alain, Ben, and will be discussed in forthcoming talk by

ANNALISA!!!