Thermostats and reciprocity (`http://ipparco.roma1.infn.it`)

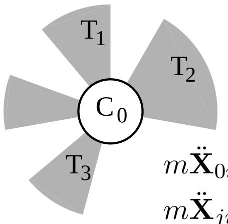
Franqui conference in honor of Pierre Gaspard's prize

An important development in non equilibrium emerged from simulations since the early 1980's (Nosé, Hoover,Evans-Morriss, Cohen): [1, 2, 3, 4] identification of averages of phase space contraction with entropy production rate.

I dare say that it might be as fundamental as the recognition that temperature is identified with average kinetic energy (Bernoulli, Herapath, Waterstone, Krönig).

Here I discuss problems and ambiguities on the matter.

General thermostats model



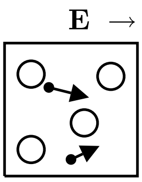
$\mathbf{X}_0, \mathbf{X}_1, \ldots, \mathbf{X}_n$

$$m\ddot{\mathbf{X}}_{0i} = -\partial_i U_0(\mathbf{X}_0) - \sum_j \partial_i W_j(\mathbf{X}_0, \mathbf{X}_j) + \mathbf{E}_i(\mathbf{X}_0)$$
$$m\ddot{\mathbf{X}}_{ji} = -\partial_i U_j(\mathbf{X}_j) - \partial_i W_j(\mathbf{X}_0, \mathbf{X}_j) - \alpha_j \dot{\mathbf{X}}_{ji}$$

multipliers α_j imply $K_j = \frac{m}{2}\dot{\mathbf{X}}_j^2$ are exactly constants of motion with values $K_j = \frac{3}{2} N_j k_B T_j$, $j = 1, \ldots, n$.

$$\alpha_j(\mathbf{X}, \dot{\mathbf{X}}) = -\frac{(Q_j + \dot{U}_j)}{3N_j k_B T_j}, \qquad Q_j \stackrel{def}{=} -\dot{\mathbf{X}}_j \cdot \partial_{\mathbf{X}_j} W_j(\mathbf{X}_0, \mathbf{X}_j)$$
$$\sigma(\mathbf{X}, \dot{\mathbf{X}}) = \sum_{j>0} \frac{(Q_j + \dot{U}_j)}{k_B T_j}, \qquad -\text{“divergence”}$$

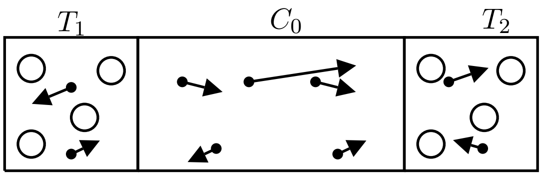
Examples



periodic boundary ("*wire*")

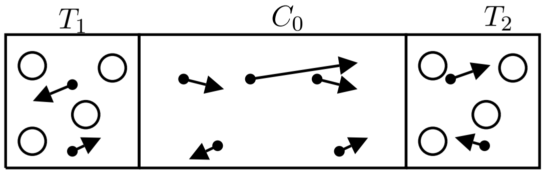
$m\ddot{\mathbf{x}} = \mathbf{E} - \alpha\dot{\mathbf{x}}$

(1) Modern version of classical Drude's model for electric conductivity.



(2) A model for thermal and electric conduction.

Imagine upper and lower walls of the central container identified (realizing a periodic boundary condition) and a constant field of intensity E: two forces conspire and the parameters $\mathbf{F} = (T_2 - T_1, E)$ characterize their strength: matter and heat currents flow.



Alternative models and approaches:
1) infinite thermostats (Ruelle 99, Jarzinsky 99,..,[5, 6]
2) stochastic thermostats (Kurchan 98, Lebowitz-Spohn, Maes 99, Gaspard 06, .. [7, 8, 9, 10])
3) infinite quantum: Feynman-Vernon 63, Eckmann-Pillet-Rey-Bellet 99, ..[11, 12])
4) finite quantum: GG 08, [13, 14]
5) equilibrium-to-equilibrium (Jarzinsky 97, Andrieux-Gaspard 08, [15, 16]

Finite thermostats are best suited for simulations and as a general conjecture statistical properties should be "independent" of thermostats.

Virtually always attention devoted to Onsager reciprocity & Green-Kubo

Microscopic motions are in all possible empirical senses “chaotic”.
Paradigm of chaotic motions are the hyperbolic transitive systems.

Chaotic hypothesis (Ruelle 76, Cohen-G 95,[17, 18]) *Attracting sets for mechanical systems are smooth surfaces on which motion is smooth, hyperbolic and transitive.*

It might be at first disturbing. But disturbing assumptions are common:
Periodicity with equal period (“monocyclicity”) of the motions was employed in the derivation of the second law from the action principle in Boltzmann.

It was considered also by Clausius, Maxwell, Helmholtz as the basis of the early works on the mechanical interpretation of the second law,

CH $\Rightarrow$
if initial data x are randomly chosen, near enough to an attracting set *and* with a distribution with (arbitrary) density:

$$\langle G\rangle = \lim_{T\to\infty}\frac{1}{T}\sum_{j=0}^{T-1} G(S^j x) = \int G(y)\mu(dy), \qquad \text{with probability 1}$$

where $x \to Sx$ is obtained by timing observations on a selected event.

The main result and the power of CH is revealed by its implication of a rigorous formulation of a *coarse graining theory* (GG 94,00,05,08, [19, 20, 21, 13].

It turns *rigorously* the SRB distribution into strochastic process and the time evolution into a *Markov chain*, (Sinai 68,94 Bowen 70, Ruelle 73, [22, 23, 24]).

Thus *making possible* and *without approximations* to treat the dynamics by stochastic methods.

The original fluctuation theorem (Cohen-G 95) and the general theory of reciprocity have been based on it.

Suppose *reversibility* (above models are such)

$$IS_t = S_{-t}I, \quad I^2 = 1, \qquad \text{isometry}$$

Dissipativity: $\langle\sigma\rangle_{SRB} = \sigma_+ > 0$.

dimensionless (finite time) phase space average contraction

$$p = \frac{1}{\tau}\sum_{j=0}^{\tau-1}\frac{\sigma(S^j x)}{\sigma_+}, \;\; or \;\; p = \frac{1}{\tau}\int_0^\tau \frac{\sigma(S_t x)}{\sigma_+}dt$$

"*pattern*" $t \to \varphi(t)$, $t \in [0,\tau]$ and

$$I_\varepsilon\varphi(t) = \varepsilon\varphi(\tau - t)$$

as it *time-reversed pattern* with parity $\varepsilon = \pm 1$, "*antipatterns*".

Fluctuation theorem: *For observables* $(F_1,\ldots,F_n)$ *with parities* ε_j *and for patterns* $(\varphi_1,\ldots,\varphi_n)$, ($n=0$ Cohen-G 95, $n>0$ GG 97, [18, 25])

$$\frac{prob(F_j(S_tx)\sim_\delta \varphi_j(t),p)}{prob(F_j(S_tx)\sim_\delta I_{\varepsilon_j}\varphi_j(t),-p)}\Big|_{SRB}\sim_{\tau\to\infty} e^{\tau\sigma_+ p}$$

A simple consequence (Bonetto 99, [26]) is an "entropy theorem"

$$\langle e^{-P\tau}\rangle_{SRB}\sim 1,\qquad P\stackrel{def}{=}\frac{1}{\tau}\int_0^\tau \sigma(S_tx)dt\equiv p\sigma_+$$

analogous to the work theorems (Jarzinsky 99, Crooks 99, [15, 27]), but different"
It is *asymptotic* (rather than time-indep.) and for *stationary* (rather than equilibrium) states. Analogous to earlier results ($n=0$), also *not dealing with stationary states*, Bokhov-Kuzovlev 81, Evans-Searles 94, [28, 29].

Colorfully .. *relative probabilities of patterns observed in a time interval of size* τ *and in presence of an average entropy production* p *are the same as those of the corresponding anti-patterns in presence of the opposite average entropy production rate*,

or ... *it "suffices" to change the sign of the entropy production to reverse the arrow of time*,

... *a waterfall will go up, as likely as we see it going down, in a world in which for some reason, or by the deed of a Daemon, the entropy creation rate has changed sign during a long enough time.*

We can also say that the *motion on an attractor is reversible, even in the presence of dissipation, once the dissipation is fixed.*

Variations of this property keep being rediscovered.

FT extends Green-Kubo and Onsager reciprocity (GG 97, [30]) if:

$$(1)\quad j_i(x) = \frac{\partial\sigma(x)}{\partial E_i},\quad (2)\quad J_i = \langle j_i\rangle_{SRB},\quad (3)\quad \underline{\textbf{if } \sigma(x) = 0 \textbf{ for } \mathbf{E} = 0}$$

$$\Rightarrow\quad L_{ij} \stackrel{def}{=} \frac{\partial J_j}{\partial_{E_i}}|_{\mathbf{E}=0} = L_{ji},\qquad L_{ij} = \frac{1}{2}\int_{-\infty}^{\infty}\langle j_i(S_t x) j_j(x)\rangle dt$$

which follow from FT when it degenerates into triviality ($\mathbf{E} = 0$).

Questions: it is possible that (3) fails
(a) $\frac{\partial\sigma(x)}{\partial E_i} = 0$;
(b) $\sigma|_{\mathbf{E=0}} \neq 0$.

Does this restrict the interpretation of phase space contraction as entropy production rate? Does FT always constitute an extension of GK?

Remark: phase space contraction *depends* on the coordinate system and *therefore it cannot have a direct physical meaning.*

In the case of the above finite thermostats

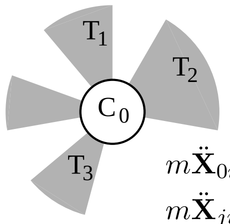
$$\sigma(x) = \sum_{j>0} \frac{Q_j + \dot{U}_j}{k_B T_j} = \varepsilon(x) + \frac{d}{dt} \sum \frac{U_j}{k_B T_j} = \varepsilon(x) + \dot{V}$$

$$\frac{1}{\tau} \int_0^\tau \sigma(S_t x) = \frac{1}{\tau} \int_0^\tau \varepsilon(S_t x) + \frac{1}{\tau}(V(\tau) - V(0)) \to \sigma_+ = \varepsilon_+$$

This kind of relations indicates that *at best* we can only expect that long time averages of σ have a physical meaning and be identified with entropy production rates.

Changing coordinates or metric alters σ by a *time derivative*, as in the example above: no effect on long time averages.

To obtain the GK formulae from FT it is necessary to see if
(1) currents can be generated by a function which satisfies FT and
(2) vanishes at $\mathbf{E}=0$. Again



$$\mathbf{X}_0, \mathbf{X}_1, \ldots, \mathbf{X}_n$$

$$m\ddot{\mathbf{X}}_{0i} = -\partial_i U_0(\mathbf{X}_0) - \textstyle\sum_j \partial_i W_j(\mathbf{X}_0, \mathbf{X}_j) + \mathbf{E}_i(\mathbf{X}_0)$$
$$m\ddot{\mathbf{X}}_{ji} = -\partial_i U_j(\mathbf{X}_j) - \partial_i W_j(\mathbf{X}_0, \mathbf{X}_j) - \alpha_j \dot{\mathbf{X}}_{ji}$$

$$Q_j \stackrel{def}{=} -\dot{\mathbf{X}}_j \cdot \partial_{\mathbf{X}_j} W_j(\mathbf{X}_0, \mathbf{X}_j) \qquad \sigma(\mathbf{X}, \dot{\mathbf{X}}) = \sum_{j>0} \frac{(Q_j + \dot{U}_j)}{k_B T_j}$$

$$\sigma_{\mathbf{E}=0} \neq 0, \qquad \partial_{E_i}\sigma \equiv 0$$

So σ does not seem right. However if H_0 is total energy (kin.+poten.)

Altering σ by a time derivative $\sigma \to \sigma - \beta \dot{H}_0$ (for any β) gives (by the "*vis viva theorem*")

$$\dot{H}_0 = \mathbf{E} \cdot \dot{\mathbf{X}}_0 - \sum_{j>0} \alpha_j \dot{\mathbf{X}}_j^2 = \mathbf{E} \cdot \dot{\mathbf{X}}_0 + \sum_{j>0} (Q_j + \dot{U}_j)$$

$\Rightarrow$ phase space contraction is *statistically equivalent* to

$$\overline{\sigma}(x) = \sigma(x) - \beta \dot{H}_0(x) = \sum_{j>0} \frac{Q_j + \dot{U}_j}{k_B T_j} - \beta\, \mathbf{E} \cdot \dot{\mathbf{X}}_0 - \beta \sum_{j>0} (Q_j + \dot{U}_j)$$

hence to $\varepsilon(x) = \sum_{j>0} \frac{Q_j}{k_B T_j}$, the *entropy production..*
Therefore $\overline{\sigma}$ *satisfies the* FT and *at the same time*

$$j_j(x) = \frac{\partial \overline{\sigma}(x)}{\partial T_j} = -\frac{Q_j}{k_B T_j^2}, \qquad j_i(x) = \frac{\partial \overline{\sigma}(x)}{\partial E_i} = -\frac{1}{k_B T} \dot{\mathbf{X}}_{0,j}$$

it generates all thermodynamic currents

Remark that $\overline{\sigma}(x)$ actually is the phase space contraction of the distribution on phase space with weight $e^{-\beta H_0(x)}$

$$\overline{\mu}(dx) = const\, e^{-\beta H_0(x)} \prod_{j>0} \delta(K_j(x) - \frac{3}{2} N_j T_j)\, dx$$

which is not the SRB distribution. *Unless* $T_j = T$ for all j and $\mathbf{E} = \mathbf{0}$: then it becomes the invariant distribution is (Evans-Morriss 90)

$$\mu_0(dx) = const\, e^{-\beta H_0(x)} \prod_{j>0} \overline{\delta}(K_j(x) - \frac{3}{2} N_j T)\, dx.$$

The generating function for the currents: $\overline{\sigma} = \sum_{j>0} \frac{Q_j+\dot U_j}{k_B T_j} - \beta\,\mathbf{E}\cdot\dot{\mathbf{X}}_0 - \beta\sum_{j>0}(Q_j+\dot U_j)$ *vanishes for vanishing "thermodynamic forces"*

$$\mathbf{F} = (T_1 - T, \ldots, T_n - T, E_1, \ldots, E_q) = \mathbf{0}$$

Since it satisfies the FT and vanishes at 0 forces *it follows*, (GG 97), [31], that the above currents satisfy reciprocity and Green-Kubo.

Besides the derivation of GK other applications:
(1) Heat conduction (Dorfman-Gaspard-Gilbert 02, Eckmann-Young 06, Gaspard-Gilbert 08, [32, 33, 34])
(2) Macroscopic non equilibrium properties Derrida-Lebowitz-Speer 02, Bertini et al. 01), [35]
(3) Applications to nanosystems (Gaspard 06)[9]

Heuristic construction and meaning of SRB. Coarse graining.

$\Rightarrow$ symbolic dynamics. $\exists\ \mathcal{E} = (E_0, \ldots, E_q)$ partition with "transition" or "compatibility" matrix

$$M_{\xi\xi'} = 1, \text{ if } SE^0_\xi \cap E^0_{\xi'} \neq \emptyset, \qquad M_{\xi\xi'} = 0 \text{ otherwise}$$

(1) transitive ($M^{\overline{\ell}}_{\xi\xi'} > 0$)..
(2) Markovian: $1 \longleftrightarrow 1$ correspondence btwn compatile sequences and points (but a zero volume set).

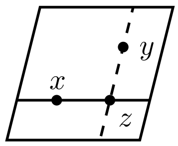
Call E_ξ "coarse cells"

(a) If $\boldsymbol{\xi} = (\ldots, \xi_{-1}, \xi_0, \xi_1, \ldots)$, $M_{\xi_i\,\xi_{i+1}} \equiv 1 \;\;\longleftrightarrow \exists\, x$ and $S^i x \in E_{\xi_i}$.

(b) If $\boldsymbol{\xi}, \boldsymbol{\xi}'$ corresp. x, x' and agree between $-\tau$ e $\tau \Rightarrow d(x, x') \le Ce^{-\lambda n}$

(c) E_ξ is foliated by W_s (W_i), smooth & connected, with histories eventually equal in the future (past) and $x, y \in W_s \Rightarrow d(S^n x, S^n y) \le Ce^{-n\lambda}$.

(d) If $x, y \in E_\xi \Rightarrow z = W_i(x) \cap W_s(y) \Rightarrow d(S^k y, S^k z) \xrightarrow[k\to\infty]{} 0$ exponent.



W_i is asymptotically attracting.

Let τ so large that *all* interesting observ. F are constant in the cells $(\widetilde{\boldsymbol{\xi}} \stackrel{def}{=} (\xi_{-\tau}, \ldots, \xi_\tau))$

$$E(\widetilde{\boldsymbol{\xi}}) \stackrel{def}{=} S^\tau E_{\xi_{-\tau}} \cap S^{\tau-1} E_{\xi_{-\tau+1}} \cap \ldots \cap S^{-\tau} E_{\xi_\tau} = \text{“}\textit{coarse cells}\text{”}$$

Problem: time evolution *cannot be a permutation* (cells too large)

Immagine phase space discretized (Boltzmann) in *microcells*. As in simulations: a point $\to$ 64 bits per each of the $\mathcal{N}$ coordinates: $2^{64}\mathcal{N}$.

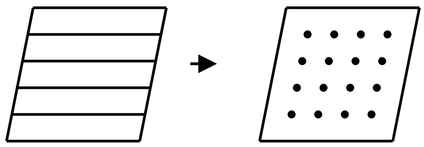
We wish $\langle F\rangle$.

The set $\mathcal{A}$ of recurrent points is the *attractor*. Transitivity (generalization of “ergodic hypothesis”) $\Rightarrow$ 1-cycle permutation.

Then averages are computed with a uniform distribution!

$$\langle F\rangle = \frac{\sum_{\widetilde{\boldsymbol{\xi}}}\mathcal{N}(\widetilde{\boldsymbol{\xi}})F(\widetilde{\boldsymbol{\xi}})}{\sum_{\widetilde{\boldsymbol{\xi}}}\mathcal{N}(\widetilde{\boldsymbol{\xi}})}$$

In the discrete representation $\mathcal{A}$ appears, in each coarse cell, as a family of points regularly arranged on a finite number of unstable manifolds



The number $\mathcal{N}(\widetilde{\boldsymbol{\xi}})$ is subject to a strong compatibility constraint.

If $x \in E(\widetilde{\boldsymbol{\xi}})$ prefixed, let $\Lambda_i(\widetilde{\boldsymbol{\xi}})$ the coefficient of expansion of the surface $W_i(x)$ for the map $S^{2\tau}$ (as map of $S^{-\tau}x$ into $S^{\tau}x$).

$$\text{Compatibility} \Rightarrow \mathcal{N}(\widetilde{\boldsymbol{\xi}}) = \mathit{cost}\,\Lambda_i(\widetilde{\boldsymbol{\xi}})^{-1}$$

hence if $\lambda_i(\widetilde{\boldsymbol{\xi}}) \stackrel{def}{=} \log\Lambda_i(\widetilde{\boldsymbol{\xi}})$

$$\langle F\rangle = \frac{\sum_{\widetilde{\boldsymbol{\xi}}} e^{-\lambda_i(\widetilde{\boldsymbol{\xi}})}F(\widetilde{\boldsymbol{\xi}})}{\sum_{\widetilde{\boldsymbol{\xi}}} e^{-\lambda_i(\widetilde{\boldsymbol{\xi}})}}$$

espressing the SRB distribution.

Applications? Fluctuation theorem of CG (*very different from* Evans-Searles), Onsager reciprocity, Green-Kubo.

Can count the number of microcells! equal to entropy in equilibrium, NOT a function of state otherwise. *No entropy defined out of equilibrium.* (Ga 01) [36]

If evolution is reversible (as in above models) $\exists I$ such that $I^2 = 1$, $IS = S^{-1}I$. Then $\lambda_i(I\widetilde{\boldsymbol{\xi}}) = -\lambda_s(\widetilde{\boldsymbol{\xi}})$
Hence if $p = \frac{1}{\tau}\sum_{j=0}^{\tau-1}\frac{\sigma(S^j x)}{\sigma_+}$, $\sigma_+ = \langle\sigma\rangle > 0$

$$\frac{P_\tau(p)}{P_\tau(-p)} = \frac{\sum_{\widetilde{\boldsymbol{\xi}},p\,\text{fixed}} e^{-\lambda_i(\widetilde{\boldsymbol{\xi}})}}{\sum_{\widetilde{\boldsymbol{\xi}},-p\,\text{fixed}} e^{-\lambda_i(\widetilde{\boldsymbol{\xi}})}} = \frac{\sum_{\widetilde{\boldsymbol{\xi}},p\,\text{fixed}} e^{-\lambda_i(\widetilde{\boldsymbol{\xi}})}}{\sum_{\widetilde{\boldsymbol{\xi}},p\,\text{fixed}} e^{-\lambda_i(I\widetilde{\boldsymbol{\xi}})}} = \frac{\sum_{\widetilde{\boldsymbol{\xi}},p\,\text{fixed}} e^{-\lambda_i(\widetilde{\boldsymbol{\xi}})}}{\sum_{\widetilde{\boldsymbol{\xi}},p\,\text{fixed}} e^{\lambda_s(\widetilde{\boldsymbol{\xi}})}}$$

$= e^{\tau\, p\, \sigma_+}$ because $-\lambda_i(\widetilde{\boldsymbol{\xi}}) - \lambda_s(\widetilde{\boldsymbol{\xi}}) = p\sigma_+\tau$.

In terms of large deviations (*Fluct. Theorem*): $\exists p^*$

$$\zeta(-p) = \zeta(p) - p\sigma_+, \qquad \forall p \in (-p^*, p^*)$$

no parameters, model independent (provided reversible).

Verifiable in simulations and, in principle, in experiments, because of the interpretation of σ as entropy creation rate.

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