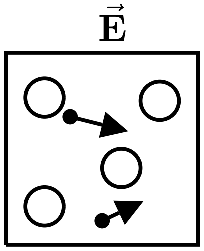
Chaotic hypothesis and coarse graining
(http://ipparco.roma1.infn.it)

In complex systems (gases, fluids) motions are as a rule chaotic. This means that not only: $\lim_{t\to\infty}\frac{1}{t}\sum_{j=1}^{t}F(S^jx)$ exists for a.a. x but

$$\lim_{t\to\infty}\frac{1}{t}\sum_{j=1}^{t}F(S^jx)=\int F(y)\mu(dy)$$

The dist. probab. on phase space μ describes a *state*. If evolution S is not Hamilt. μ is a *nonequilibrium stationary state*.

Example 1: Drude's Model (1899)
Example 2: Heat conduction.



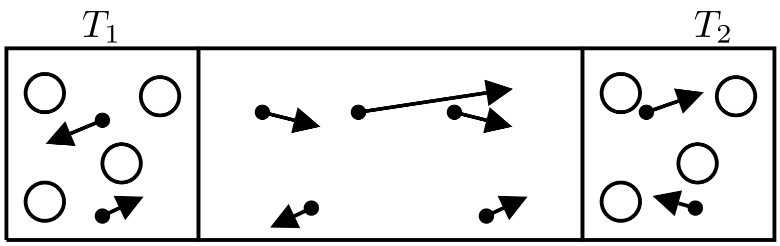
El. Cond.

periodic b.c. ("*wire*")

$m\ddot{\mathbf{x}} = \mathbf{E} +$ collision rule

elastic + rescal. velo. to $|\dot{\mathbf{x}}| = \sqrt{\frac{3}{m} k_B T}$

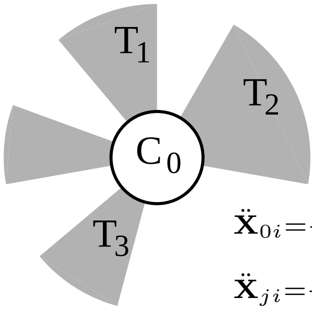
Problem: $\langle \dot{\mathbf{x}} \rangle = cE$? (Ohm). Theorem if $N = 1$ (CELS).



Term. Cond.

Fourier law? Open problem with conjectures (no?)

A general thermostat model



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

$$\ddot{\mathbf{X}}_{0i} = -\partial_i U_0(\mathbf{X}_0) - \sum\nolimits_j \partial_i U_j(\mathbf{X}_0, \mathbf{X}_j) + \mathbf{E}_i(\mathbf{X}_0)$$

$$\ddot{\mathbf{X}}_{ji} = -\partial_i U_j(\mathbf{X}_j) - \partial_i U_j(\mathbf{X}_0, \mathbf{X}_j) - \alpha_j \dot{\mathbf{X}}_{ji}$$

$$\frac{m\dot{\mathbf{X}}_j^2}{2} = \frac{3}{2} k_B T_j \, N_j, \qquad Q_j = -\dot{\mathbf{X}}_j \cdot \partial_{\mathbf{X}_j} U_j(\mathbf{X}_0, \mathbf{X}_j)$$

$$\alpha_j = \frac{Q_j + \dot{U}_j}{3 k_B T_j N_j}$$

Efficient? when? Phase Volume contraction $\Rightarrow$ divergence

$$\sigma = \varepsilon + \dot{V}, \qquad \varepsilon \stackrel{def}{=} \sum_{j \ge 1} \frac{Q_j}{k_B T_j}, \quad V \stackrel{def}{=} \sum_{j \ge 1} \frac{U_j}{k_B T_j}$$

Kinetic interpretation of entropy creation:

$$S - E \stackrel{def}{=} \frac{1}{\tau}\int_0^\tau \sigma\, dt - \frac{1}{\tau}\int_0^\tau \varepsilon\, dt = \tfrac{V(\tau)-V(0)}{\tau} \xrightarrow[\tau\to\infty]{} 0$$

E and S have *intrinsically* equal average $\langle\varepsilon\rangle \equiv \langle\sigma\rangle \;\Rightarrow\; (\tau\to\infty)$
equal statistics for $p = \frac{E}{\langle\varepsilon\rangle}$ and $p' \stackrel{def}{=} \frac{S}{\langle\sigma\rangle}$.

Nonsense to attribute any meaning to V: ε has physical meaning and can be measured. V is *arbitrary* (coordinate dependent!)

Chaotic Hypothesis:
The attractor for mechanical systems is hyperbolic, regular, transitive

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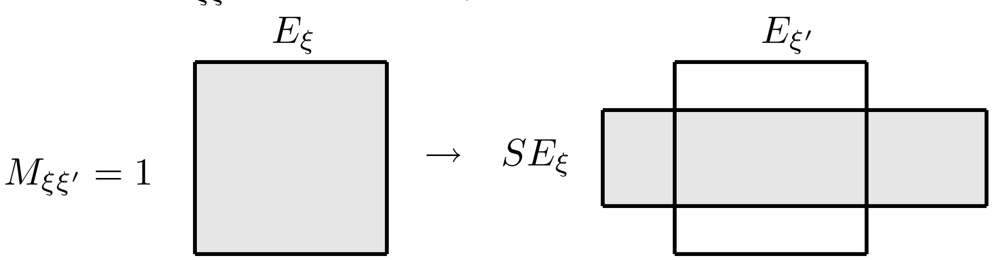
Analogous to the *Ergodic Hypotesis* (which it implies): $\mu =$ SRB.

CH $\Rightarrow$ Coarse graining can be made precise !

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

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

transitive ($M^{\overline{\ell}}_{\xi\xi'} > 0$). Call E_ξ "coarse cells".

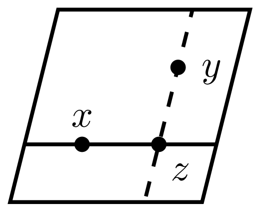


(a) If $\boldsymbol{\xi} = (\ldots, \xi_{-1}, \xi_0, \xi_1, \ldots)$, $M_{\xi_i\,\xi_{i+1}} \equiv 1 \;\;\longleftrightarrow\; \exists\, x$ and $S^i x \in E_{\xi_i}$.

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

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

(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.



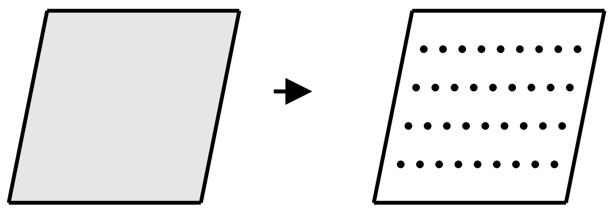
W_i is asymptotically attracting *while its surface is expanded.*

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)

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



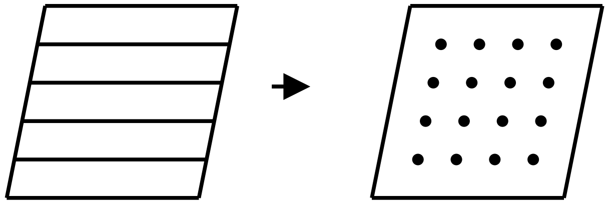
The set $\mathcal{A}$ of recurrent points is the *attractor*. Transitivity (generalization of "ergodic hypothesis") $\Rightarrow$ 1-cycle permutation.
The attractor is still expanding: if $x \in E(\widetilde{\boldsymbol{\xi}})$ prefixed, let

$$\Lambda_i(\widetilde{\boldsymbol{\xi}}) = |\det \partial S^{2\tau}(\widetilde{\boldsymbol{\xi}})_i|$$

the expns. coeff. of surface $W_i(x)$ for $S^{2\tau}$ (as map of $S^{-\tau}x$ into $S^{\tau}x$).
Then its points are spread over a surface larger by a factor $\Lambda_i(\widetilde{\boldsymbol{\xi}})$.
nevertheless all microcells are changed into others which already exist *and dynamics just permutes the microcells.*
Transitivity $\Rightarrow$ cycle is just one cycle: hence $\langle F\rangle$ is computed

$$\langle F\rangle = \frac{\sum_{\widetilde{\boldsymbol{\xi}}}\mathcal{N}(\widetilde{\boldsymbol{\xi}})F(\widetilde{\boldsymbol{\xi}})}{\sum_{\widetilde{\boldsymbol{\xi}}}\mathcal{N}(\widetilde{\boldsymbol{\xi}})} \qquad \text{with a uniform distribution!}$$

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 as no microcells must be generated in spite of the strong expansion $\Lambda(\widetilde{\boldsymbol{\xi}})$.

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

hence the SRB distribution is

$$\langle F\rangle = \frac{\sum_{\widetilde{\boldsymbol{\xi}}} e^{-\lambda_i(\widetilde{\boldsymbol{\xi}})} F(\widetilde{\boldsymbol{\xi}})}{\sum_{\widetilde{\boldsymbol{\xi}}} e^{-\lambda_i(\widetilde{\boldsymbol{\xi}})}}, \qquad \lambda_i(\widetilde{\boldsymbol{\xi}}) \stackrel{def}{=} \log \Lambda_i(\widetilde{\boldsymbol{\xi}})$$

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

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 $p = \frac{1}{\tau}\sum_{j=0}^{\tau-1}\frac{\sigma(S^j x)}{\sigma_+}$, $\sigma_+ = \langle\sigma\rangle > 0$

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

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

This is a large deviations theorem (*Fluct. Theorem*).

no parameters, model independent (provided reversible).

Comments

(1) *Verifiable* in simulations and, in principle, in experiments, because of the interpretation of σ as entropy creation rate: provided care is paid to perform the experiments on a time small compared to the time scale where friction becomes relevant and reversibility is lost unless a detailed understanding of the dissipation is undertaken.

(2) *Once more* it appears that the unphysical difference between the mathematical notion of phase space contraction and the physically measurable entropy creation rate is not relevant as the result holds for ε.

(3) Even when V is unbounded (as it can in some models) the FT has been formulated *timed observations*, *i.e.* for maps. And of course observations are always timed at events which are not singular.