Chaotic hypothesis, Thermostats, SRB distributions
(http://ipparco.roma1.infn.it)

Thermodynamics → equilibrium → states ≡ dist. probab. on phase space
Non Equilibrium: stationary state: distrib. probab. as well

Aim: look for "universal" relations translating structural properties like:

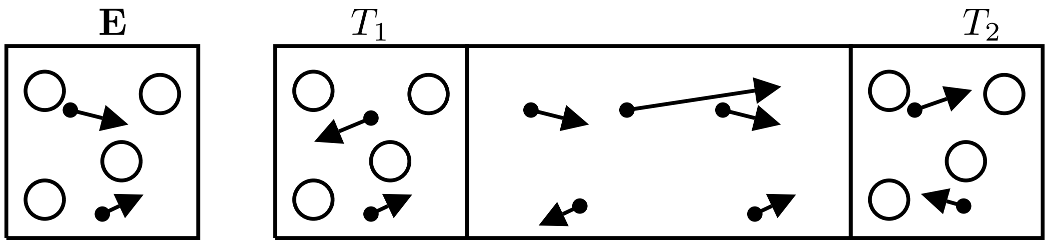
$$\text{Hamiltonian } H = K + U, \ \& \ K = \sum_{i=1}^{N} \frac{1}{2} m \dot{\mathbf{x}}_i^2, \quad U = \sum_{i<j} \Phi(\mathbf{x}_i - \mathbf{x}_j)$$

+ ergodic hypothesis ⇒ Second Law (Boltzmann: trivial identity for 1 degree of freedom but not for 10^{23}).

Example 1: Drude's Model (1899)

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

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



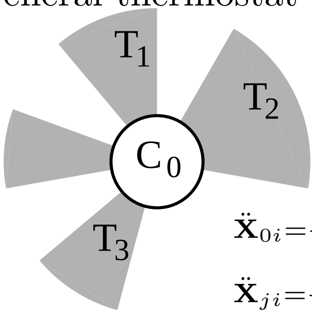
El. Cond. *Term. Cond.*

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

Example 2: Heat conduction. Fourier law?

Open problem. A conjecture ("YES", "NO").

General thermostat model



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

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

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

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

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

Efficient? when? Phase Volume contraction ⇒ 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:

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

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 $p' \stackrel{def}{=} \frac{S}{\langle\sigma\rangle}$.

If chaotic (hyperbolic, regular, transitive) p' (**hence** p) satisfies "*large deviations*", $\exists\, \zeta(p)$ analytic in (p_1, p_2), convex, max at $\langle p\rangle \equiv 1$

$$P_\tau(p\in[a,b]) \simeq e^{\tau\,\max_{[a,b]}\zeta(p)}, \qquad \forall a,b\in(p_1,p_2)$$

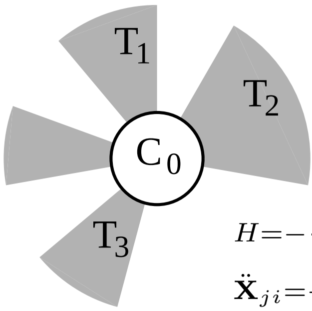
if $\zeta(p)$ quadratic at 1 $\Rightarrow$ Central limit theorem.

Chaotic Hypothesis

The attractor for mechanical systems is hyperbolic, regular, transitive

Analogous to the *Ergodic hypotesis* (which it implies)

Quantum Mechanics Finite thermostats



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

$$H = -\frac{\hbar^2}{2}\Delta_{\mathbf{X}_0} + U_0(\mathbf{X}_0) + \sum_{j>0}\Big(U_{0j}(\mathbf{X}_0, \mathbf{X}_j) + U_j(\mathbf{X}_j) + K_j\Big)$$

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

H operator on $L_2(\mathcal{C}_0^{3N_0})$, symm. or antisymm. waves Ψ,

Dynamical System phase space is $\big(\Psi, (\{\mathbf{X}_j\}, \{\dot{\mathbf{X}}_j\})_{j>0}\big)$:

$$-i\hbar\dot{\Psi}(\mathbf{X}_0) = (H\Psi)(\mathbf{X}_0),$$

$$\ddot{\mathbf{X}}_j = -\Big(\partial_j U_j(\mathbf{X}_j) + \langle \partial_j U_j(\mathbf{X}_0, \mathbf{X}_j)\rangle_\Psi\Big) - \alpha_j \dot{\mathbf{X}}_j \quad j > 0$$

Constraint K_j constant $\Rightarrow$

$$\alpha_j \stackrel{def}{=} \frac{\langle W_j\rangle_\Psi - \dot{U}_j}{2K_j}, \qquad W_j \stackrel{def}{=} -\dot{\mathbf{X}}_j \cdot \partial_j U_{0j}(\mathbf{X}_0, \mathbf{X}_j)$$

$$\sigma(\mathbf{x},\dot{\mathbf{x}}) \equiv \varepsilon(\mathbf{X}, \dot{\mathbf{X}}) + \dot{V}(\mathbf{X}) = \sum_{j>0} \frac{Q_j}{k_B T_j} + \dot{V}$$

Consistency: single thermostat is SRB equivalent to Gibbs?

Chaotic hypothesis $\Rightarrow$ unique statistics: $\forall x$ up to 0 volume and $\forall\, F$

$$\frac{1}{\tau}\sum_{j=0}^{\tau-1} F(S^j x) \xrightarrow[\tau\to\infty]{} \int F(y)\mu(dy)$$

$\mu \stackrel{def}{=}$ *SRB statistics*: concentrated on volume 0 if $\langle\sigma\rangle \stackrel{def}{=} \sigma_+ > 0$

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

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

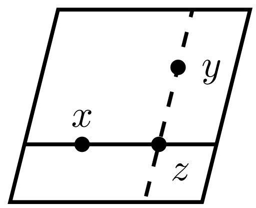
transitive ($M^{\overline{\ell}}_{\xi\xi'} > 0$). Call E_ξ "coarse cells".

(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.

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

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

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: $2^{64}\mathcal{N}$.

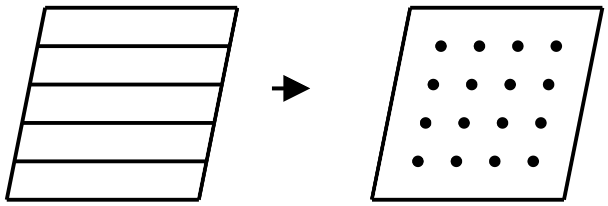
We wish $\langle F \rangle$.

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

Then average 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 $S^{\tau}x$).

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

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

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.