Entropy, FT, Irreversibility

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How much irreversible is a process $\mu_0 \to \mu_\infty$?
Question seems to require a notion of entropy

Entropy is naturally defined only for equilibrium

Recent controversial proposal is to define (only) *entropy creation* and identify it with the phase space contraction

$$\dot{x} = f(x)$$

Chaotic Hypothesis: *Motion on the attractor can be regarded as "hyperbolic" (Anosov)*
(Ruelle 73, Cohen-G 95)

(*Ambitious* $\to$ identification btwnn Equilibrium and Nonequilibrium $\Rightarrow$ ergodic)

Th *If evolution is hyperbolic a statistics μ of motion exists and is unique:*

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T F(S_t x) \stackrel{def}{=} \int_M \mu(dy)\, F(y)$$

"SRB distribution". Admits a formal expression!

Extension to nonequilibrium of Boltzmann–Gibbs

$+$ *reversibility, i.e.* $I^2 = 1$, $IS_t = S_{-t}I \to$ **FT**

$\sigma(x) = -diverg(x) \equiv -\sum \partial_{x_i} f_i(x)$ *and* $\sigma_+ \stackrel{def}{=} \langle\sigma\rangle_{SRB}$

and $p \equiv p(x) \stackrel{def}{=} \frac{1}{\tau}\int_{-\frac{\tau}{2}}^{\frac{\tau}{2}} \frac{\sigma(S_t x)}{\sigma_+} dt$
dimensionless phase space contraction". Then:

TH: FT *If evolution hyperbolic+reversible then*
$\mu(p(x) \in \Delta) = e^{\tau \max_{p\in\Delta} \zeta(p) + O(1)}$
and
$\zeta(-p) = \zeta(p) - p\sigma_+ \qquad |p| < p^*$

or $\frac{P(-p)}{P(p)} \simeq e^{-p\sigma_+\tau}$
(Cohen,Evans,Morriss (exp) Cohen,G (theory)
This is only an example of theorem. One more:

$F_1(x), \ldots, F_n(x)$ even/odd: $F_i(Ix) = \pm F_i(x)$

"patterns": $t \to \varphi_j(t)$, $t \in (-\frac{\tau}{2}, \frac{\tau}{2})$, $j = 1, \ldots, n$

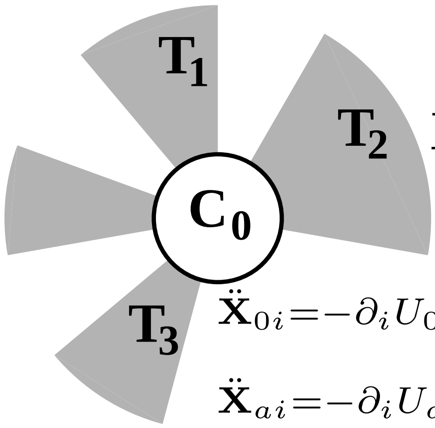
$$\frac{P_\tau\Big(F_j(S_t x) \sim \varphi_j(t), p \Big)}{P_\tau\Big(F_j(S_t x) \sim \pm\varphi_j(-t), -p \Big)} = e^{p\,\sigma_+\,\tau + O(1)}, \ |p| < p^*$$

$P_\tau =$ SRB probability; for all $f, f_j, \varphi_j, n \Rightarrow$!

If $\sigma_+ \to 0$? $\Rightarrow$ (Onsager reciprocity)

$$\partial_A \langle \partial_B \sigma \rangle|_{A,B=0} \equiv \partial_B \langle \partial_A \sigma \rangle|_{A,B=0}$$

Why is $\sigma(x)$ "entropy"? How to connect with Physics ? (Experim. or Simul.). Example:



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

$$\ddot{\mathbf{X}}_{0i} = -\partial_i U_0(\mathbf{X}_0) - \sum\nolimits_a \partial_i U_a(\mathbf{X}_0, \mathbf{X}_i) + \mathbf{F}_i$$

$$\ddot{\mathbf{X}}_{ai} = -\partial_i U_a(\mathbf{X}_a) - \partial_i U_a(\mathbf{X}_0, \mathbf{X}_i) - \alpha_a \dot{\mathbf{X}}_a$$

$$\alpha_a = \textit{Gauss for } K_a = \frac{1}{2} \sum\nolimits_i \dot{\mathbf{X}}_{ia}^2 = \frac{3}{2} k_B T_a \, N_a$$

$$\alpha_a = (\textit{exercise}) = \frac{W_a - \dot{U}_a}{3 N_a k_B T_a}$$

$$W_a = -\sum \dot{\mathbf{X}}_a \cdot \boldsymbol{\partial}_{\mathbf{X}_a} U_a(\mathbf{X}_0, \mathbf{X}_a), \, W_a = \dot{Q}_a = \text{heat}$$

Divergence

$$\sigma(\mathbf{X}) = \scriptstyle{(exercize)} \textstyle = \sigma_0(\mathbf{X}) + \dot{U}(\mathbf{X})$$

$$\sigma_0(\mathbf{X}) = \sum_{a=1}^{n} \frac{\dot{Q}_a}{k_B T_a} \frac{3N_a - 1}{3N_a} = \sum_{a=1}^{n} \frac{\dot{Q}_a}{k_B T_a}$$

$$U(\mathbf{X}) = \sum_{a=1}^{n} \frac{\dot{U}_a}{k_B T_a} \frac{3N_a - 1}{3N_a}$$

If volume $V^N \times R^{3N}$ changes

$$\sigma^\Gamma(\mathbf{X}) = \sigma_0(\mathbf{X}) + \dot{U} - N \frac{\dot{V}_t}{V_t}$$

EPR,Ja 99: ∞-thermostats, no K_a-constraint

Assume U_a bounded and thermostats *efficient*

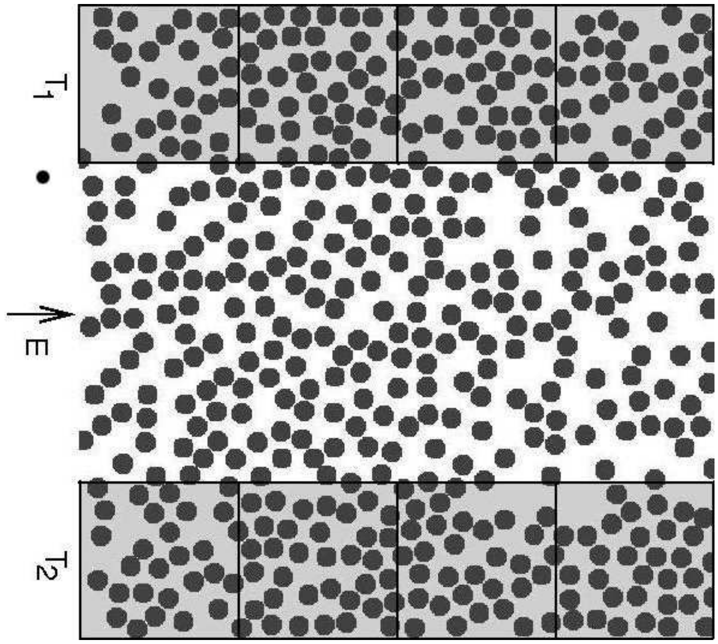
$\lim_{t\to\infty} \frac{1}{t}\int_0^t F(S_t\mathbf{X}) = \int_{\mathcal{F}} F(\mathbf{Y})\,\mu(d\mathbf{Y})$, then

$\sigma_+ = \langle\sigma\rangle_\mu \equiv \langle\sigma_0\rangle + \lim_{t\to\infty} \frac{U(t)-U(0)}{t} \equiv \langle\sigma_0\rangle$

CH $\rightarrow$ FT : $\zeta(-p) = \zeta(p) - p\sigma_+$

$p = p_0 + \frac{U(t)-U(0)}{t\sigma_+} \Rightarrow FT\ for\ p_0!$

$\frac{U(t)-U(0)}{t} \rightarrow 0$ on large time scale ! (CvZ,BGGZ) but σ_+ and p_0 bear no more reference to thermostats and have time scale of $O(surface)$



Efficient thermostat ?

Def Irreversibility time scale for process Π

$\varepsilon(X) \stackrel{def}{=} \sigma_0(\mathbf{X}) - N\frac{\dot V_t}{V_t}$

Quasi static $\Pi:\ \mathbf{F}(t) = \mathbf{F}_0 + (1-e^{-\gamma t})(\mathbf{F}_\infty - \mathbf{F}_0)$

Stationary μ_0 evolves to μ_t and to μ_∞.

$\mu_{srb,t}$ = SRB parameters "frozen" at value taken at time t. Let *irreversibility time scale* for Π

$\frac{1}{\tau(\Pi)} \stackrel{def}{=} \frac{1}{N^2}\int_0^\infty \big(\langle\varepsilon_t\rangle_{\mu_t} - \langle\varepsilon_t^0\rangle_{\mu_{srb,t}}\big)^2 dt$

If quasi static $\tau(\Pi) = O(\gamma^{-1} \log \gamma^{-1}) \xrightarrow[\gamma\to 0]{} \infty$ ($i.e.$ $\to$ reversible)

If "Joule-Thomson" with vol. doubling at speed w it is $\tau(\Pi) = O(\frac{L}{w})$

If "Joule-Thomson" with volume *suddenly* larger $\tau(\Pi) = 0$

If "Joule-Thomson" with volume side from L to $L(1+\delta)$ at speed w: $\tau(\Pi) = \frac{L}{w\delta}$