

FT and Irreversibility time scale

*F.Bonetto (Georgia Tech),
A.Giuliani (Princeton),
F.Zamponi (ENS-Paris)*

“Work,dissipation and fluctuations in nonequilibrium physics”

Bruxelles 22-225 March, 2006

How much irreversible a process from μ_0 to μ_∞ ?

Need “Entropy creation”: via **FT**

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

(*Ambitious* → identification btwnn
Equilibrium and Nonequilibrium ⇒ ergodic)

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

Be $F_1(x), \dots, F_n(x)$ even/odd: $F_i(Ix) = \pm F_i(x)$
Let $\sigma(x) = -\text{divergence}(x)$ and $\sigma_+ \stackrel{\text{def}}{=} \langle \sigma \rangle_{SRB}$

Given τ and “patterns” $t \rightarrow \varphi_i(t)$, $t \in (-\frac{\tau}{2}, \frac{\tau}{2})$

$$p = \frac{1}{\tau} \int_{-\frac{\tau}{2}}^{\frac{\tau}{2}} \frac{\sigma(S_t x)}{\sigma_+} dt$$

“dimensionless phase space contraction”

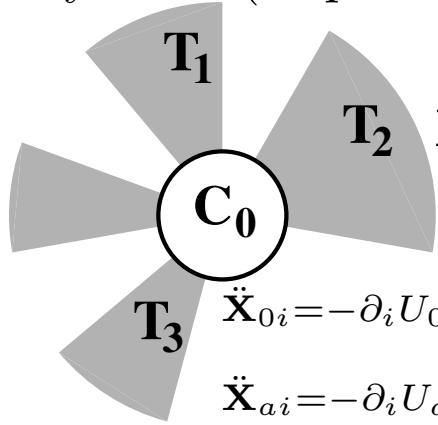
$$\frac{P_\tau(\forall j F_j(S_t x) \sim \varphi_j(t), p)}{P_\tau(\forall j F_j(S_t x) \sim \pm \varphi_j(-t), -p)} = e^{p\sigma_+ \tau + O(1)}, \quad |p| < p^*$$

P_τ = SRB probability; or ($n = 0$)

$$\frac{P_\tau(p)}{P_\tau(-p)} = e^{\zeta(p)\tau} \text{ and } \zeta(-p) = \zeta(p) - p\sigma_+$$

FT ↑↑↑↑↑ (Cohen,Evans,Morriss (exp) Cohen,G
(theory)

Physics ? (Experiment or Simulation).



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

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

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

$$\alpha_a = \text{Gauss for } K_a = \frac{1}{2} \sum_i \dot{\mathbf{X}}_{ia}^2 = \frac{3}{2} k_B T_a N_a$$

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

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

Divergence

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

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

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

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*

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

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

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

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

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

Def Irreversibility time scale for process Π

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

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

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

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

If quasi static $\tau(\Pi) = O(\gamma^{-1} \log \gamma^{-1}) \xrightarrow[\gamma \rightarrow 0]{} \infty$ (*i.e.*
 \rightarrow 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 : $\tau(\Pi) = \frac{L}{w\delta}$