Hyperbolic systems, fluctuation theorems
NESS construction

Question: Is Thermodynamics extendible to nonequilibrium phenomena?

Minimal program: extension to stationary states

Temperature,Entropy, Energy ... can be defined ?

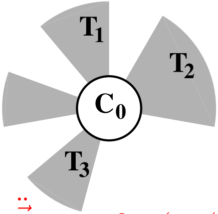
dissipation is necessary.

$\Rightarrow$ system interacts with *thermostats*.

Thermostats models? ∞ sustaining a temperature *gradient*.

ambient space has to be 3 dimensional

Major advance finite thermostats (Hoover,Evans '980s).



$$U_i = \sum_{jk} v(q_k - q_j)$$

$$W_{0i} = \sum_{j\in C_0, k\in T_i} v(q_k - q_j)$$

$$\alpha_i = \frac{\sum_{j\in C_0,k\in T_i}(\partial_{q_k} v(q_k-q_j) - \dot U_k)}{k_B T_k}$$

$$\ddot{\vec X}_0 = -\partial_{\vec X_0}(U_0(\vec X_0) + \sum_{i>0} W_{0i}(\vec X_0, \vec X_i)) + \vec E(\vec X_0)$$

$$\ddot{\vec X}_i = -\partial_{\vec X_i}(U_i(\vec X_i) + W_{0i}(\vec X_0, \vec X_i)) - \alpha_i \dot{\vec X}_i$$

α_i s.t. $\frac{m}{2}\sum_{i>0}\dot{\vec X}_i^2 = \frac12 N_i k_B T_i$ const: $\alpha_i = \frac{L_i - \dot U_i}{N_i k_B T_i}$

Prelim.: does it matter? if $d \le 3$ & smooth pair interactions

Theorem: *a.a. data $\vec X$ chosen with a distribution in which the thermostats are in a Gibbs state with temperatures T_i evolved into $\vec X(t)^{[n]}$ by letting move only particles in a ball of radius $r2^n$ with or without $a_i\dot{\vec X}_i$ converge to the SAME $\vec X^\infty$, exponentially fast at fixed distance from 0.* (Presutti, GG)

Open: does the evolution lead to a stationary distribution?

NEQ Ruelle's principle for fluids: $\exists$ a single natural NESS: because dynamic *hyperbolic*.

Chaotic hypothesis: (Cohen, G) *Motions on the attracting set of a chaotic system can be regarded as motions of a smooth transitive reversible hyperbolic system.*

Mathematical meaning: There exist reversible Markovian partitions $\mathcal{P} = (P_1, \ldots, P_n) \Rightarrow$ general properties.

MP $\Rightarrow$ *History* of x on $\mathcal{P}$, $\vec{\sigma} = \{\sigma_i\}_{i=0}^{\infty}$ s.t. $S^i x \in P_{\sigma_i}$ defines adapted coordinates for x

FT: The stationary distr. of the random variable

$$p = \frac{1}{\tau}\sum_{k=0}^{\tau}\frac{s(S^k\vec{X})}{\langle\, s\,\rangle_{srb}}, \qquad Prob(p\in\Delta) = e^{\tau\max_{p\in\Delta}\zeta(p)+o(\tau)}$$

then $\frac{Prob(p)}{Prob(-p)} = e^{-p\tau\langle\, s\,\rangle}$: more precisely exact symmetry

$$\zeta(-p) = \zeta(p) - p\,\langle\, s\,\rangle_{srb}$$

Importance: $s(\vec{X})$, hence p has a physical interpretation: *i.e.* it is the *entropy increase of the thermostats*.

Experimentally accessible and the Fluctuation Relation is model independent; possibly first after Onsager reciprocity.

Time reversal leads to many other FRs.

If $F_1(\vec{X}),\ldots,F_n(\vec{X})$ are n TR-odd obs., $(F_i(Ix) = -F_i(x))$, given n patterns $\varphi_1(t),\ldots,\varphi_n(t)$ then

If $F_1(\vec{X}),\ldots,F_n(\vec{X})$ are n TR-odd obs. ($F_i(Ix)=-F_i(x)$), given n patterns $\varphi_1(t),\ldots,\varphi_n(t)$ then

$$\frac{Prob(\{F_i(S^k\vec{X})\stackrel{\varepsilon}{=}\varphi_i(k)\}_{k=\tau}^{\tau},p)}{Prob(\{F_i(S^k\vec{X})\stackrel{\varepsilon}{=}-\varphi_i(-k)\}_{k=\tau}^{\tau},-p)}=_{\tau\to\infty} e^{p\,\tau\,\langle\, s\,\rangle}$$

again no free parameters (and independent on F_i).

"*All needed to reverse time is to reverse entropy production*". also $\Rightarrow$ OR & Green-Kubo.

How the CH can be viewed from Physics? it allows to define precisely coarse graining, to count phase space points, to better understand of entropy and finally to a "natural proposal" of quantitative meas. of quasi-static processes.

Coarse graining on a MP $\mathcal{P}=\{P_1,P_2,\ldots,P_s\}$;

MP $\to$ code by $\{\sigma_i\}_{i=-\infty}^{\infty}$ s.t. $x\longleftrightarrow\{\sigma_i\}_{i=-\infty}^{\infty}$ s.t. $S^ix\in P_{\sigma_i}$

Refine $\mathcal{P}\to\mathcal{P}_n$ s.t. "all" F are constants on sets of $\mathcal{P}_n$

Sets in $\mathcal{P}_n = \{P(\sigma_{-n},\ldots\sigma_n) \stackrel{def}{=} \cap_{-n}^{n} S^{-i}P_{\sigma_i}\}_{\vec\sigma}$

The $P_{\sigma_{-n},\ldots\sigma_n} \equiv P(\vec\sigma)$ will be called coarse grained cells.

The SRB is a distribution with weight $w(\vec\sigma)$ for $P(\vec\sigma)$ and admits an explicit formula

$$w(\vec\sigma) = e^{-\Lambda_{u,n}(\vec\sigma)} \;\Rightarrow\; \mu_{SRB}(P(\vec\sigma)) = \frac{e^{-\Lambda_{u,n}(\vec\sigma)}}{\sum_{\vec\sigma'} e^{-\Lambda_{u,n}(\vec\sigma')}}$$

Interpretation ($\frac12$-heuristic): in simulations phase space is discrete and evolution is a map on a finite space.

Discard nonrecurrent points (*i.e.* transient, present in any code): remain those on the "attractor" $\mathcal{A}$.

Thier number in $\mathcal{A}\cap P(\vec\sigma)$ is the fraction of the total $\mathcal{N}$

$$\mathcal{N}(\vec\sigma) = \mathcal{N}\mu_{SRB}(P(\vec\sigma))$$

and evolution is a one cycle permutation of $\mathcal{A}$, "ergodicity"

This unifies equilibrium and nonequilibrium:

In both cases the stationary dist. is equal weight of the phase space points, *i.e.* SRB $\supset$ Boltzmann.

Becomes possible therefore to count the number of points: is it nonequilibrium Entropy ??

(My) answer NO!: both in equilibrium and nonequilibrium the count is ambiguous: it depends on the precision "ε" of discretization.

BUT equil. ambiguity = an additive constant $($"$3N \log \hbar$"$)$ independent on the state.

Not so for NESS is state dependent

Nevertheless $S_{\mathcal{P},\varepsilon} = k_B \log \mathcal{N}_{\mathcal{P},\,\mathcal{A},\,\varepsilon}$ is maximal among all distributions on the attractor.

Simply as it corresponds to equal weights: hence it can play the role of Lyapunov function measuring the distance of an evolving distribution to the SRB; just as in equilibrium !!

What about processes? transforming μ_{ini} into another μ_{fin}? under external parameters $\Phi(t)$ changes of (forces, thermostats temperatures, volume, &tc) as $0 \le t \le +\infty$.

At $0 < t < \infty$ time evolution $x = (\dot{\vec{X}}, \vec{X}) \to x(t) = S_{0,t}x$ is non autonomous evolution. Initial state evolves into μ_t

$$\langle\, F \,\rangle_{\mu_t} = \int_{\mathcal{F}(t)} \mu_t(dx) F(x) \stackrel{def}{=} \int_{\mathcal{F}(0)} \mu_0(dx) F(S_{0,t}^{-1} x)$$

Imagine $\Phi(t)$ stepping from $\Phi(0)$ to $\Phi(\infty)$. Clearly

$$\langle\, F \,\rangle_{\mu_{srb}(t)} \neq \langle\, F \,\rangle_{\mu_t}$$

In the previous model phase space contraction is

$$s(\dot{\vec{X}}, \vec{X}) = \sum_a \frac{\dot{Q}_a}{k_B T_a} - N\frac{\dot{V}_t}{V_t} - \sum_a \frac{\dot{U}_a}{k_B T_a}$$

which dimensionally is a $time^{-1}$.

It is natural (GG) to introduce the quantity

$$t^{-1}_{irreversibiiy} = \frac{1}{N^2}\int_0^{+\infty} \Big(\langle\, s(t)\,\rangle_{\mu_t} - \langle\, s(t)\,\rangle_{SRB,t}\Big)^2 dt$$

By Chaotic Hypothesis μ_t evolve to $\mu_{SRB,t}$ exponentially fast under the "frozen evolution".

Therefore the integral will converge.

The slower the evolution the smaller the integral: it will $\to 0$ as evolution slows down:

$$t_{irreversibility} \to +\infty$$

Interpretation:

$t_{irreversibility}$ = time to "realize" the process is irreversible

Example: Joule-Thomson: (gas expansion in a piston)

S = section; $H_t = H_0 + w\,t$ distance base-moving lid;

$\Omega = S\,H_t$ increases at rate $N\frac{w}{H_t}$.

Hence $\langle\, s_t \,\rangle_t$ is $-N\frac{w}{H_t}$, while $s_t^{srb} \equiv 0$.

$T = \frac{L}{w}$ process duration (to increase height by L)

$$t^{-1}_{irreversibility} = N^{-2}\int_0^T N^2\Big(\frac{w}{H_t}\Big)^2\,dt \xrightarrow[T\to\infty]{} w\frac{L}{H_0(H_0+L)}$$

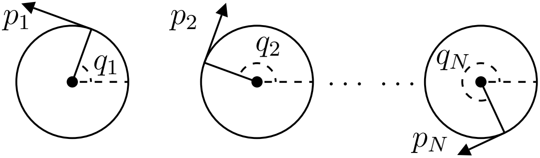
immediately, if $w = \infty$, irreversibility becomes apparent
never, if $w \to 0$: quasi static $\equiv \infty$-slow.

In any event "quasi staticity" becomes quantitative notion

In the latter example it is customary to estimate the degree of irreversibility at the lift of the lid by the *thermodynamic equilibrium entropy* change between initial and final states.

BUT Not quantitative

It is also not inconceivable a quantitative study of the irreversibiliy of attempts at realizing Carnot cycles.



Representation of N rotators $\vec{q} = (q_1, \ldots, q_N) \in T^N$ phase space.

On 1 act torque τ, damping ξ, noise $\dot{w}$, n.n. potential

$$2gV \cos q_i + g'V \cos(q_i - q_{i+1}) + 2gV \cos q_{i+1}$$

Problem: find the stationary state, if any

Simulations exist, no theory. Then
particular case $N = 1$,

Forced pendulum with noise and friction (gravity$= 2Vg$)

Stochastic equation on $T^1 \times R$:

$$\dot{q} = \frac{p}{J}, \qquad \dot{p} = 2gV\sin q - \tau - \frac{\xi}{J}p + \sqrt{\frac{2\xi}{\beta}}\dot{w}$$

$\dot{w}$ white noise with $dw^2 = (w(t+dt) - w(t))^2 = dt$
β noise temperature^{-1}, J=inertia (constants).

Stationary $F(p,q)dpdq$: $\Rightarrow$ the PDE $\mathcal{L}^*F = 0$

$$\mathcal{L}^*F = -\Big\{\Big(\frac{p}{J}\partial_q F(q,p) - (-2gV\sin q + \tau)\partial_p F(q,p)\Big) - \xi\,\Big(\beta_0^{-1}\partial_p^2 F(q,p) + \frac{1}{J}\partial_p(p\,F(q,p))\Big)\Big\}$$

Gen. results: interesting simulations, [1], and theory, [2]

(1) exists a smooth solution $F \in L_2(dpdq)$, [2]

(2) positive $\quad F(q,p) = \frac{e^{-\frac{\beta}{2J}p^2}\rho(p,q)}{\sqrt{2J\beta^{-1}}} = G(p)\rho(p,q)$, [2]

(3) exponential approach from $\delta(p,q)$, [2]

(4) $\rho(p,q) \in L_2(G(p)dpdq)$

Hence $\rho(p,q) = \sum_{n=0}^{\infty} \rho_n(q) \ :p^n:$ with

$:p^n: \stackrel{def}{=} \left(\frac{J\beta^{-1}}{2}\right)^{\frac{n}{2}} H_n(\frac{p}{\sqrt{2J\beta^{-1}}})$ (Wick,Hermite polynomials)

or in dimensionless form

$$\sigma_n(q) \stackrel{def}{=} \rho_n(q)\xi^n n!, \qquad \eta \stackrel{def}{=} \beta\xi^2/J, \qquad \beta\tau, \qquad \beta V,$$

Problem: "Construct $\rho_n(q)$" so that $\mathcal{L}^* F = 0$

Hermite poly. rules:

$$p : p^n :=: p^{n+1} : + \frac{J}{\beta} n \ : p^{n-1} : \qquad \partial_p : p^n := n \ : p^{n-1} :$$

If $\sigma_n(q) = \overline{\sigma}_n + \widetilde{\sigma}_n(q)$, $\qquad \overline{\sigma}_n \overset{def}{=}$ average of σ_n

$$\mathcal{L}^* G(p)\rho(p,q) \equiv \mathcal{L}^* \left(G(p) \sum_{n=0}^{\infty} \rho_n(q) : p^n : \right)$$

by substitution

$$\begin{aligned} \partial\widetilde{\sigma}_n = & -\eta(n-1)\Big(\partial\widetilde{\sigma}_{n-2} + \beta\widetilde{\partial U\widetilde{\sigma}_{n-2}} + \beta\partial U\overline{\sigma}_{n-2} \\ & + \beta\tau\widetilde{\sigma}_{n-2} + \widetilde{\sigma}_{n-1}\Big) \\ \overline{\sigma}_n = & -\left(\overline{\beta\partial U\widetilde{\sigma}_{n-1}} + \beta\tau\,\overline{\sigma}_{n-1}\right) \end{aligned}$$

Idea: possibly σ_n are analytic in g ??

$$\begin{aligned} \widetilde{\sigma}_n(q) =& g\widetilde{\sigma}_n^{[1]}(q) + g^2\widetilde{\sigma}_n^{[2]}(q) + \dots \\ \overline{\sigma}_n =& \overline{\sigma}_n^{[0]} + g\overline{\sigma}_n^{[1]} + g^2\overline{\sigma}_n^{[2]} + \dots \end{aligned}$$

Fix an order R in the expansion in powers of g

Theorem: *Given $R > 0$ there is $\varepsilon_R > 0$ such that if $\xi^{-1}, \beta\tau < \varepsilon_R$ ("large viscosity, small forcing") then*

(1) the order $r \geq 0$ coeff. $\rho_n^{[r]}(q)$ of formal Taylor expansion for $\rho_n(q)$ in powers of g can be constructed for $r \leq R$.

(2) Fourier's coefficients $\rho_{n,k}^{[r]}$ vanish for $|k| > r$ and satisfy

$$\xi^n |\rho_{n,k}^{[r]}| \leq A_r \frac{(C|k|)^n}{n!} e^{-c|k|}, \qquad \forall r \leq R, \forall k$$

for A, C suitably chosen R-dependent.

Unless convergence is proved we cannot even be sure that $\sum_{r=0}^{R} g^r \sum_{n=0}^{\infty} \rho_n(q) : p^n :=$ Taylor exp. $\rho(p,q)$ to order R.

Question: is this a sign that $\sigma_n(q)$ is not analytic?

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