Nonequilibrium statistical mechanics

Equilibrium: Hamiltonian

$$\ddot{\underline{q}}_i = -\partial_{\underline{q}_i} V(\underline{q}), \quad (\dot{\underline{q}}, \underline{q}) \equiv x \in \text{phase space}$$

States: $\mu_{U,V}$ = Liouville (microcan.)

Transformations: quasi static. Thermostats.

Nonequilibrium: Non conservative systems

$$\ddot{\underline{q}}_i = -\partial_{\underline{q}_i} V(\underline{q}) + E\, \underline{g}(\underline{q}) - \underline{\vartheta}_i^E(\underline{q}, \dot{\underline{q}})$$

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Molecular dynamics $\to$ mechanical thermostats

(Nosé–Hoover, Gauss, infinite, stoch.)

States: $\mu = \mu_{U,V,E,\ldots}$ = stationary distrib, (which?) s.t. aside from a 0–volume

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T F(S_t x)dt = \int_\Omega F(y)\mu(dy)$$

Mechanical thermostats: heat? entropy?

$$W = \langle E\,\underline{g}\,(\,\underline{q}\,) \cdot \underline{\dot{q}}\,\rangle_{time} = \langle\,\underline{\vartheta}^{\,E} \cdot \underline{\dot{q}}\,\rangle_{time} = Q$$

Q is identified with "*heat production rate*"
From various examples emerges a definition of *entropy production rate* $k_B\sigma_+$

$$\sigma_+ = \langle divergence\rangle = \langle\partial_{\underline{\dot{q}}} \cdot \underline{\vartheta}^{\,E}(\,\underline{q}\,,\,\underline{\dot{q}}\,)\rangle \ge 0$$

$W = Q$ by stationarity

$$\Big[\frac{d}{dt}\Big(\frac{\underline{\dot{q}}^{\,2}}{2} + V(\,\underline{q}\,)\Big) \equiv E\,\underline{g}\,(\,\underline{q}\,) \cdot \underline{\dot{q}} - \underline{\vartheta}^{\,E} \cdot \underline{q}\,\Big]$$

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obviously $\sigma_+ > 0$ implies that it will not be possible to define "entropy" *of the system*: if entropy content, *i.e.* a conserved quantity identified with entropy, existed then it should be $-\infty$ if $\sigma_+ > 0$.

Temperature: $\Theta = \frac{Q}{k_B \sigma_+}$

I take these as *definitions* of interesting mechanical quantities

Are names consistent with equilibrium?

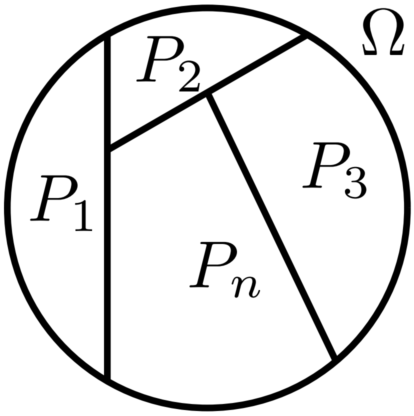
Which is μ?

(Ruelle 1970's, Cohen, G. 1995)

Which is μ? Chaotic hypothesis:

A chaotic multiparticle system can be regarded as a transitive Anosov system.

esoteric? Meaning: "coarse graining possible on all scales"



History:

$$
\begin{array}{rcl}
x & \to & (\ldots i_{-1}, i_0, i_1, \ldots) \\
S^k x & \in & P_{i_k} \\
S & = & \text{Timed evolution}
\end{array}
$$

Given a precision $\gamma > 0 \, \exists \mathcal{P} = (P_1, P_2, \ldots)$

(1) "cells" $P_{i_{-T},\ldots,i_T}$= set of x with i_j

(2) cells $\neq \emptyset$ iff $i_k \to i_{k+1}$ possible

$\quad$ *i.e.* $SP^0_{i_k} \cap P^0_{i_{k+1}} \neq \emptyset$

Microscopic states $\longleftrightarrow$ *states of infnite spin chains with nearest neighbor hard cores*

Key result (Sinai, Ruelle,Bowen)

Liouville volume μ_0 *is a Gibbs dist. with short range potential*

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Φ_- Φ' Φ_+

time ev. = left shift $\leftarrow$

Hence

$S^k\mu_0 \xrightarrow[k\to\infty]{} \mu_+ =$ SRB and

$S^k\mu_0 \xrightarrow[k\to-\infty]{} \mu_-$

Chaot. hyp. extends ergodic hyp.:

gives the statistics of almost all initial data and implies ergodic hyp. +

exponential fast approach to stationarity

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Universal properties? example Boltzmann heat theorem

States: $\mu_{U,V}$ (microc.) $\Rightarrow$ def: $P(U,V), \Theta(U,V)$
change U,V by dU, dV

$$\frac{dU + PdV}{\Theta} = exact \longleftrightarrow \partial_V \frac{1}{\Theta} = \partial_U \frac{P}{\Theta}$$

Reversible systems: isometry I and

$$S^2 = 1, \qquad IS = S^{-1} I$$

$I =$ time reversal (*e.g.* T, PT, PCT *or more complicate*).

Average entropy production (if $\sigma_+ > 0$):

$$p_\tau(x) = \frac{1}{\tau\sigma_+} \sum_{k=-\tau/2}^{\tau/2} \sigma(S^k x)$$

Results (Sinai) p is multifractal:

$$\Pi_\tau(p\in\Delta)=e^{\tau\,\max_{p\in\Delta}\zeta(p)+O(1)}$$

for $|p|<c\,\sigma_+$ and $\zeta(p)$ is analytic in p.
because SRB is a Gibbs state of 1*–dim Ising system with short range potential.*

. *Fluctuation theorem* for reversible maps

$$\zeta(-p)=\zeta(p)-p\sigma_+,\qquad |p|<p^*$$

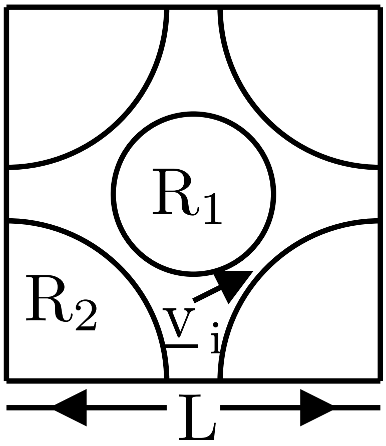
parameterless and universal

(discovered in molecular dynamics, 1993 Evans-Cohen-Morriss, theory Cohen-G., 1995)
More general: $F_1,\ldots,F_n$ odd time rev.
let $t\to\varphi_1(t),\ldots,\varphi_n(t)$ be n "patterns" $t\in[-\frac{\tau}{2},\frac{\tau}{2}]$ and let $I\varphi_j(t)\stackrel{def}{=}\varphi_j(-t)$

$$\frac{\Pi_\tau(F_1\simeq\varphi_1,\ldots,F_n\simeq\varphi_n,p)}{\Pi_\tau(F_1\simeq I\varphi_1,\ldots,IF_n\simeq\varphi_n,-p)}=e^{\tau p\sigma_+}$$

$\forall F_1,\ldots,F_n.\Rightarrow$ Onsager reciprocity and Green–Kubo for $\sigma_+\to 0$

Example *Drude's conduction theory*



$\ddot{\underline{\mathrm{q}}}_{\mathrm{i}} = \mathrm{E}\,\underline{\mathrm{u}} - \underline{\vartheta}_{\mathrm{i}} + \mathrm{coll}$

speed renorm to $\sqrt{3k_B\Theta}$

or keep constant speed

$\underline{\vartheta}_{\mathrm{i}} = \alpha(\dot{\underline{\mathrm{q}}})\,\dot{\underline{\mathrm{q}}}_{\mathrm{i}}$

$\alpha(\dot{\underline{q}}) = \frac{E\sum \underline{u}\cdot\underline{q}_i}{\sum \dot{\underline{q}}_i^2}$ and $\sum \dot{\underline{q}}_i^2 = 3Nk_B\Theta$

so that

$$W = \langle\, \underline{\vartheta} \cdot \underline{\dot q}\, \rangle = E\langle J\rangle = Q$$

$$\sigma_+ = \langle div\rangle = (3N-1)\frac{E\langle J\rangle}{3Nk_B\Theta} \sim \frac{Q}{k_B\Theta}$$

$\zeta(p)$ describes *the current fluctuations*

Tests: 1) numerical, 2) in nature

1) global seems ok. Local ? few examples: lattices of Anosov maps

Lattice (*e.g.* 1 dim):

$$\bullet \qquad \bullet_{\xi}^{\underline{\varphi}_\xi} \; \ldots \quad \bullet \quad \ldots \bullet \qquad \bullet \qquad \xi \in V \subset \mathcal{Z}^d$$

$$(S\,\underline{\varphi}\,)_\xi = S_0\,\underline{\varphi}_{\,\xi} + \varepsilon\,\delta(\,\underline{\varphi}_{\,nn(\xi)})$$

If reversible def. *local phase space contr.*

$$\sigma_{V_0}(\,\underline{\varphi}_{\,V}) = -\log|\det\partial_{\underline{\varphi}_{\,V_0}} S(\,\underline{\varphi}\,)_{V_0}|$$

$$p_{\tau,V_0}(\,\underline{\varphi}\,) \stackrel{def}{=} \frac{1}{\tau\langle\sigma_{V_0}\rangle}\sum_{-\tau/2}^{\tau/2}\sigma_{V_0}(S^k\,\underline{\varphi}\,)$$

Then

$\langle \sigma_{V_0} \rangle = V_0 \sigma^0_+ + O(\partial V_0)$

$\tau\zeta(p) = V_0 \tau \zeta^0(p) + O(\partial(V_0 \times [-\frac{\tau}{2}, \frac{\tau}{2}]))$

$\zeta^0(-p) = \zeta^0(p) - p\sigma^0_+$

i.e.

entropy production fluctuations behave in an analogous way as the density fluctuations in equilibrium: they scale with the space–time volume, (G.).

2) Tests in natural systems

(I) measurements in a "small region" of Q = dissipat. per unit time

(II) Check that $p \stackrel{def}{=} \frac{1}{\tau}\int_{-\frac{\tau}{2}}^{\frac{\tau}{2}} Q(t)$ has a linear symmetry

$\zeta(p) = \zeta(-p) + cp$

One then identifies $\frac{\langle Q\rangle}{k_B c} \stackrel{def}{=} \Theta$ *effective temperature of the thermostat*

Granular materials (very weak friction: Feitosa–Menon)

Fluid turbulence (very strong friction: Ciliberto)

Problems

(a) Reversibil.: essential? (Bonetto-G)

(b) Local fluctuation relations in more general systems (with boundary only forcing/dissipation)? (Bonetto-Lebowitz)

(c) strong friction? (G, Rondoni-Segre)

(d) soluble models? (Derrida-Lebowitz-Speer, Bertini-DeSole-Gabrielli-Jona-Landim)

(e) When are 2 thermostats equivalent? (She-Jackson, Evans-Sarman, G)

Example: Drude's conduction models

$\ddot{\underline{q}}_i = E\,\underline{u} - \nu\,\dot{\underline{q}}_i, \qquad \ddot{\underline{q}}_i = E\,\underline{u} - \alpha(\,\dot{\underline{q}}\,)\,\dot{\underline{q}}_i,$

Look in a volume $V_0 \subset V$ and consider an observable F_{V_0} then *if energy is tuned so that* $\nu = \langle\alpha\rangle$

$$\frac{\langle F_{V_0}\rangle_{\mu_\nu}}{\langle F_{V_0}\rangle_{\mu_\alpha}} \xrightarrow[V\to\infty]{} 1$$

(f) Stochastic thermostats (Kurchan, Lebowitz-Spohn)

(g) Infinite (Hamiltonian classical or quantum) thermostats (Eckmann-Pillet-ReyBellet, Ruelle).

(h) Boundary only dissipation: is $\sigma_{V_0} = 0$ if $V_0 \subset V$? Two definitions

(I) (G)

$\sigma_{V_0}(x_{V_0}) = -\frac{1}{\tau_0} \log\det \partial_{x_{V_0}} S_{\tau_0}(x_{V_0}, x_{V_0^c})$

with τ_0 large enough so that a disturbance at the boundary of V_0 travels to the center ($\sim L_0/(speed\ of\ sound)$)

(II) (Ruelle)

$$\sigma_{V_0}(x_{V_0}) = -\frac{1}{\tau_0}\log\langle\det\partial_{x_{V_0}} S_{\tau_0}(x_{V_0}, x_{V_0^c})\rangle\Big|_{\tau_0=0}$$

with the average computed with the SRB distribution conditioned to x_{V_0} in V_0.