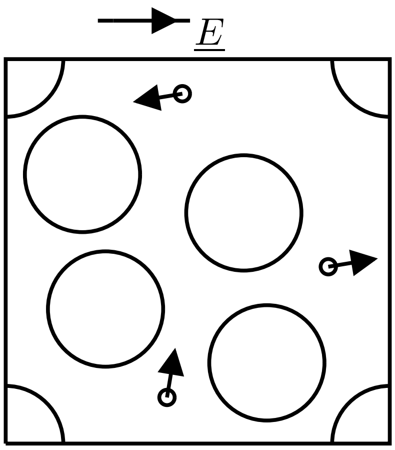
Nonequilibrium Stationary States

System subject to nonconservative forces: hence to thermostats. Example



$\underline{E}$ external non conservative force

$$m\,\underline{\ddot{x}}_i = \underline{F}_i + \underline{E} - \underline{\vartheta}_i$$

$\underline{\vartheta}$ thermostat force

$\underline{\vartheta}$ thermostat models

(1) $\underline{\vartheta}_i = -\nu\,\underline{p}_i$ (viscous thermostat)

(2) $\underline{\vartheta}_i = -\alpha\,\underline{p}_i \qquad \alpha = \frac{\sum \underline{\dot{x}}_i \cdot \underline{E}}{\sum \underline{p}_i^2/m}$ (Gaussian thermostat)

(3) anelastic $\sqrt{\eta}$ = restitution coefficient ($\underline{v}\cdot\underline{n} \to -\sqrt{\eta}\,\underline{v}\cdot\underline{n}$

(4) renormalize $|\underline{v}_i|$ after each collision to $|\underline{v}'_i| = \sqrt{\frac{d}{2}\frac{k_BT}{m}}$

(5) stochastic thermostat and infinite reservoir thermostat (Rey Bellet)

Thermostats $\longleftrightarrow$ phase space contraction $\sigma = -\mathrm{div}\,\underline{\vartheta} = -\sum \partial_{\underline{p}_i}\underline{\vartheta}_i(x,p)$

(1) $\sigma = \nu\,N\,d$

(2)$\sigma = \frac{\sum \underline{E}\cdot\underline{\dot{x}}_i}{k_BT}\frac{L}{k_BT_\vartheta} \qquad$ if $\qquad dNk_BT \stackrel{def}{=} \sum \frac{\underline{p}_i^2}{2m}$

(3) $\sigma = \sqrt{\eta}\nu_{collision} \stackrel{def}{=} \frac{L}{k_BT_\vartheta}\ \ldots.$

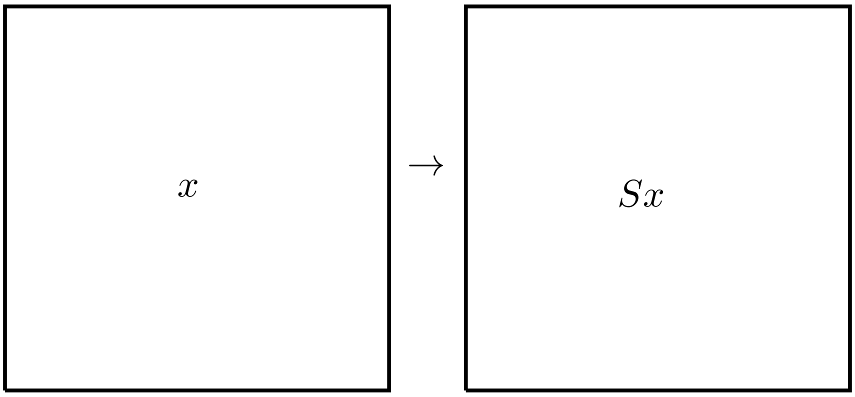
In general $\sigma = \sum \underline{p}_i \cdot \partial_{\underline{p}_i}\underline{F}_i \stackrel{def}{=} \frac{\sum \underline{F}_i\cdot\underline{\dot{x}}_i}{k_BT_\vartheta}$

Thermostats (1), (3) are irreversible while (2) is reversible *i.e.* it generates a dynamics S_tx such that $IS_t = S_{-t}I$ wih $I(p,x) \stackrel{def}{=} (-p,x)$.

One says that motion *has a well defined statistics* μ if

$\frac{1}{T}\sum_{n=0}^{T-1} F(S^n x) \xrightarrow[T\to\infty]{} \int \mu(dy)\, F(y)$ for (a.s.) all x

Assumption: (*Chaotic hypothesis* (M, S) is such that



(1) *covariance*

(2) x *"hyperbolic"*

(3) *dense orbit*

(Ruelle 73, Cohen, G, 95)

Consequence: a.a. initial data x have statistics μ independent on x: SRB–statistics

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In equilibrium: $\Rightarrow$ ergodicity $\Rightarrow$ statistical mechanics

For instance: in the conservative case the stationary states are characterized by two parameters U, V: $\mu = \mu_{U,V}$. And *Boltzmann's heat theorem* follows

Let $p(U, V)$ be the $\mu_{U,V}$ average momentum transfer to walls

Let $T(U, V)$ be the $\mu_{U,V}$ average kinetic energy

Then $\frac{dU+p(U,V)dV}{T}$ = exact (hence = dS): **a parameterless universal relation**

Are there such consequences in nonequlibrium? when the chaotic hypothesis becomes the chaotic hypothesis?

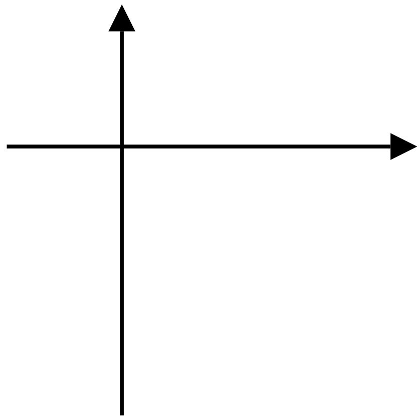
A "*nonequilibrium ensemble*" is a collection of probability distributions on phase space which are stationary and are parameterized by macroscopic parameters like U, V, E in the example and by the thermostat force.

Experimentally discovered property (Evans,Cohen,Morriss, 93) in nunerical study of a *reversible* system of 54 particles. Define the observable

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

has probability of being between p and $p+dp$ proportional to $e^{-\tau\zeta(p)+\ldots}$ and $\zeta(p)$ verifies the "Fluctuation Relation"

$$\zeta(-p) = \zeta(p) - p\sigma_+ \qquad (\text{“}FR''\text{)}$$



This is a theorem in systems verifying the chaotic hypothesis (Cohen,G, 95).

Several experimental (numerical) checks

Nonnumerical tests attempted but, so far, not successfully (difficulty of observing such large fluctuations)

Need a "local fluctuation result" (G98).

Chain (or d-dimensional lattice) of "*Arnold cat maps*"

$$\bullet^{\underline{\varphi}_0}_{0} \qquad \bullet^{\underline{\varphi}_1}_{1} \qquad \bullet^{\underline{\varphi}_2}_{2} \ldots \qquad \ldots \bullet^{\underline{\varphi}_{V-1}}_{V-1}$$

where

$$\underline{\varphi}'_j = \begin{pmatrix} \varphi'_{j1} \\ \varphi'_{j2} \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \varphi_{j1} \\ \varphi_{j2} \end{pmatrix} + \eta \begin{pmatrix} \delta_1(\underline{\varphi}_j) \\ \delta_2(\underline{\varphi}_j) \end{pmatrix} + \varepsilon \begin{pmatrix} f_1(\underline{\varphi}_{nn(j)}) \\ f_2(\underline{\varphi}_{nn(j)}) \end{pmatrix}$$

where f_j depends on nearest neighbors only (eg $f_1 = \cos(\varphi_{j+1,1} - 2\varphi_{j,1} + f_{j-1,1})$

For $\eta \neq 0$ and ε small the system is chaotic (for most f, δ) and dissipative *uniformly* in the size V of the system.

$$-\log\det \partial S_\varepsilon(\underline{\varphi})\partial\underline{\varphi} = \sigma(\underline{\varphi}) \quad \text{has} \quad \langle\sigma\rangle = \sigma_+ V$$

$$\sigma_{V_0} = \log\det \frac{\partial S_{V_0}(\underline{\varphi}_{V_0}\underline{\varphi}_{V_0^c})}{\partial\underline{\varphi}_{V_0}}$$

Th.: if $p = \frac{1}{V_0\tau}\sum_{-T/2}^{T/2}\sigma_{V_0}(S^j\underline{\varphi})$ then the probability is $e^{-V_0\tau\zeta(p)}$ and

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

Real systems are almost always modeled by *non reversible thermostsats*

Equivalence conjectures.