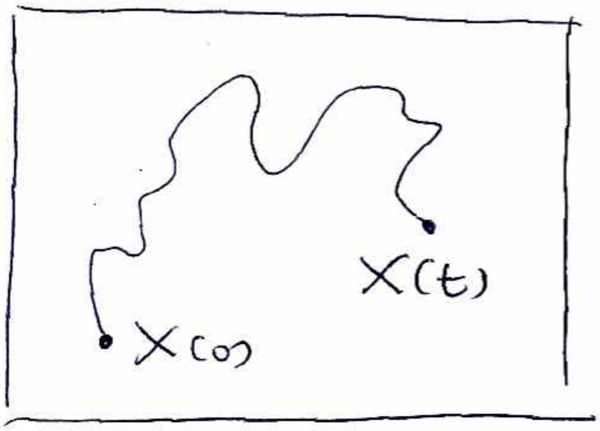
Ensembles

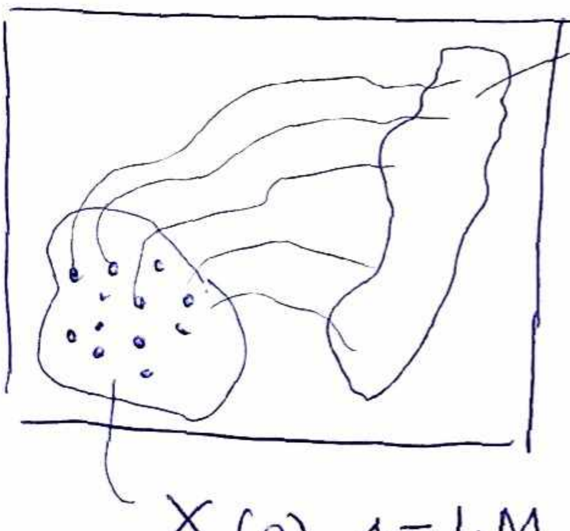
Single evolution



time average

$$(\bar{f})_T = \frac{1}{T}\int_0^t dt\, f(X(t))$$

ensemble of initial data

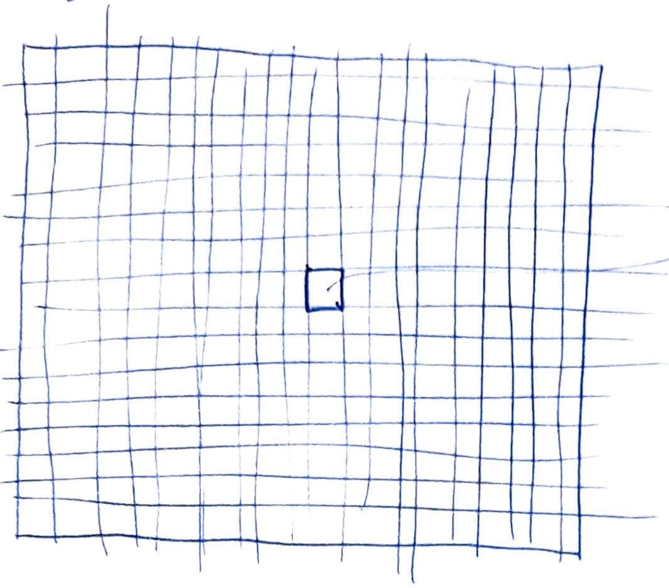


define average on an ensemble as

$$\langle f(0)\rangle = \lim_{M\to\infty} \frac{1}{M}\sum_{1}^{M} f(X_i(0)) \quad \text{at time } t=0$$

$$\langle f(t)\rangle = \lim_{M\to\infty} \frac{1}{M}\sum_{1}^{M} f(X_i(t)) \quad \text{at time } t>0$$

discrete phase space on hyper cubes of volume Δx



α-th cell of "volume" Δx

$\alpha = 1, \mathcal{M}$

in each cell the observable f take a definite value

$$f(x) = f_\alpha \quad \forall\, x \in \alpha\text{-th cell}$$

then

$$\frac{1}{M}\sum_{i=1}^{M} f(x_i) = \frac{1}{M}\sum_{\alpha=1}^{\mathcal{M}} f_\alpha n_\alpha$$

# of points of ensembles that fill the α-th cell

for very small cell's volume

$$\lim_{M\to\infty} \sum_{i=1}^{M} f(x_i) = \lim_{\substack{\Delta x\to 0\\ M\to\infty}} \frac{1}{M\Delta x}\sum_\alpha \Delta x\, n_\alpha f_\alpha$$

$$\lim_{M\to\infty} \frac{1}{M}\sum_{i=1}^{M} f(x_i) = \boxed{\int dx\, \rho(x)\, f(x)}$$

since $\sum_{\alpha=1}^{\mathcal{M}} n_\alpha = M$ $\qquad \sum_\alpha \rho_\alpha \Delta x = \sum_\alpha \frac{n_\alpha \Delta x}{M\Delta x} = 1$

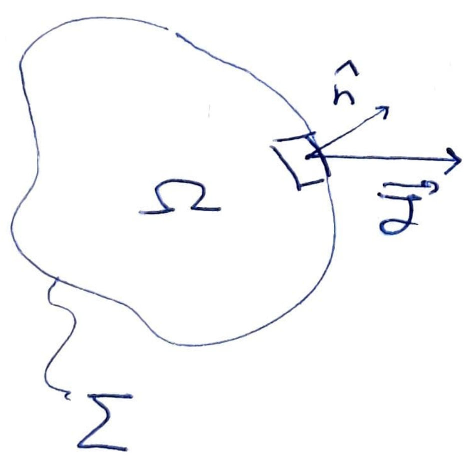
Liouville's theorem (Motion of ensemble)

$$\begin{cases} \dot{p} = -\dfrac{\partial H}{\partial q} \\ \dot{q} = \dfrac{\partial H}{\partial p} \end{cases} \Rightarrow \text{variation in time of } \rho(\overbrace{p\,q}^{x}\,t)$$

$$\underbrace{\frac{d}{dt}\int_{\Omega} d\Gamma\, \rho(x,t) = -\int_{\Sigma} \vec{J}\cdot\hat{n}\, d\Sigma}_{\text{"Mass" conservation}}$$

Stoke's theorem

$$\int_{\Sigma} \vec{J}\cdot\hat{n}\, d\Sigma = \int_{\Omega} d\Gamma\, \mathrm{div}\, \vec{J}$$



$$\vec{J} = \rho\, \vec{v}$$

"density" "velocity"

$$\vec{J} = \begin{pmatrix} \rho \dot{q} \\ \rho \dot{p} \end{pmatrix} \begin{matrix} \} 3N \\ \} 3N \end{matrix} \Big\} \text{ 6N coordinates}$$

$$\operatorname{div} \vec{J} = \frac{\partial}{\partial q}(\rho \dot{q}) + \frac{\partial}{\partial p}(\rho \dot{p}) =$$

$$= \frac{\partial \rho}{\partial q} \dot{q} + \cancel{\rho \frac{\partial \dot{q}}{\partial q}} + \frac{\partial \rho}{\partial p} \dot{p} + \cancel{\rho \frac{\partial \dot{p}}{\partial p}}$$

Hamilton's equations

$$\frac{\partial \dot{q}}{\partial q} = -\frac{\partial^2 H}{\partial q \partial p} \qquad \frac{\partial \dot{p}}{\partial p} = \frac{\partial^2 H}{\partial p \partial q}$$

$$\operatorname{div} \vec{J} = + \frac{\partial \rho}{\partial q} \frac{\partial H}{\partial p} - \frac{\partial \rho}{\partial p} \frac{\partial H}{\partial q} = + \{\rho, H\}$$

Poisson's parentheses

$$\{\rho, H\} = \frac{\partial \rho}{\partial q} \frac{\partial H}{\partial p} - \frac{\partial \rho}{\partial p} \frac{\partial H}{\partial q}$$

$$\int_\Omega d\Gamma \frac{\partial \rho}{\partial t} = -\int d\Gamma \left(+ \{\rho, H\} \right)$$

$$\boxed{\frac{\partial \rho}{\partial t} = -\{\rho, H\}}$$ Liouville

notice that for a generic phase-space function ...

$$\frac{df}{dt} = \frac{\partial f}{\partial q}\dot{q} + \frac{\partial f}{\partial p}\dot{p} + \frac{\partial f}{\partial t}$$

$$\frac{df}{\partial t} = \{f, H\} + \frac{\partial f}{\partial t}$$

just the opposite sign of ρ evolution

that means that for the distribution function the total derivative i.e. the derivative along the trajectory is zero!

$$\frac{d\rho}{dt} = 0 \qquad \boxed{\frac{\partial \rho}{\partial t} = -\{\rho, H\}}$$

in quantum mechanics ...

an operator $\hat{A}$ evolves (in the Heisenberg's picture) as

$$\hat{A}(t) = e^{+\frac{i}{\hbar}Ht} A \, e^{-\frac{i}{\hbar}Ht}$$

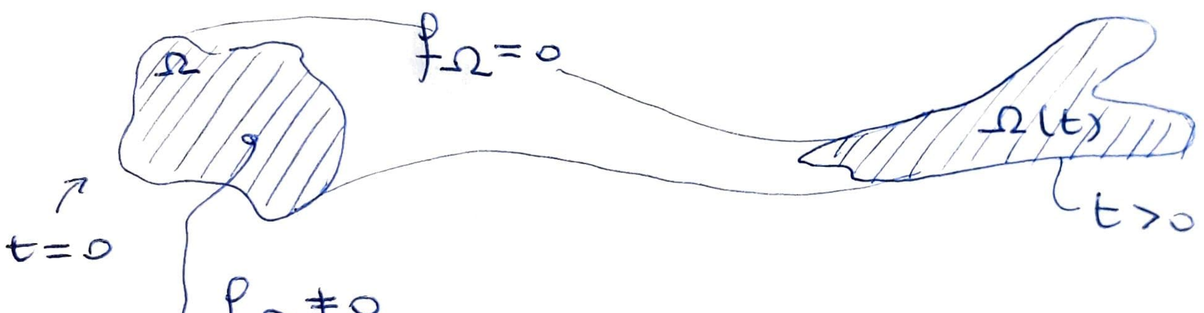
$$\frac{d\hat{A}}{dt} = +\frac{i}{\hbar}[H, A] = -\frac{i}{\hbar}[A, H]$$

$$\boxed{\{\ldots, \ldots\} \Longleftrightarrow -\frac{i}{\hbar}[\ldots, \ldots]}$$

Conservation of "volumes" of phase space in Hamiltonian systems

to select a "volume" in phase space define the charateristic function

$$f_\Omega(x) = \begin{cases} x \subset \Omega \neq 0 \\ x \not\subset \Omega = 0 \end{cases}$$



take this function as the $t=0$ $f(x,0) = f_\Omega(x)$ in the Liouville's evolution of Hamiltonian system

the volume at $t=0$ is

$$\Omega(0) = \int_\Omega dp(0)\, dq(0)$$

the volume at time t

$$\Omega(t) = \int dp(t)\, dq(t)$$

the relation btw $\Omega(0)$ & $\Omega(t)$ involves a Jacobian J

$$\underbrace{\int dp(t)\, dq(t)}_{\Omega(t)} = J \underbrace{\int dp(0)\, dq(0)}_{\Omega(0)}$$

$$dp(t)\,dq(t) = J(t)\,dp(0)\,dq(0)$$

$$J(t) = \frac{\partial(p(t), q(t))}{\partial(p(0), q(0))} = \begin{vmatrix} \frac{\partial p}{\partial p(0)} & \frac{\partial p}{\partial q(0)} \\ \frac{\partial q}{\partial p(0)} & \frac{\partial q}{\partial q(0)} \end{vmatrix}$$

time dependent

$$\frac{dJ}{dt} = \frac{d}{dt}\left(\frac{\partial p}{\partial p(0)}\frac{\partial q}{\partial q(0)} - \frac{\partial p}{\partial q(0)}\frac{\partial q}{\partial p(0)}\right)$$

$$= \frac{\partial \dot p}{\partial p(0)}\frac{\partial q}{\partial q(0)} + \frac{\partial p}{\partial p(0)}\frac{\partial \dot q}{\partial q(0)} - \frac{\partial \dot p}{\partial q(0)}\frac{\partial q}{\partial p(0)} - \frac{\partial p}{\partial q(0)}\frac{\partial \dot q}{\partial p(0)}$$

(a) (b)

$$= \underbrace{\begin{vmatrix} \frac{\partial \dot p}{\partial p(0)} & \frac{\partial \dot p}{\partial q(0)} \\ \frac{\partial q}{\partial p(0)} & \frac{\partial q}{\partial q(0)} \end{vmatrix}}_{(a)} + \underbrace{\begin{vmatrix} \frac{\partial p}{\partial p(0)} & \frac{\partial p}{\partial q(0)} \\ \frac{\partial \dot q}{\partial p(0)} & \frac{\partial \dot q}{\partial q(0)} \end{vmatrix}}_{(b)}$$

$$\frac{\partial \dot p}{\partial p(0)} = \frac{\partial \dot p}{\partial p}\frac{\partial p}{\partial p(0)} + \frac{\partial \dot p}{\partial q}\frac{\partial q}{\partial p(0)}$$

$$(a) = \begin{vmatrix} \underbrace{\frac{\partial \dot p}{\partial p}\frac{\partial p}{\partial p(0)}}_{a} + \underbrace{\frac{\partial \dot p}{\partial q}}_{\lambda}\frac{\partial q}{\partial p(0)} & \underbrace{\frac{\partial \dot p}{\partial p}\frac{\partial p}{\partial q(0)}}_{b} + \frac{\partial \dot p}{\partial q}\frac{\partial q}{\partial q(0)} \\ \underbrace{\frac{\partial q}{\partial p(0)}}_{c} & \underbrace{\frac{\partial q}{\partial q(0)}}_{d} \end{vmatrix}$$

$$= \begin{vmatrix} a + \lambda c & b + \lambda d \\ c & d \end{vmatrix} = \begin{vmatrix} a & b \\ c & d \end{vmatrix}$$

the same holds for (b) thus

$$\frac{dJ}{dt} = \underbrace{\begin{vmatrix} \frac{\partial \dot p}{\partial p}\frac{\partial p}{\partial p(0)} & \frac{\partial \dot p}{\partial p}\frac{\partial p}{\partial q(0)} \\ \frac{\partial q}{\partial p(0)} & \frac{\partial q}{\partial q(0)} \end{vmatrix}}_{(a)} + \underbrace{\begin{vmatrix} \frac{\partial p}{\partial p(0)} & \frac{\partial p}{\partial q(0)} \\ \frac{\partial \dot q}{\partial q}\frac{\partial q}{\partial p(0)} & \frac{\partial \dot q}{\partial q}\frac{\partial q}{\partial q(0)} \end{vmatrix}}_{(b)}$$

Now use

$$\left(\begin{vmatrix} ka & kb \\ c & d \end{vmatrix} = k \begin{vmatrix} a & b \\ c & d \end{vmatrix} \right)$$

$$\frac{dJ}{dt} = \frac{\partial \dot p}{\partial p} J + \frac{\partial \dot q}{\partial q} J$$

Hamilton's equation got a $-$ sign!

$$\begin{cases} \dot q = \frac{\partial H}{\partial p} \\ \dot p = -\frac{\partial H}{\partial q} \end{cases} \qquad \begin{aligned} \frac{\partial \dot q}{\partial q} &= \frac{\partial^2 H}{\partial q \partial p} \\ \frac{\partial \dot p}{\partial p} &= -\frac{\partial^2 H}{\partial p \partial q} \end{aligned}$$

therefore

$$\frac{dJ}{dt} = 0 \Rightarrow J = \text{Const in time!}$$

and since $J(0) = 1 \Rightarrow J = 1 \Rightarrow \Omega(t) = \Omega(0)$

(Q.E.D)

Stationary distribution

Ensemble of initial data will evolve according Liouville's theorem

$$\frac{\partial \rho}{\partial t} = \{H, \rho\} = \frac{\partial H}{\partial q}\frac{\partial \rho}{\partial p} - \frac{\partial H}{\partial p}\frac{\partial \rho}{\partial q}$$

a stationary distribution ρ_{stat} is such that

$$\rho_{stat}(\cancel{t}) \Rightarrow \frac{\partial \rho_{stat}}{\partial t} = 0$$

$$\rho = \rho_{stat} \iff \{H, \rho_{stat}\} = 0$$

a possible choice is

$$\rho_{stat}(pq) = f(H(qp))$$

because

$\{H, f(H)\} = 0$ (as in QM $\hat{H}$ commutes with a generic $f(\hat{H})$)

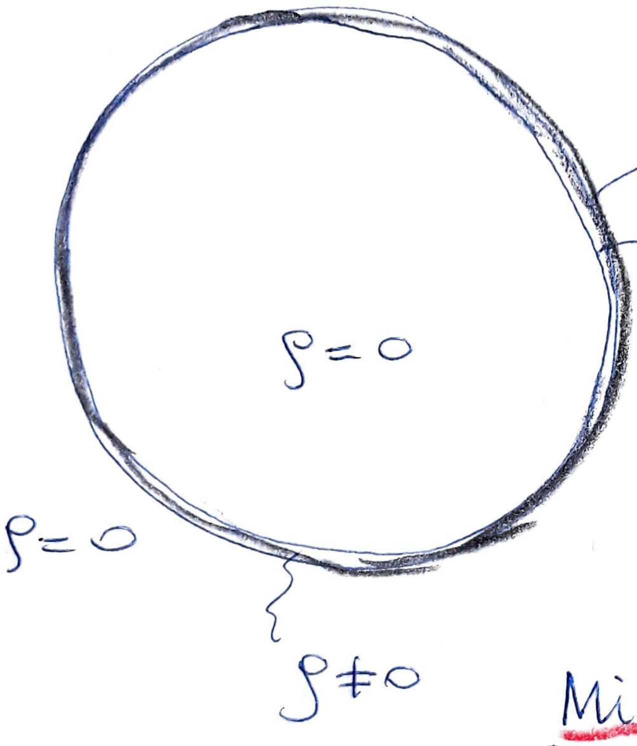
But for an isolated system

$H = E$ is conserved

thus for an isolated system

$p, q \mid H = E \qquad \rho_{stat} = \text{const}$

$p, q \mid H \neq E \qquad \rho_{stat} \neq 0$



"small" Δ
i.e. Δ not
extensive

Micro Canonical
Distribution

$$\rho_{stat}(pq) = \frac{\Delta(H-E)}{\int d^{3N}p\, d^{3N}q\, \Delta(H-E)}$$

$$\Delta(H-E) = \begin{cases} 1 & E \leq H \leq E+\Delta \\ 0 & \text{otherwise} \end{cases}$$

Ergodic theorems (unuseful)

Ergodic System — Definition

$$\lim_{T\to\infty} \bar{f}_T = \int d\Gamma\, \rho_{eq}(x) f(x)$$

- independent on $X(0)$ $\forall f$
- independent on the trajectory — def

I) Birkhoff th.

- Dynamics will give rise to a limited motion
- $f(x)$ is integrable with weight ρ_{eq}
- $\exists$ almost everywhere the limit

$$\lim_{T\to\infty} \bar{f}_T$$

then

a) $\bar{f}_{T\to\infty}$ is indep $X(0)$

b) $\bar{f}_{T\to\infty}$ may depend on trajectory

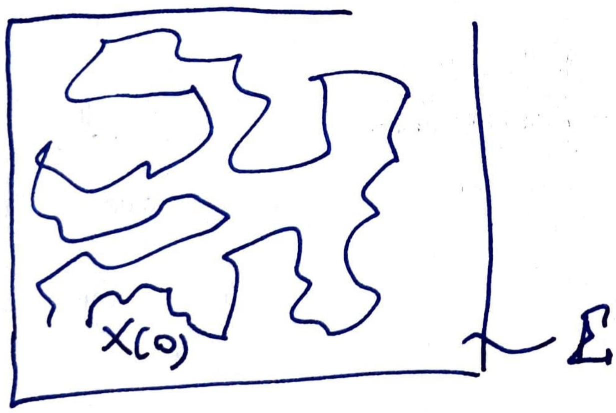
II Birkoff

+ to other hypothesys of BK 1

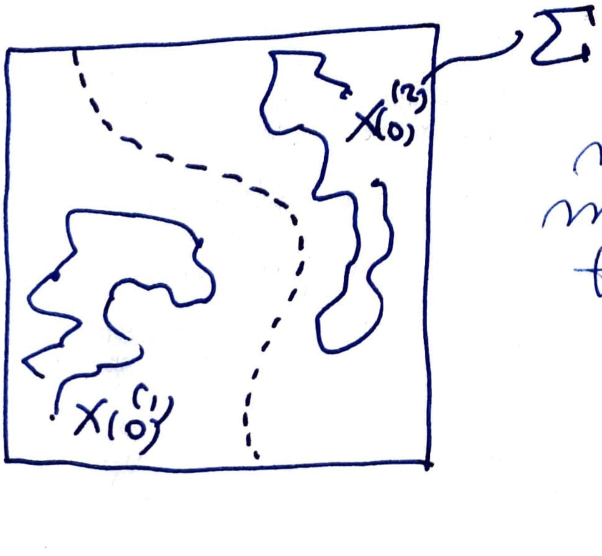
Metrically transitivity i.e.

- Σ cannot by divided in parts such that they are disconnected by mechanical motion

then the system is ergodic



metrically transitive



non metrically transitive

Ergodicity & Mixing

Ergodicity

for <u>any</u> phase function $f(x)$

a) $\exists$ time average for almost all initial data

$$\overline{(f)}_T = \lim_{T\to\infty} \frac{1}{T}\int_0^T dt\, f(X(t))$$

b) if $\overline{(f)}$ exists then

$$\overline{(f)} = \int dx\, \rho_{sta}(x) f(x)$$

where ρ_{stat} is constant on the surface $H=E$

Mixing

a system is mixing if for <u>any</u> phase function $f(x)$ and <u>any</u> initial $\rho(x,0)$

$$\lim_{t\to\infty} \langle f(t)\rangle = \int dx\, \rho(x,t) f(x) = \int dx\, \rho_{stat}(x) f(x)$$

Mixing is stronger than ergodicity

Ergodicity $\not\to$ Mixing but
Mixing $\longrightarrow$ Ergodicity

Mixing $\lim_{t\to\infty} \langle f(t) \rangle = \int dx\, \rho_{st}(x) f(x) \quad \forall f$

$\forall \rho(x,0)$

now formally $\boxed{P(B) = \int dA\, P(B|A)\, P(A)}$

$$\rho(x,t) = \int d\bar{x}\, \rho(x,t|\bar{x},0)\, \rho(\bar{x},0)$$

for a deterministic evolution if $X(t)$ is the evolution choosing an ensemble such that

$\rho(\bar{x},0) = \delta(\bar{x} - x_0)$ i.e. all elements of the ensemble departs from the same initial condition

then

$$\rho(x,t) = \rho(x,t|x_0,0) = \delta(x - X(t))\Big|_{X(0)=x_0}$$

is a single dummy trajectory

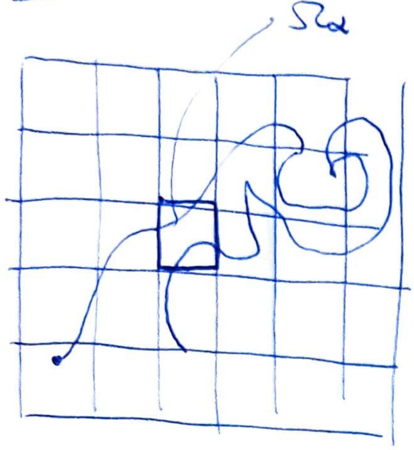
$$\bar{f} = \lim_{T\to\infty} \int_0^T dt\, f(X(t))\Big|_{X(0)=x_0} = \int dx \left(\underbrace{\lim_{T\to\infty} \frac{1}{T} \int_0^T dt\, \delta(x - X(t))\Big|_{X(0)=x_0}}_{\rho(x,t)!} \right) f(x)$$

$\boxed{\lim_{T\to\infty} \frac{1}{T} \int_0^T dt\, \rho(x,t) = \rho_{st}(x)}$ and

$$\bar{f} = \int dx\, \rho_{st}(x)\, f(x)$$

Alternative def of ergodicity

An ergodic system spend a time τ in the volume $\Omega \supset \Gamma$ which is proportional to Ω



divide the Γ in M cell

if the cells are small

$$f(x) \quad x_\alpha \supset \Omega_\alpha \simeq f(x_\alpha)$$

$$\overline{(f)}_T = \frac{1}{T}\int_0^T dt\, f(x(t))$$

$$\overline{(f)}_T \simeq \frac{1}{T}\sum_{\alpha=1}^{M} n_\alpha \tau_\alpha f(x_\alpha)$$

time spent in the α-th cell

# of times the system is in the cell (α-th) $n_\alpha \geq 0$

The system is ergodic therefore

$$\lim_{T\to\infty} \sum_{\alpha=1}^{M} \frac{n_\alpha \tau_\alpha}{T} f(x_\alpha) = \sum_\alpha \rho_{stat}(x_\alpha) f(x_\alpha) \Omega_\alpha$$

small volume

this is valid for any f therefore

total time τ

$$\lim_{T\to\infty} \frac{n_\alpha \tau_\alpha}{T} = \rho_{stat}(x_\alpha)\Omega_\alpha$$

const $\sim \frac{1}{\Gamma}$ available volume

total time spent on volume Ω $\rightarrow$ $\frac{\tau}{T} = \frac{\Omega}{\Gamma}$ — volume / total volume

Measured time

Chaos in dynamical systems

Chaos is the sensitivity ~~of~~ dynamical evolution to small differences in initial data.

Let's consider 2 initial date

$X(0) \longrightarrow x(t)$

$X(0)+\delta \longrightarrow x'(t)$

for a chaotic system $X'(t)$ departs exponentially from $X(t)$

let

$|x'(t) - X(t)| \propto e^{\lambda t}$

there should be a proportionality factor of the same dimensions as x which go to zero as $\delta \to 0$ therefore we choose for small δ

$$|x'(t) - x(t)| = \delta e^{\lambda t}$$

In this case

$$\lambda = \frac{1}{t} \ln \frac{|x'(t) - x(t)|}{\delta}$$

to generalise this argument let us define

$$\boxed{\lambda = \lim_{t \to \infty} \lim_{\delta \to 0} \frac{1}{t} \ln \frac{|x'(t) - x(t)|}{\delta}}$$

the Lyapunov exponent

Chaoticity is a property of dynamical system which can occur in low dimensional systems and is not directly related to irreversibility of a macroscopic system.

However generally speaking systems with more than 3 particles are chaotic (in presence of interaction)

Liapunov exponent

Suppose that we have

1) $|x'(0) - x(0)| < \varepsilon$ at time $t=0$

we hae chaos if

2) $|x'(t) - x(t)| \propto e^{\lambda t}$ with $\lambda > 0$

Let us consider

$|x'(t) - x(t)| = \varepsilon e^{\lambda t}$ (constant)

constant < 1 such that at $t=0$ (1) is fulfilled the constant will be unessential

$$|x'(t) - x(t)| = k\varepsilon e^{\lambda t}$$

$$\lambda = \frac{1}{t} \ln\left[\frac{|x'(t) - x(t)|}{k\varepsilon}\right]$$ depends on time!

or

$$\boxed{\lambda(t) = \frac{1}{t} \ln \frac{|x'(t) - x(t)|}{|x'(0) - x(0)|}}$$

the Liapunov exponent is defined as

$$\lambda = \lim_{t \to \infty} \lim_{x'(0) \to x(0)} \frac{1}{t} \ln \frac{|x'(t) - x(t)|}{|x'(0) - x(0)|}$$

<u>in this order!</u>

first $x'(0) \to x(0)$

then $t \to \infty$

<u>Discrete maps</u>

$$\underline{x}_{n+1} = f(\underline{x}_n)$$

Vector d-dimensional

time is discrete

f LINEAR is trivial

f non LINEAR

Consider a $d = 1$ map

"initial time"

$$x_1 \longrightarrow x_{n+1} \qquad n = (n+1) - 1$$

$$x'_1 \longrightarrow x'_{n+1}$$

$$\frac{1}{n} \ln \frac{|x'_{n+1} - x_{n+1}|}{|x'_1 - x_1|} = \frac{1}{n} \ln \frac{|f(x'_n) - f(x_n)|}{|x'_1 - x_1|} = \lambda_n$$

consider $n=1$

$$\lambda_1 = \ln \left| \frac{f(x_1')-f(x_1)}{x_1'-x_1} \right|$$

consider $x_1' > x_1$

$$\lambda_1 = \ln \left(\frac{df}{dx}\right)_{x=x_1}$$

now generalise

$$\lambda_m = \ln\left|\left(\frac{df}{dx}\right)_{x=x_m}\right|$$

perform the time average

$$\lambda = \lim_{n\to\infty} \frac{1}{n}\sum_{1}^{m}{}_{m}\, \lambda_m$$

$$= \lim_{n\to\infty} \frac{1}{n}\sum_{1}^{n}{}_{m}\, \ln\left|\left(\frac{\partial f}{\partial x}\right)_{x=x_m}\right|$$

Now for a <u>linear map</u>

$\left(\frac{\partial f}{\partial x}\right)\Big|_{x=x_m}$ indep of x_m

$$\lambda = \ln c$$

and $c<0$ to have a stable map!

check

logistic Map

$$x_{n+1} = r\, x_n (1 - x_n)$$

parameter

depending on r there can or canot be chaos

Conservation of volumes in a discete-time map: the Arnold's cat map

let $0 \leq q \leq L$; $0 \leq p \leq L$

and

$$\begin{cases} \tilde{q}_{t+1} = 2q_t + p_t \\ \tilde{p}_{t+1} = q_t + p_t \end{cases} \quad \text{and} \quad \begin{cases} q_{t+1} = \mathrm{mod}(\tilde{q}_{t+1}, L) \\ p_{t+1} = \mathrm{mod}(\tilde{p}_{t+1}, L) \end{cases}$$

e.g. if $\tilde{p}_{t+1} = 1,2$ and $L = 1$ then $p_{t+1} = 0,2$

$$\begin{pmatrix} q_{t+1} \\ p_{t+1} \end{pmatrix} = \begin{bmatrix} 2 & 1 \\ 1 & 1 \end{bmatrix} \begin{pmatrix} q_{t+1} \\ p_{t+1} \end{pmatrix} \mod L$$

$$dq_{t+1}\, dp_{t+1} = J\, dq_t\, dp_t$$

$$J = \begin{vmatrix} 2 & 1 \\ 1 & 1 \end{vmatrix} = 2 - 1 = 1$$

Arnold's cat map preserves volumes

Separable Hamiltonians

(and the role of observables)

$$H = \sum_{1}^{N}{}_{n} H_n (q_n\, p_n)$$

$$\begin{cases} \dot{q}_k = \dfrac{\partial H}{\partial p_k} = \dfrac{\partial H_k}{\partial p_k} \\ \dot{p}_k = -\dfrac{\partial H}{\partial q_k} = -\dfrac{\partial H_k}{\partial q_k} \end{cases}$$

$\{H, H_n\} = 0 \quad \forall n \quad H_n$ constant of motion

no equipartition & no ergodicity - (stricto sensu) for a special observable which select only some of the variables $\{q_m, p_m\}$ the average over time $\neq$ average are stationary ensemble

N disconnected ensembles

Example

$$H = \sum_{1}^{N}{}_{n} \frac{p_n^2}{2m_n} + \frac{1}{2} m_n \omega_n^2 q_n^2$$

$$\begin{cases} q_n = A_n \cos(\omega_n t + \varphi_n) \\ p_n = -m_n \omega_n A_n \sin(\omega_n t + \varphi_n) \end{cases}$$

Solution

Energy of a single "mode" m is

$$E_m = \frac{1}{2} m_n \omega_n^2 A_m^2$$

and is constant

now let's consider a single function

$$f_m(q_m(t), p_m(t))$$

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T dt\, f_m\left(A_m \cos(\omega_n t + \varphi_m), -m_n\omega_n A_m \sin(\omega_n t + \varphi_m)\right)$$

$$= \int_0^{2\pi} d\varphi_m\, f_m\left(A \cos(\varphi_m), -m_n\omega_n A_m \sin(\varphi_m)\right)$$

but averaging over the phase means

average over surface of constant

Mode energy

But each mode energy is conserved

Interaction is needed for equipartition

However I can always start from a typical initial data which conserves the total energy and consider the sum functions

$$f(x) = \Sigma_n f_n(q_n, p_n)$$

then on probability on random initial data

Khinchin (Khintchine) theorem

$$\mathrm{Prob}\left(\left| \frac{(\bar{f})}{\langle f \rangle_{stat}} - 1 \right| > \frac{k_1}{N^{1/4}} \right) < \frac{k_2}{N^{1/4}}$$

this is not ergodicity but is "ergodicity" in probability as $N \to \infty$

We must consider observables which cumulates the state of all the constituents of a large system

A. J. Khinchin "Mathematical foundations of Statistical Mechanics" (Dover publications, 1960)