**First step:** Take a classical dynamical system of N particles with $\vec{q}$ = 3N coord. of all particles

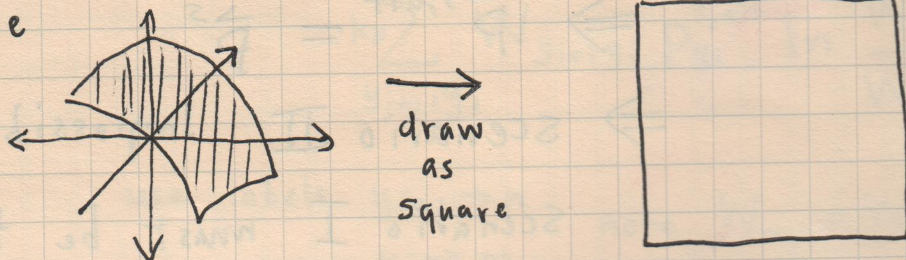
$\vec{p}$ = 3N momenta of all particles

System confined to finite volume V, no gain/loss of energy from outside (isolated).

total energy $E = H(\vec{q}, \vec{p})$ conserved

$\uparrow$ Hamiltonian

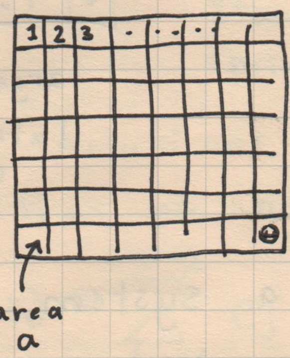
For a given E, the equation $E = H(\vec{q}, \vec{p})$ defines a $6N-1 \equiv D$ dimensional surface in phase space



Divide up this constant energy phase space into area elements, label them $\nu = 1, \ldots\ldots, \Theta(E)$ of area $a$ (small)

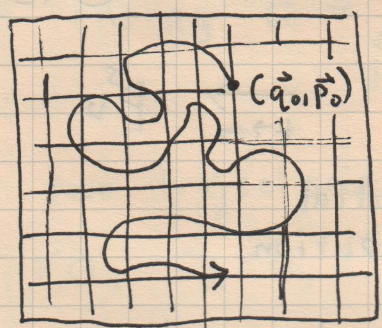
$\uparrow$ func. of $E$ (and $a$)

phase space surface of constant $E$




we say system is in "state" $\nu$ if $(\vec{q}, \vec{p})$ falls inside element $\nu$

Classical mechanics starting w/ energy $E$ at initial point $(\vec{q}_0, \vec{p}_0)$ is a path on this surface.

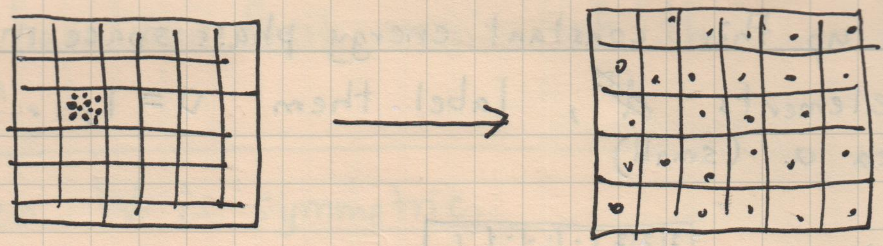



Keep in mind this system is deterministic! (no randomness assumed)

To justify stat. mech, we want a system where all trajectories (except maybe for a set of measure zero) are:

- ergodic: as $t \to \infty$ every state $\nu$ will be visited, no matter how small $a$ is
- mixing: if at $t=0$ several similar trajectories are initiated in any state $\nu_0$, they will diverge quickly (exponentially in time) so that when $t \to \infty$ the $(\vec{q}, \vec{p})$ of these trajectories are distributed equally among all states (hallmark of a chaotic system!)

__note:__ mixing is a stronger subset of ergodic mixing:



$t=0$
initial dist. of $(\vec{q},\vec{p})$

large $t$
later dist. of $(\vec{q},\vec{p})$

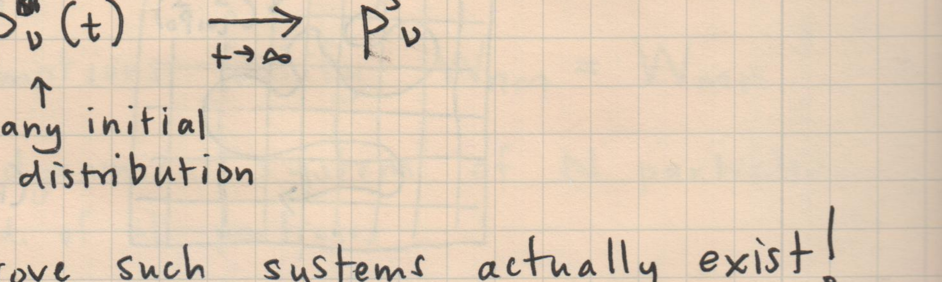
If one could find such a system, then one could generate a microcanonical ensemble by just waiting: a ~~collection of~~ stationary probability distribution $p^s_\nu = \dfrac{1}{\Theta(E)}$ = same for all $\nu$

Mixing entails $p^{0}_\nu(t) \xrightarrow[t\to\infty]{} p^s_\nu$
↑
any initial distribution

Not so easy to prove such systems actually exist!

1953-55: Fermi, Pasta, Ulam (FPU) and Tsingou conduct first ever physics computer simulation (on MANIAC I in Los Alamos) looking for this mixing behavior

Test system:
coupled harmonic oscillators




spring constants $k$
mass $m$ at position $X_i(t) = l_i + x_i(t)$

equations of motion:

$$m\ddot{x}_i = \underbrace{\left[ k(x_{i+1}-x_i) + k(x_{i-1}-x_i) \right]}_{\text{Standard spring forces}} \left[ 1 + \alpha\,(x_{i+1}-x_{i-1}) \right]$$

↑ nonlinear perturbation

<u>when $\alpha = 0$</u>, solutions ~~have~~ can be written as superposition of normal modes:

$$x_i(t) = \sum_{j=1}^{N-2} c_j\, \xi_i^{(j)}(t)$$

$\omega = \sqrt{\frac{k}{m}}$

where $\xi_i^{(j)}(t) = \cos\left(\frac{j\pi\omega t}{(N-1)}\right) \sin\left(\frac{ij\pi}{N-1}\right)$

total energy $E = \sum_{j=1}^{N-2} \underbrace{c_j^2\, \epsilon^{(j)}}$ ↳ energy of jth mode

Can choose two trajectories, one with

$c_1 \neq 0,\ c_2 = 0,\ \ldots,\ c_{N-2} = 0$

other with

$c_1 = 0,\ c_2 \neq 0,\ c_3 = 0,\ \ldots,\ c_{N-2} = 0$

and same $E$, and they will ~~never come close to each other~~ stay in separate parts of phase space, never mixing (energy in each mode a constant of motion)

$c_j(t)$ becomes time-dependent

FPU tried $\alpha \neq 0$, creating "interactions" among modes, so energy (and amplitude) began spreading from one mode to another, but when they waited...

~~not all modes~~

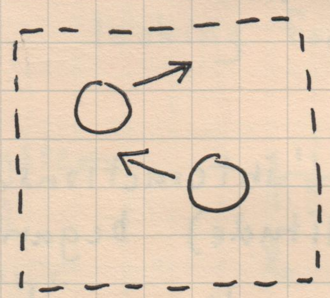
all modes <u>did not</u> become equally likely, but the system followed complex quasiperiodic patterns if you start 100% in mode 1, eventually return to case where 99% of energy is in mode 1, etc., and you never reach high $j$ modes

$\Rightarrow$ Major mystery! $\Rightarrow$ no ergodicity, no mixing

1954-1963: Kolmogorov, Arnold, Moser (KAM) theorem proves that for weak interparticle interactions, quasiperiodic behavior persists near the unperturbed (zero interaction) trajectories.

To get ergodic + mixing you need strong interactions ~~in~~ in a many particle system.

1970: Yakov Sinai (2014 Abel prize) makes breakthrough, proving that two hard disks on 2D square w/ periodic boundaries are ergodic + mixing.
(hard disk = $\infty$ repulsion on overlap = strong interaction)



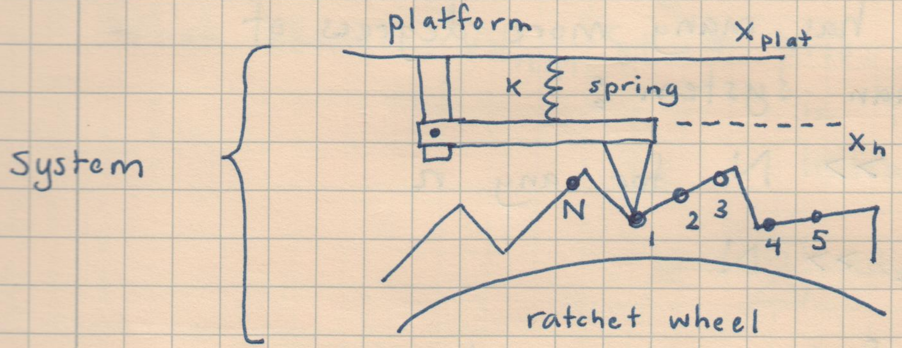
"Sinai billiard"

system exhibits chaotic trajectories, allowing for mixing

slow progress: $N \geq 2$ d-dim. spheres is almost proven to be ergodic

To connect these ideas to matrix W, consider a "total" system composed of small subsystem (call simply "system") + rest (the "environment").

Famous example from Feynman: ratchet + pawl

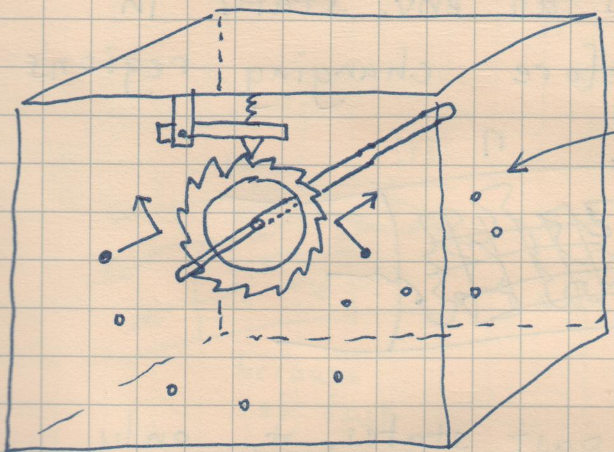



L = natural length of spring

$x_n$ = pawl pos. in nth state

positions of wheel = discrete states (discretize for simplicity)

system energy in state $n$ : $E_n = \frac{1}{2}k\left(x_{plat} - x_n - L\right)^2$



isolated box filled w/ fluid or gas ("environment")

$E_{tot} = E_n + E_n^{env}$

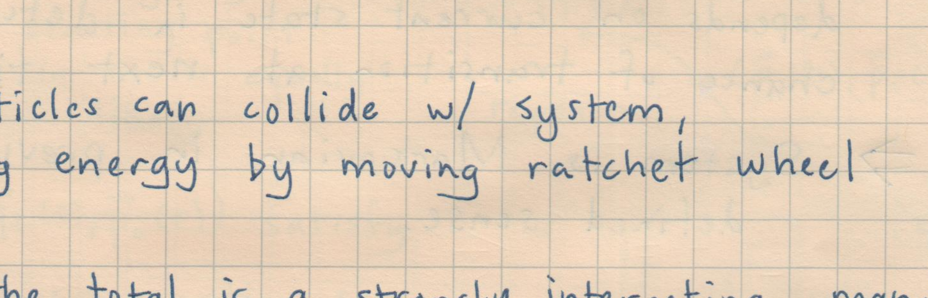
$\Downarrow$ constant

energy of fluid when sys is in state $n$

fluid particles can collide w/ system, exchanging energy by moving ratchet wheel

Assume the total is a strongly interacting, many particle system which is ergodic + mixing.

for total, $E_{tot}$ manifold




diff. regions correspond to diff. sys states

all env. states when sys is in state 1

$\Theta_{tot}$ = tot. number of states on $E_{tot}$ manifold

$\Theta_n$ = number of states of the environment when system is in state $n$

Clearly $\Theta_{tot} = \sum_{n=1}^{N} \Theta_n$

Assumptions:

- environment has many more degrees of freedom than system:

  $\Theta_n \gg N$ for any $n$

  $\Rightarrow \Theta_{tot} \gg N$

- mixing is fast: when a trajectory crosses from states $m \to$ state $n$ region, it quickly explores all env. states in state $n$ region before changing regions

so each subregion of manifold mixes fast compared to $\delta t$ of Markov description


$\Rightarrow$ Dynamics "forgets" past states, & only depends on current state in determining chance of transition at next time step

$\Rightarrow$ System is Markovian in previously defined sense.

- if we wait long enough, $p_\nu(t) \to \frac{1}{\Theta_{tot}} \equiv p^s_\nu$ as $t \to \infty$

for any total state $\nu$

hence $p_n(t)$ = prob. to be in system state $n$ $= \sum_{\nu \in \text{set corr. to } n} p_\nu(t) \longrightarrow \frac{\Theta_n}{\Theta_{tot}}$

Thus an ergodic + mixing total physical system gives remarkable result for stationary probability:

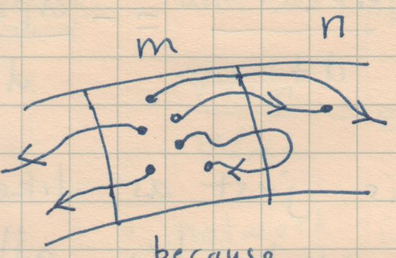
$$P_n^s = \frac{\Theta_n}{\Theta_{tot}}$$

large compared to mixing time in each state

What about $W_{nm}\,\delta t$ = prob. to go from $m \to n$ in time $\delta t$, given initial start in $m$

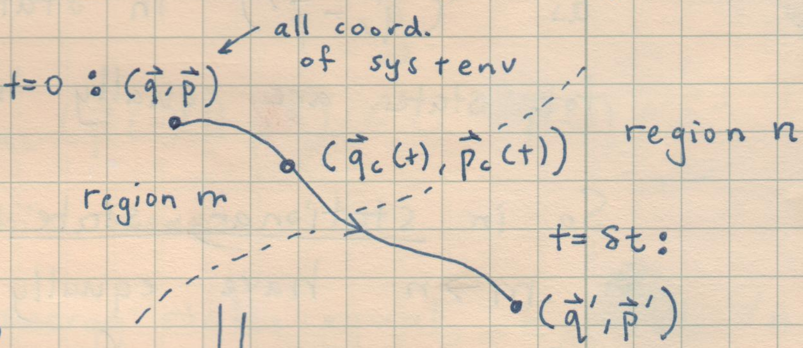
~~$= \sum$ all paths that start in~~

$$= \frac{\#\text{ classical trajectories that start in } m\text{, end in } n \text{ after time } \delta t}{\#\text{ classical trajectories that start in } m\text{, end anywhere after time } \delta t}$$

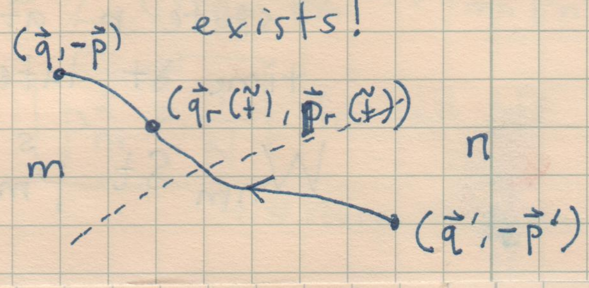



because of fast mixing, any starting point in m is equally likely

Very interesting property of classical trajectories: <u>time reversal symmetry</u>




$\Downarrow$ if such a trajectory exists, then "reverse" solution also exists!




Proof: Let $(\vec{q}_c(t), \vec{p}_c(t))$ satisfy Hamilton's equations:

$$\frac{d\vec{q}_c}{dt} = \frac{\partial \mathcal{H}}{\partial \vec{p}_c}, \quad \frac{\partial \vec{p}_c}{\partial t} = -\frac{\partial \mathcal{H}}{\partial \vec{q}_c}$$

with $\mathcal{H} = \frac{\vec{p}_c^{\,2}}{2m} + U(\vec{q}_c)$

then "reverse" solution

$$\vec{q}_r(\tilde{t}) \equiv \vec{q}_c(t-\tilde{t}), \quad \vec{p}_r(\tilde{t}) \equiv -\vec{p}_c(t-\tilde{t})$$

also obeys same equations of motion:

$$\mathcal{H} = \frac{\vec{p}_c^{\,2}}{2m} + U(\vec{q}_c) \rightarrow \mathcal{H} = \frac{\vec{p}_r^{\,2}}{2m} + U(\vec{q}_r) \quad \text{unchanged}$$

$$\frac{\partial \vec{q}_c}{\partial t} = \frac{\partial \mathcal{H}}{\partial \vec{p}_c} \rightarrow -\frac{d\vec{q}_r}{d\tilde{t}} = -\frac{\partial \mathcal{H}}{\partial \vec{p}_r} \quad \text{same}$$

$$\text{using} \quad \frac{d\vec{q}_c(t-\tilde{t})}{dt} = -\frac{d\vec{q}_c(t-\tilde{t})}{d\tilde{t}} = -\frac{d\vec{q}_r}{d\tilde{t}}$$

$$\frac{\partial \vec{p}_c}{\partial t} = \frac{\partial \mathcal{H}}{\partial \vec{p}_c} \rightarrow \frac{d\vec{p}_r}{dt} = -\frac{\partial \mathcal{H}}{\partial \vec{q}_r} \quad \text{same}$$

$$\text{using} \quad \frac{d\vec{p}_c(t-\tilde{t})}{dt} = -\frac{d\vec{p}_c(t-\tilde{t})}{d\tilde{t}} = \frac{d\vec{p}_r}{d\tilde{t}}$$

Note starting point $(\vec{q}, \vec{p})$ is just as likely as $(\vec{q}', -\vec{p}')$ in stationary state, b/c all tot. states are equally likely when $t \to \infty$.

So in <u>stationary state</u> all transitions from $m \to n$ have equally likely reverse transitions from $n \to m$. (ensures <u>microscopic reversibility</u>)

| | | |
|---|---|---|
| prob. to see state m, then state n at time $\delta t$ later | = | prob. to see state n, then state m $\delta t$ later |

$$W_{nm}\,\delta t\, p_m^s = W_{mn}\,\delta t\, p_n^s$$

Hence $\boxed{W_{nm}\, p_m^s = W_{mn}\, p_n^s}$ for any $(n,m)$ where $W_{nm} \neq 0$

↳ a property called <u>detailed balance</u>

Since $p_m^s = \dfrac{\Theta_m}{\Theta_{tot}}$, $p_n^s = \dfrac{\Theta_n}{\Theta_{tot}}$

$\Rightarrow \dfrac{W_{nm}}{W_{mn}} = \dfrac{\Theta_n}{\Theta_m}$ useful property of $W$ matrix entries

$\Rightarrow$ also ensures all networks are MR (+ hence consistent w/ uniqueness of $\vec{p}^{\,s}$)