Applications of the Maxwell-Boltzmann distr.

- barometric formula
- equipartition thm:

If we can neglect potential energy, then every degree of freedom receives on average $\frac{1}{2}kT$ of kinetic energy.

Ex molecules oscillate, bend, rotate

$T_1 = Q_1 \times \mathbb{R}^d$ or $T Q_1$

Ex $Q_1 = \mathbb{R}^3 \times SO(3)$

rot. velo

$$H = \frac{p^2}{2m} + \frac{1}{2} \underline{\omega}^T I \underline{\omega}$$

tensor of inertia

quadr.

$$H(x) = x^T A x$$

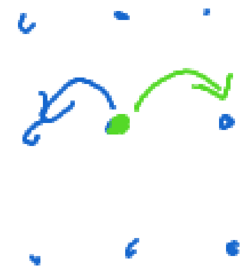
$\Rightarrow$ Maxw.-Boltzm. distr.

$$\rho_1(x) = \frac{1}{Z} e^{-\beta x^T A x} = \frac{1}{Z} e^{-\beta \sum a_j \bar{x}_j^2}$$

$$\langle a_j \bar{x}_j^2 \rangle = a_j \sigma_j^2 = \frac{1}{2\beta} = \underline{\frac{1}{2} kT} .$$

$$\beta a_j = \frac{1}{2\sigma_j^2}$$

The Ising Model



no dynamics

W. Lenz 1920, E. Ising 1925

$\mathbb{R}^3 \to \mathbb{Z}^d, \quad \underline{i} \in \mathbb{Z}^d, \quad \sigma_{\underline{i}} = \pm 1$

$$\Lambda = \Lambda_L = \{\underline{i} = (i_1, \dots, i_d) \in \mathbb{Z}^d : |i_k| < \tfrac{L}{2} \ \forall k\}$$

$$\Omega = \{+1, -1\}^{\Lambda} = \{(\sigma_{\underline{i}})_{\underline{i}}\}$$

$$= \{\sigma : \Lambda \to \{+1, -1\}\}$$

$$H(\sigma) = -J \sum_{\underline{i},\underline{j} : |\underline{i}-\underline{j}|=1} \sigma_{\underline{i}} \sigma_{\underline{j}} \quad , \quad J > 0$$

canonical ensemble:

$$\mathbb{P}_\beta(\sigma) = \frac{1}{Z} e^{-\beta H(\sigma)}$$

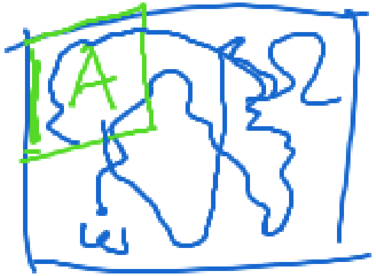
Ergodicity and Mixing

Def A MPDS $(\Omega, \mathcal{F}, \mathbb{P}, T)$ (say, in cont. time) is ergodic iff $\forall A \in \mathcal{F}$ and for almost all $\omega \in \Omega$

$$\lim_{\tau \to \infty} \frac{1}{\tau} \lambda \{ t \in [0, \tau] : T^t \omega \in A \} = \mathbb{P}(A).$$

(λ = Lebesgue meas.)

ω spends time in A according to size



Thm The following are equivalent:

(i) T^t is ergodic

(ii) $\forall f \in L^1(\Omega)$ and almost all ω

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T dt\, f(T^t_\omega) = \mathbb{E} f$$

time average = ensemble average

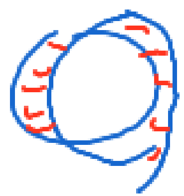
(iii) Every conserved quantity is almost const.

$f : \Omega \to \mathbb{R}$, $\quad f(x) = c$ for almost all x

(iv) Every invariant set has either measure 0 or measure 1.

(v) Every set that is invariant up to null sets has meas. 0 or 1.

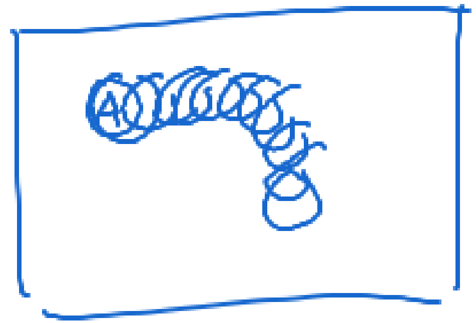
i.e. $\mathbb{P}(\; T^t A \,\triangle\, A) = 0 \}$



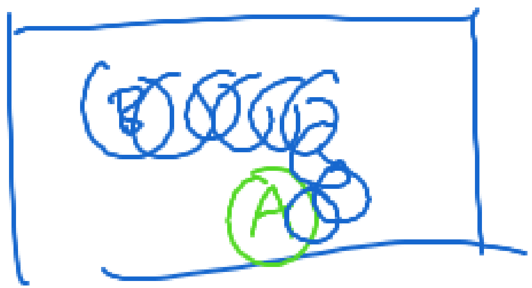
$A \triangle B = (A \setminus B) \cup (B \setminus A)$.

(vi) For every $A \subseteq \Omega$ with $\mathbb{P}(A) > 0$,

$$\mathbb{P}\left(\bigcup_{t>0} T^t A \right) = 1.$$



(vii) If $A, B \subseteq \Omega$ have $\mathbb{P}(A) > 0$ and $\mathbb{P}(B) > 0$, then $\exists t > 0$: $\mathbb{P}(A \cap T^t B) > 0$.



Ex $\Omega = \text{circle} = S^1 = \{ z \in \mathbb{C} : |z| = 1 \}$

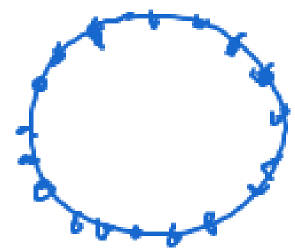
$T^t z = e^{it} z$

ergodic.

Ex discrete time $(t \in \mathbb{Z})$ $T^t \omega$ 'visits all regions in Ω acc. to their sizes'

Ex $\Omega = S^1$, $Tz = e^{i\alpha} z$

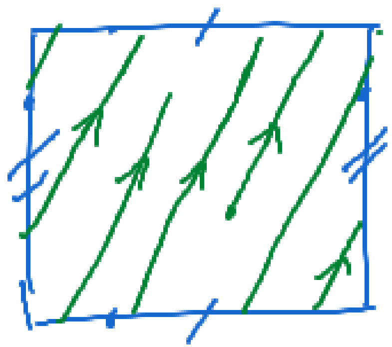
ergodic iff $\alpha \notin \pi \mathbb{Q}$



Ex n-dim torus $\mathbb{T}^n = (S^1)^n$

motion in fixed direction

$n=2$



ergodic for most directions

Ex hard sphere gas in $\Lambda \subset \mathbb{R}^3$, N spheres radius a

is believed to be ergodic on every Γ_E.

ergodic components = subsets of Ω
on which T is erg.

<u>Thm</u> Every MPDS where $(\Omega, \mathcal{F}, \mathbb{P})$ is sufficiently regular (Lebesgue space) can be essentially uniquely decomposed into ergodic components.

<u>Rem</u>

Mixing

Def A MPDS is mixing iff $\forall A, B \in \mathcal{F}$:

$$\lim_{t\to\infty} \mathbb{P}(A \cap T^t B) = \mathbb{P}(A)\,\mathbb{P}(B)$$

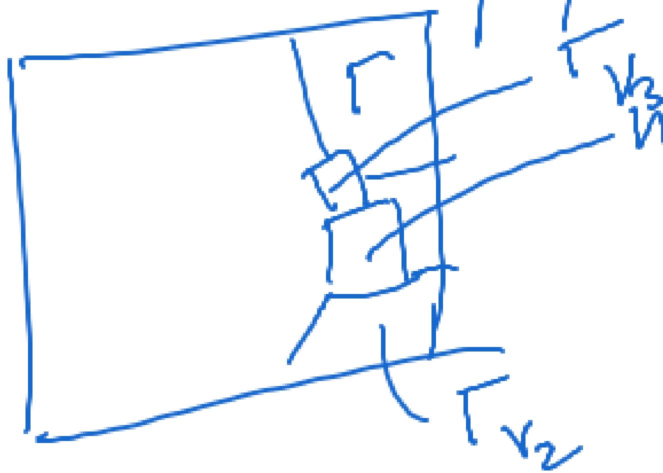
<u>Rem</u> Ergodicity (or mixing)
is neither necessary nor
sufficient for thermodynamic
behavior.

mixing plays a role for macro
randomness

Macro States, Macro Variables, Thermal Eq., and Entropy

macro appearance = macro state

~~macro~~ not sharply defined



macro set Γ_ν

macro variable $M_j : \Gamma \to \mathbb{R}$

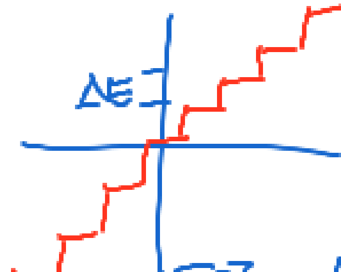
inaccuracy ΔM_j , $M_j : \Gamma \to \Delta M_j \mathbb{Z}$

$$M_j(x) = M_j(x') \iff$$ look macro the same

$\Gamma_\nu = \{ x \in \Gamma : M_j(x) = \nu_j \; \forall j \}$

partition of Γ.

<u>Ex</u> $g(H(x)) = M_1(x)$ g



$g(E) = [E/\Delta E]\,\Delta E$

$[s]$ = nearest int

In particular

$$\Gamma_{mc} = \{ x \in \Gamma : \ E \leq H(x) \leq E + \Delta E \}$$

Γ_ν form a partition of Γ_{mc}.