Spin Systems & Phase Transitions

① Introduction

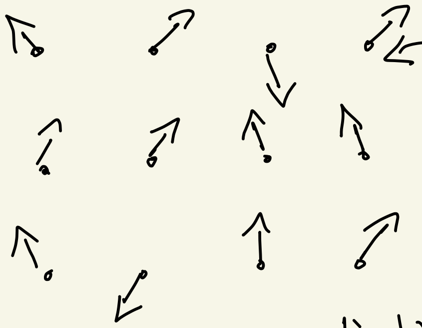
1 Statistical Mechanics

Mathematical derivation of macroscopic (thermodynamic) properties of physical systems from microscopic descriptions.

Ex: $1\,cm^3$ of iron has $\approx 10^{23}$ atoms

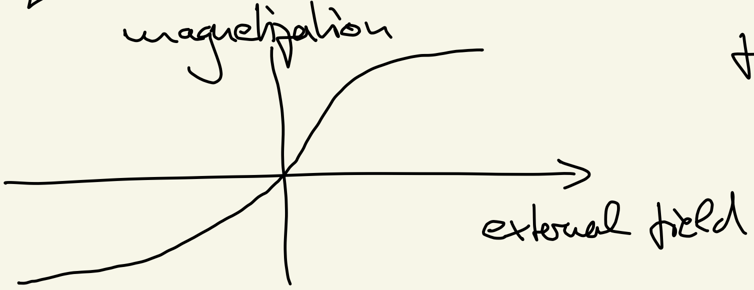
Micro: Individual atom with certain states

Macro: Magnetization of whole iron block



← atom with spin (many variables)

Spin system = configuration of particles with spins



few variable: volume, temperature, external magnetic field

Ansatz: (Gibbs, Boltzmann, Maxwell 2nd half of 19th century)

Conceive macroscopic states as probability measures on micro states $\omega \in \Omega$

2 Equilibrium

Macroscopic systems at equilibrium minimizes free energy:

$$\underbrace{\sum_{\omega\in\Omega} H(\omega)\,p(\omega)}_{\text{expected energy under } p} + \underbrace{\sum_{\omega\in\Omega} p(\omega)\log p(\omega)}_{\text{entropy of } p \ (S(p))} = F(p)$$

$H(\omega)$: energy of ω

$p(\omega)$: probability of microstate $\omega\in\Omega$

We compute the minimizer in case $|\Omega|<\infty$

$\sum v(\omega)=0$

$$\frac{1}{\varepsilon}\left(F(p+\varepsilon v)-F(p)\right)$$

$$=\frac{1}{\varepsilon}\left(\varepsilon\sum_{\omega\in\Omega}H(\omega)v(\omega)+\sum_{\omega\in\Omega}(p+\varepsilon v)(\omega)\log\big((p+\varepsilon v)(\omega)\big)-\sum_{\omega}p(\omega)\log p(\omega)\right)$$

$$=\sum_{\omega\in\Omega}H(\omega)v(\omega)+\frac{1}{\varepsilon}\sum_{\omega\in\Omega}p(\omega)\log\frac{p(\omega)+\varepsilon v(\omega)}{p(\omega)}$$

$$+\sum_{\omega\in\Omega}v(\omega)\log\big(p(\omega)+\varepsilon v(\omega)\big)\Big)$$

$\approx \frac{1}{\varepsilon}\sum p(\omega)\left(\varepsilon\frac{v(\omega)}{p(\omega)}\right)$

$= \sum v(\omega) = 0$

$$\xrightarrow{\varepsilon\to 0}\ \sum_{\omega\in\Omega}H(\omega)v(\omega)+\sum_{\omega\in\Omega}v(\omega)\log p(\omega)$$

$$=\sum_{\omega\in\Omega}v(\omega)\Big(H(\omega)+\log p(\omega)\Big)=0 \quad \forall v$$

$$\Rightarrow H(\omega)+\log p(\omega)=c \quad \text{for some } c\in\mathbb{R}$$

$$p(\omega)=e^{c}e^{-H(\omega)}$$

$$1=\sum p(\omega)=e^{c}\sum e^{-H(\omega)} \Rightarrow e^{c}=\frac{1}{\sum e^{-H(\omega)}}$$

$$\rho(\omega) = \frac{e^{-H(\omega)}}{\sum_{\eta\in\Omega} e^{-H(\eta)}}$$

Hamiltonian

Partition function

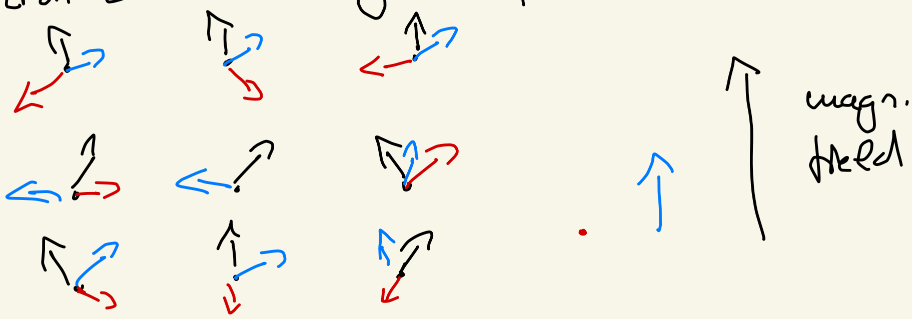
Gibbs measures

3 Phase transition

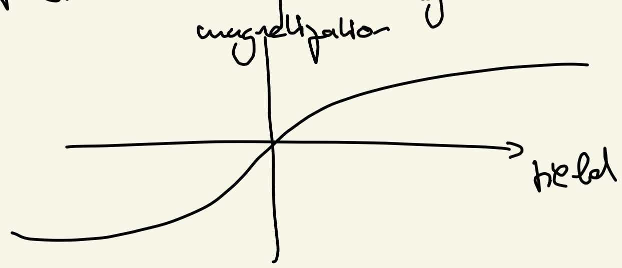
Roughly, phase transitions are discontinuities of macroscopic systems under parameter changes.

Ex: Paramagnetism vs Ferromagnetism

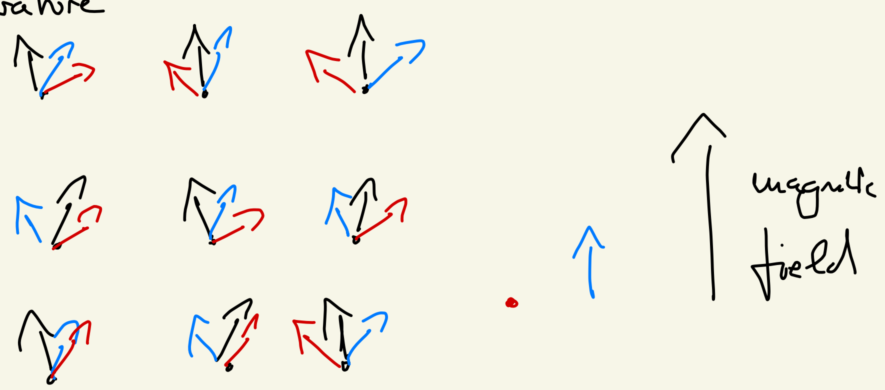
Consider iron block at high temperature



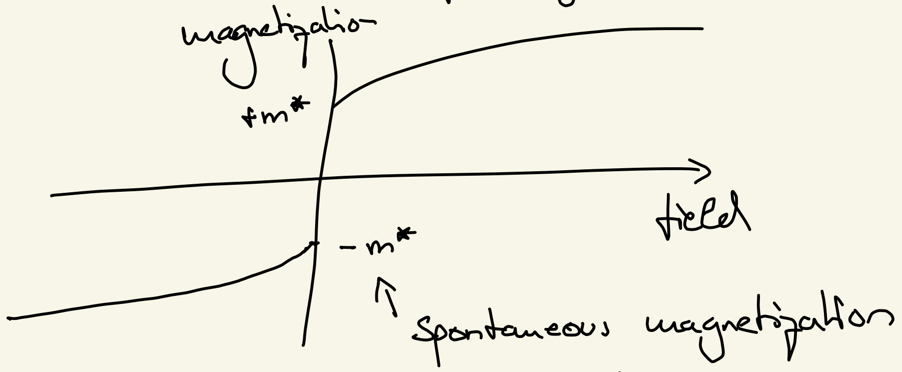
Loss of order <-> paramagnetic behavior



Low temperature



persistence of order $\Longleftrightarrow$ ferromagnetic behavior



first-order phase transition (Pierre Curie 1895)

Other phase transitions: 1) Liquid-vapor transition
2) Bose-Einstein condensation

<u>Ensembles</u>: 1) <u>Microcanonical ensemble</u>: the macro state is the uniform distribution on $\omega \in \Omega$ with $H(\omega) = U$ (fixed energy for every microstate)

2) <u>Canonical ensemble</u>: macro states are Gibbs measure

$$p(\omega) = \frac{1}{\sum_{\eta \in \Omega} e^{-\beta H(\eta)}} \underbrace{e^{-\beta H(\omega)}}_{\text{Boltzmann weight}}$$

$\beta \in \mathbb{R}$ interpreted as the inverse temperature chosen s.t. $\sum H(\omega) p(\omega) = U$ (fixed expected energy)

3) <u>Grand canonical ensemble</u> : macro state is a Gibbs measure of the form

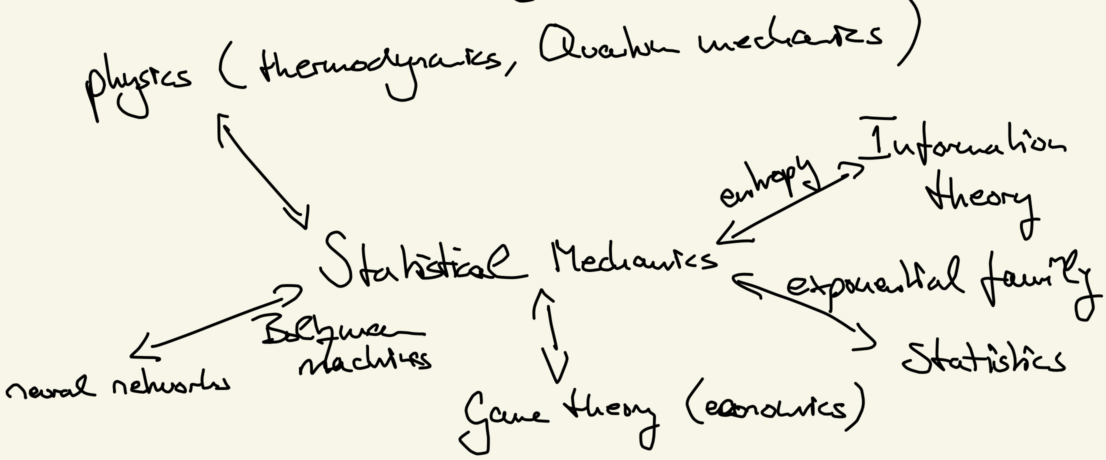
$$p(\omega) = \frac{1}{\sum_{\eta \in \Omega} e^{-\beta H(\eta) - \mu N(\eta)}} e^{-\beta H(\omega) - \mu N(\omega)}$$

number of particles in system

$$\sum H(\omega) p(\omega) = U$$

$$\sum N(\omega) p(\omega) = N \quad \text{(expected number of particles)}$$

μ interpreted as chemical potential or external magnetic field.



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(2) Ising Model

Paradigmatic model for magnetization (Lenz 1920, Ising 25)

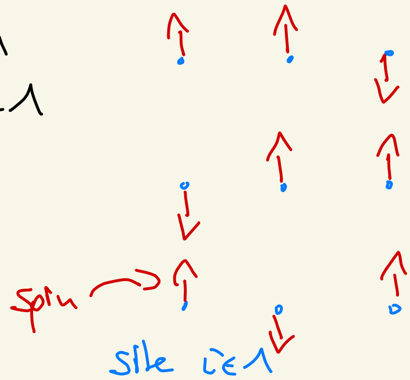
1 Definition

- Configuration space $\Omega = \{-1,1\}^{\mathbb{Z}^d}$

  $\Omega_\Lambda = \{-1,1\}^\Lambda \quad \Lambda \subset \mathbb{Z}^d \ ; \ \Lambda \subset\subset \mathbb{Z}^d$ if $|\Lambda| < \infty$

  we write $\omega = (\omega_i)_{i\in\Lambda}$ for $\omega_\Lambda \in \Omega_\Lambda$

  $\quad\uparrow$ spin ± 1 at site $i \in \Lambda$



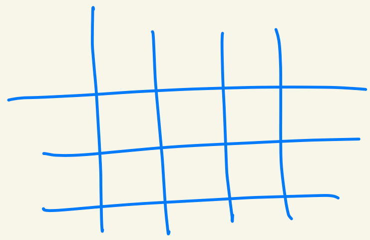
$$\Omega_\Lambda^\eta = \{\omega \in \Omega : \omega_i = \eta_i \ \forall i \notin \Lambda\}$$

boundary condition

- Nearest-neighbor edge space

$$\mathcal{E}_\Lambda = \{ \{i,j\} \subset \Lambda : i \sim j \}$$

$\quad\uparrow \|i-j\|_1 = 1$



$$\mathcal{E}_\Lambda^b = \{ \{i,j\} \subset \mathbb{Z}^d : \{i,j\} \cap \Lambda \neq \emptyset, \ i \sim j \} \quad \Lambda \subset \mathbb{Z}^d$$

boundary edges are included

Def: (Ising model)

The Ising model in $\Lambda \subset\subset \mathbb{Z}^d$ with boundary condition $\eta \in \Omega$ at parameters $\beta \geq 0$; $h \in \mathbb{R}$ is the Gibbs measure

$$\mu^{\eta}_{\Lambda;\beta,h}(\omega) = \frac{1}{Z^{\eta}_{\Lambda;\beta,h}} e^{-H_{\Lambda;\beta,h}(\omega)} \quad \text{on } \Omega^{\eta}_{\Lambda}$$

where $H_{\Lambda;\beta,h}(\omega) = -\beta \sum_{\{i,j\} \in \mathcal{E}^b_{\Lambda}} \omega_i \omega_j - h \sum_{i \in \Lambda} \omega_i$

the Hamiltonian, and $Z^{\eta}_{\Lambda;\beta,h} = \sum_{\omega \in \Omega^{\eta}_{\Lambda}} e^{-H_{\Lambda;\beta,h}(\omega)}$

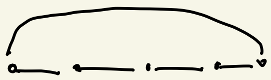
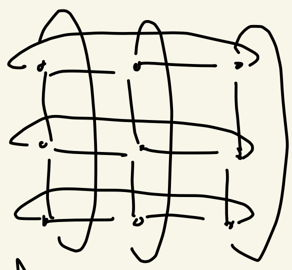
the partition function.

__Remarks:__

1) β inverse temperature
2) h external magnetic field
3) Often also defined with open or periodic boundary conditions.

Open: boundary interactions are ignored $\mu^{\emptyset}_{\Lambda;\beta,h}$

periodic: volume Λ is a torus $\mathbb{T}_n$, e.g.

$d=1$  $d=2$ 

4) ferromagnet since spin like to align

2 Magnetization

For $\omega \in \Omega$ we consider the total magnetization in $\Lambda \subset \mathbb{Z}^d$

$$M_\Lambda(\omega) = \sum_{i \in \Lambda} \omega_i$$ and the

magnetization density

$$\frac{1}{|\Lambda|} M_\Lambda(\omega) \in [-1, 1]$$ $\rightsquigarrow$ Information on average spin direction

By symmetric $\quad \mu^{\phi}_{\Lambda;\beta,0}(M_\Lambda) = 0$

zero magnetic field.

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3 Infinite temperature

Consider box $B_n = \{-n, \dots, n\}^d \subset \mathbb{Z}^d$ and $\beta \downarrow 0$

then

$$\lim_{\beta \downarrow 0} \mu^{\phi}_{B_n;\beta,0}(\omega) = \mu^{\phi}_{B_n,0,0}(\omega) = \frac{1}{|\Omega_{B_n}|}$$

for any $\omega \in \Omega_{B_n}$, ie, the equidistribution on Ω_{B_n}. Hence,

$$\mu^{\phi}_{B_n,0,0}\left(\frac{1}{|B_n|} M_{B_n} \notin [-\varepsilon,\varepsilon]\right) \to 0 \quad \text{as } n \uparrow \infty$$

by weak LLN. (Even CLT; LDP)

The magnetization density concentrates around zero for large volumes.

4 Zero temperature

Case $\beta \uparrow \infty$. Groundstate $\eta^+, \eta^- \in \Omega_{B_n}$

$\{\eta^+_i = 1 \; ; \; \eta^-_i = -1 \;\; \forall i \in B_n$

$\forall \omega \in \Omega_{B_n} \setminus \{\eta^+, \eta^-\} \;\; \exists \{i,j\} \in \mathcal{E}_{B_n}$ st. $\omega_i \neq \omega_j$

hence

$$H_{B_n,\beta,0}(\omega) - H_{B_n,\beta,0}(\eta^{\pm}) = \beta \sum_{\{i,j\} \in \mathcal{E}_{B_n}} (1 - \omega_i\omega_j) \geq 2\beta$$

$$\Rightarrow \frac{\mu^{\phi}_{B_n;\beta,0}(\omega)}{\mu^{\phi}_{B_n;\beta,0}(\eta^{\pm})} = \frac{e^{-H^{\phi}_{B_n;\beta,0}(\omega)}}{e^{-\beta H^{\phi}_{B_n,\beta,0}(\eta^{\pm})}} \leq e^{-2\beta} \to 0 \quad \text{as } \beta \uparrow \infty$$

Since $\mu^{\phi}_{B_n,\beta,0}(\eta^+) = \mu^{\phi}_{B_n,\beta,0}(\eta^-)$

$$\Rightarrow \lim_{\beta\uparrow\infty} \mu^{\phi}_{B_n;\beta,0}(\omega) = \begin{cases} \frac{1}{2} & \text{if } \omega\in\{2^+,2^-\} \\ 0 & \text{else} \end{cases}$$

<u>Remarks</u> 1) Concentration on groundstates
2) No LLN
3) Spontaneous magnetization / global order

5 Thermodynamic limit

The analysis in 3 & 4 was based on

$$\lim_{n\uparrow\infty} \lim_{\substack{\beta\uparrow\infty \\ (\beta\downarrow 0)}} \mu^{\phi}_{B_n,\beta,0}(\underset{\substack{\uparrow \\ \text{test-function}}}{f})$$

However we are interested in

$$\lim_{n\uparrow\infty} \mu^{\phi}_{B_n,\beta,0}(f)$$ the <u>thermodynamic limit</u>

at fixed $\beta\geq 0$. Which of the two pictures in 3 & 4 can be "observed"?

<u>Care needed</u>: Let

$$\Omega^k_{B_n} = \{\omega\in\Omega_{B_n} : \#\{i : \omega_i \neq 2^+_i\} = k \text{ or } \#\{i : \omega_i\neq 2^-_i\}=k\}$$

$$|\Omega^k_{B_n}| = \binom{|B_n|}{k} \; ; \quad k\leq \frac{|B_n|}{2}$$

$$H_{B_n;\beta,0}(\underset{\substack{\Uparrow \\ \Omega^k_{B_n}}}{\omega}) - H_{B_n;\beta,0}(2^{\pm}) \leq 4d\beta k$$

$$\Rightarrow \frac{\mu^{\phi}_{B_n;\beta,0}(\Omega^k_{B_n})}{\mu^{\phi}_{B_n;\beta,0}(2^{\pm})} = \sum_{\omega\in\Omega^k_{B_n}} e^{-(H_{B_n;\beta,0}(\omega)-H_{B_n;\beta,0}(2^{\pm}))}$$

$$\geq \binom{|B_n|}{k} e^{-4dk\beta} \geq \frac{1}{k!} \left(\frac{|B_n|}{2} e^{-4d\beta} \right)^k \to \infty \text{ for } n \uparrow \infty$$

Which means: Much more likely to observe misaligned configurations for all $\beta > 0$.