# Review of previous lecture (May 09)

## phase transitions for systems with continuous symmetry

for example: Heisenberg model:

$$H(\{\vec{\sigma}_i\}) = -\sum_{i=1}^{N} \vec{B}_i \cdot \vec{\sigma}_i - \sum_{\langle i,j \rangle} J_{ij}\, \vec{\sigma}_i \cdot \vec{\sigma}_j$$

$$H(\{R(\Omega)\vec{\sigma}_i\}) = H(\{\vec{\sigma}_i\})$$

long-range order only for $\underline{d > 2}$

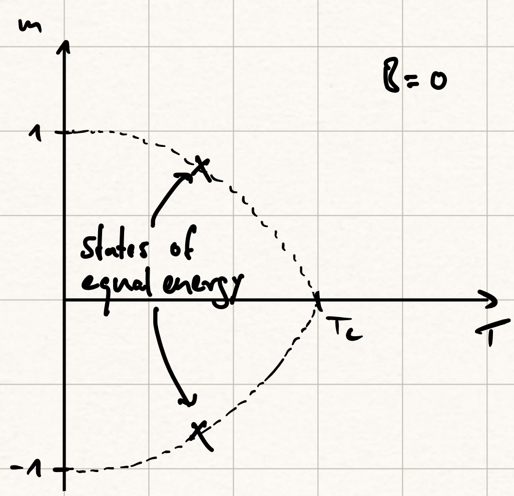
## Spontaneous symmetry breaking and ergodicity breaking

$$m = \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} \langle \sigma_i \rangle \neq 0 \quad \text{despite} \quad H(\{\sigma_i\}) = H(\{-\sigma_i\}).$$

state of system is determined by initial conditions

for $N \to \infty$ system is trapped in subpart of phase space

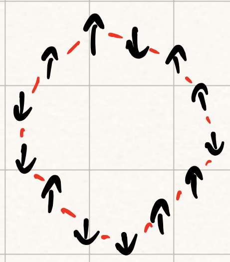
↳ ergodicity breaking



# One dimensional Ising model : exact solution

the Ising model allows to illustrate many of the key concepts of the previous sections

nearest - neighbor interaction with N spins:



$$H = -B\sum_{i=1}^{N}\sigma_i - J\sum_{\langle ij\rangle}\sigma_i\sigma_j \qquad J>0$$

we will use periodic boundary conditions: $\sigma_1 = \sigma_{N+1}$

$$Z_c = \mathrm{Tr}\, e^{-\beta H} \qquad h = \beta\cdot B\,,\quad k = \beta\cdot J$$

$$\Rightarrow Z_c(h,k) = \mathrm{Tr}\exp\left(h\cdot\sum_i\sigma_i + k\sum_i\sigma_i\sigma_{i+1}\right)$$

$$= \sum_{\sigma_1=\pm1}\sum_{\sigma_2}\sum_{\sigma_3}\cdots\sum_{\sigma_N} \exp\left[\frac{h}{2}(\sigma_1+\sigma_2)+k\sigma_1\cdot\sigma_2\right]$$
$$\exp\left[\frac{h}{2}(\sigma_2+\sigma_3)+k\,\sigma_2\cdot\sigma_3\right]$$
$$\vdots$$
$$\exp\left[\frac{h}{2}(\sigma_N+\sigma_1)+k\,\sigma_N\cdot\sigma_1\right]$$

introduce the transfer matrix : $T_{\sigma_i\sigma_{i+1}} = \exp\left[\frac{h}{2}(\sigma_i+\sigma_{i+1})+k\cdot\sigma_i\cdot\sigma_{i+1}\right]$

i.e in matrix form : $T = \begin{pmatrix} T_{11} & T_{1-1} \\ T_{-11} & T_{-1-1}\end{pmatrix} = \begin{pmatrix} e^{h+k} & e^{-k} \\ e^{-k} & e^{-h+k}\end{pmatrix}$

$$\Rightarrow Z_c(h,k) = \sum_{\sigma_1}\sum_{\sigma_2}\cdots\sum_{\sigma_N} \underbrace{T_{\sigma_1\sigma_2}T_{\sigma_2\sigma_3}\cdots T_{\sigma_N\sigma_1}}_{\text{matrix product}}$$

$$= \sum_{\sigma_1} T^N_{\sigma_1\sigma_1} = \mathrm{Tr}\left(T^N\right)$$

↳ conventional matrix trace !

the trace can be calculated by <u>diagonalizing</u> T :

$$T' = S^{-1} T S$$

and use cyclic invariance of trace : $Tr(T') = Tr(T)$.

denote eigenvalues of T by $\lambda_1$ and $\lambda_2$ :

$$\Rightarrow \quad Tr(T^N) = Tr(\underbrace{T'^N}_{\begin{pmatrix}\lambda_1 & 0\\ 0 & \lambda_2\end{pmatrix}}) = \lambda_1^N + \lambda_2^N$$

if $\lambda_1 > \lambda_2$ partition function is governed by largest eigenvalue:

$$Z_c(h,k) = \lambda_1^N \left[ 1 + \underbrace{\left(\frac{\lambda_2}{\lambda_1}\right)^N}_{\to 0 \text{ for } N\to\infty} \right] = \lambda_1^N$$

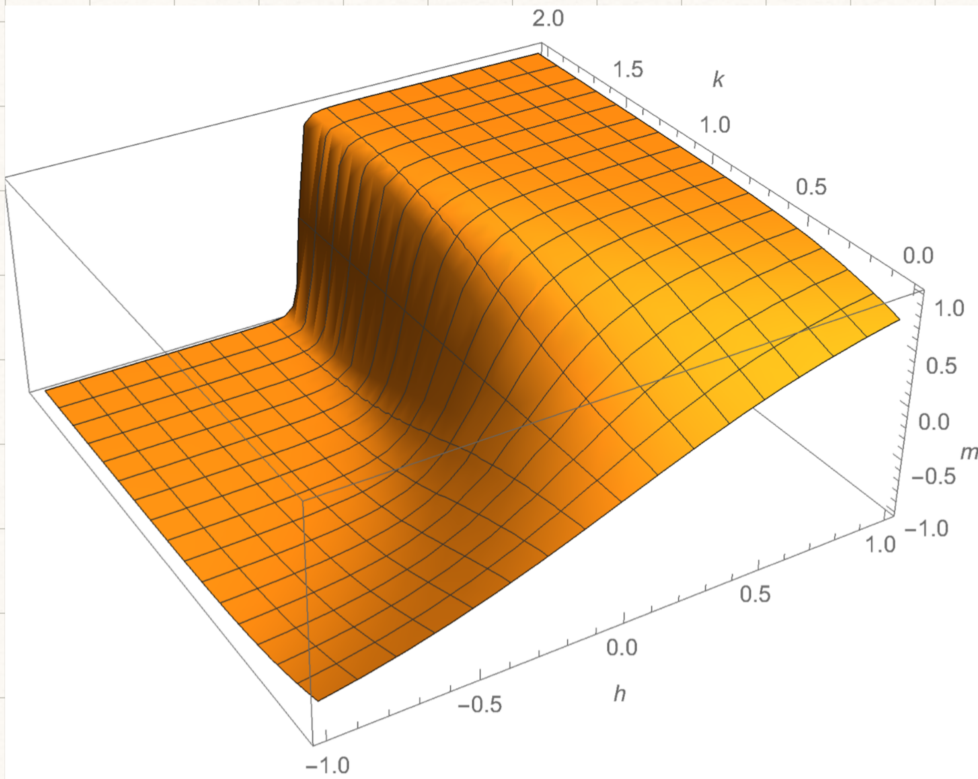
$$\Rightarrow f = \lim_{N\to\infty} \frac{F(h,k,T)}{N} = -k_B \cdot T \log \lambda_1$$

diagonalization of T gives : $\lambda_{1/2} = e^k \left( \cosh(h) \pm \sqrt{\sinh^2(h) + e^{-4k}} \right)$

$$\boxed{\Rightarrow m(h,k) = -\frac{\partial f}{\partial B} = \frac{\sinh(h)}{\sqrt{\sinh^2(h) + e^{-4k}}}}$$

for $T \to 0$ $(k \to \infty)$ we obtain :

$$m_{T=0}(h) = \frac{\sinh(h)}{|\sinh(h)|} = \begin{cases} 1 & \text{for } h > 0 \\ -1 & \text{for } h < 0 \end{cases} \qquad \text{(as above)}$$




However, no phase transition for $T>0$ (in agreement with general arguments for 1d above)

Consider $f$ for $h=0$ ($B=0$): $\lambda_+ = e^{k}\left(1+e^{-2k}\right) = 2\cosh(k)$

$$\Rightarrow \quad f(h=0,k) = -k_B \cdot T\left[k+\log\left(1+e^{-2k}\right)\right] \qquad (k=\beta\cdot J)$$

$$\Rightarrow \quad f(h=0,k) = \begin{cases} -J & \text{for } T=0 \ (k\to\infty) \\ -k_B\cdot T\log 2 & \text{for } T\to\infty \ (k=0) \end{cases}$$

cf. $F = E - T\cdot S$ $\qquad S = k_B \cdot \log 2^N$

total disorder

$\cdots\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\uparrow\downarrow\cdots$

isothermal susceptibility: $\chi_T = \frac{\partial m}{\partial B}$

"how does the magnetization $m$ change in response to a magnetic field?"

$B \to 0$, $\sinh h \sim h$

$$\to m \sim h e^{2K} = e^{2K} \frac{B}{k_B \cdot T}$$

$$\Rightarrow \chi_T = \frac{\exp\left(\frac{2J}{k_B T}\right)}{k_B T} \quad , \quad \lim_{T\to\infty} \chi_T = \frac{1}{k_B T}$$

↳ Curie law

# Spatial correlations (1d Ising model)

- spatial correlations play a key role for phase transitions
- Correlations in many-body systems can be quantified via correlation functions.
- the two-body correlation function for a spin system reads:

$$G(i,j) = \langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle \langle \sigma_j \rangle$$
$$= \langle (\sigma_i - \langle \sigma_i \rangle)(\sigma_j - \langle \sigma_j \rangle) \rangle$$

- for $B=0$ and $T>0$ we have shown that $\langle \sigma_i \rangle = 0$ for the 1d Ising model $\Rightarrow G(i,j) = \langle \sigma_i \sigma_j \rangle$

- for practical calculation of $\langle \sigma_i \sigma_j \rangle$ start with $\langle \sigma_i \sigma_{i+1} \rangle$
- in addition we allow for general $J_i$ resp $k_i$ in the Hamiltonian and consider $B=0$: $H = -\sum_i J_i \sigma_i \sigma_{i+1}$

$$\langle \sigma_i \sigma_{i+1} \rangle = Z_c^{-1} \operatorname{Tr} \sigma_i \sigma_{i+1} e^{-\beta H}$$
$$= Z_c^{-1} \frac{\partial}{\partial k_i} \operatorname{Tr} e^{k_1 \sigma_1 \sigma_2 + k_2 \sigma_2 \cdot \sigma_3 + \dots + k_{N-1} \sigma_{N-1} \sigma_N + k_N \sigma_N \cdot \sigma_1}$$
$$= Z_c^{-1} \frac{\partial}{\partial k_i} Z_c$$
$$= \frac{\partial}{\partial k_i} \log Z_c$$

$\hookrightarrow Z_c = \prod_{i=1}^{N} 2\cosh(k_i)$

$$\Rightarrow \langle \sigma_i \sigma_{i+1} \rangle = \frac{\sinh(k_i)}{\cosh(k_i)} = \tanh(k_i)$$

for calculation of general $\langle \sigma_i \sigma_j \rangle$ note that:

$$\langle \sigma_i \sigma_{i+2} \rangle = Z_c^{-1} \, \mathrm{Tr} \, \sigma_i \underbrace{\sigma_{i+1} \sigma_{i+1}}_{1} \sigma_{i+2} \, e^{-\beta H}$$

$$= \frac{\partial}{\partial k_i} \frac{\partial}{\partial k_{i+1}} \log Z_c = \tanh(k_i) \tanh(k_{i+1})$$

by induction it follows that

$$G(i, i+j) = \prod_{a=i}^{i+j-1} \tanh(k_a) \;\xRightarrow{\text{setting } k_i = k}\; G(i, i+j) = [\tanh(k)]^j$$

- at $T=0$ ($k \to \infty$) we have $\tanh(k) \to 1$, $G(i,j) = 1$ for all $j$
  $\Rightarrow$ all spins maximally correlated, long-range order
- for $T > 0$ we obtain:

$$G(i, i+j) = [\tanh(k)]^j$$
$$= e^{j \log[\tanh(k)]}$$
$$= e^{-j \log[\coth(k)]}$$

The correlation length $\xi$ is defined via

$$G(i, i+j) = e^{-j/\xi} \quad \text{here } \Rightarrow \xi = \frac{1}{\log[\coth(k)]} \qquad \left( \coth x = \frac{e^x + e^{-x}}{e^x - e^{-x}} \right)$$

- the correlation length is a measure over which distance degrees of freedom are correlated with probability $O(1)$.
- in present case $\xi$ behaves like $\xi(T) = \frac{1}{2} \exp\left(\frac{J}{k_B T}\right)$ as $T \to 0$
- around critical points $\xi$ behaves like $\xi(T) \sim (T - T_c)^{-\nu}$, i.e. a power law instead of an exponential behaviour.

## analytic properties of the free energy in the Ising model

$Z_c$ for the Ising model consists of $2^N$ positive terms for any finite $T$:

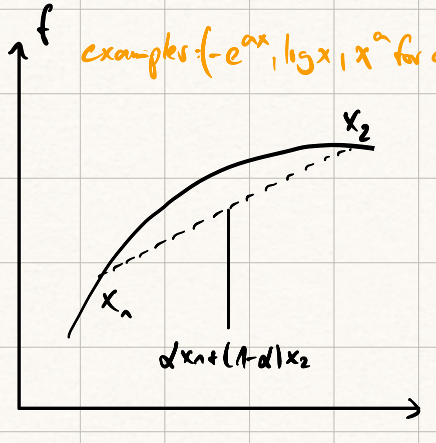
$$F = -k_B T \log Z_c = -k_B T \log \mathrm{Tr}\, e^{-\beta H} \quad , \quad f \equiv \frac{F}{N}$$

**$F<0$ ($f<0$):**
- need to show that $Z_c > 1$
- this is true if there is one spin configuration $\{\sigma_i^*\}$ for which $\langle H \rangle_* < 0$ since then $\langle e^{-\beta H} \rangle_* > 1$ for $\beta > 0$
- for $B>0$ and $J>0$ the configuration $\sigma_i^* = +1$ is such a configuration (for $B<0$, $\sigma_i^* = -1$)
- all other contributions to $Z_c > 0$ $\Rightarrow$ q.e.d.

**$F$ is analytic:** logarithm only develops singularities when argument vanishes $\Rightarrow$ q.e.d. (see above).

**$F$ and $f$ convex up in $B$:**

examples: $-e^{ax}$, $\log x$, $x^a$ for $a \in [0,1]$




$$f(\alpha x_1 + (1-\alpha) x_2) \geq \alpha f(x_1) + (1-\alpha) f(x_2)$$
$$\alpha \in [0,1]$$

for this we use the Hölder inequality:

$$\sum_i a_i^\alpha b_i^{(1-\alpha)} \leq \left(\sum_i a_i\right)^\alpha \left(\sum_i b_i\right)^{1-\alpha}$$

$$Z_c(B) = \mathrm{Tr}\left[ e^{\beta B \sum_i \sigma_i} \underbrace{e^{\beta J \sum_{\langle i,j \rangle} \sigma_i \sigma_j}}_{G[\sigma]} \right]$$

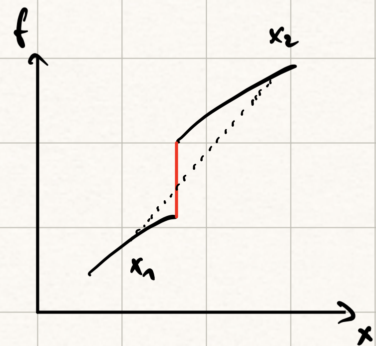
$$Z_c(\alpha B_1 + (1-\alpha) B_2) = \mathrm{Tr}\, \exp\left(\beta \alpha B_1 \sum_i \sigma_i + \beta (1-\alpha) B_2 \sum_i \sigma_i\right) G[\sigma]$$
$$= \mathrm{Tr} \left(\exp\left(\beta B_1 \sum_i \sigma_i\right) \cdot G[\sigma]\right)^\alpha \left(\exp\left(\beta B_2 \sum_i \sigma_i\right) G[\sigma]\right)^{1-\alpha}$$

$$\leq \mathrm{Tr}\left(\exp\left(\beta B_1 \sum_i \sigma_i\right) \cdot G[\sigma]\right)^{\alpha} \mathrm{Tr}\left(\exp\left(\beta B_2 \sum_i \sigma_i\right) G[\sigma]\right)^{1-\alpha}$$

$$= Z_c(B_1)^{\alpha} \; Z_c(B_2)^{1-\alpha}$$

$$\Rightarrow F(\alpha B_1 + (1-\alpha) B_2) \geq \alpha F(B_1) + (1-\alpha) F(B_2)$$

q.e.d.

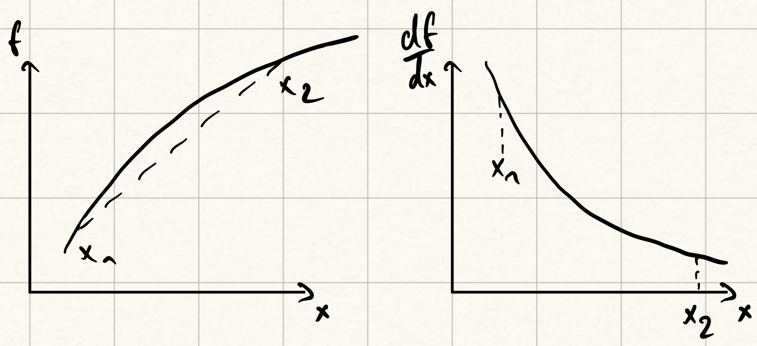


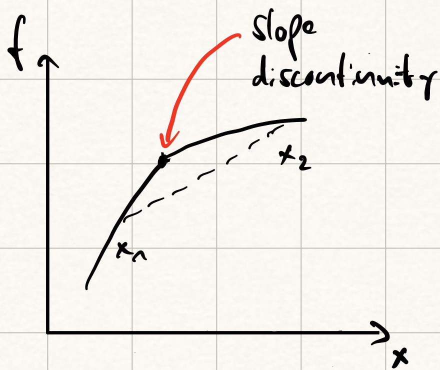

## F and f are continuous (implied by convexity)

any discontinuity violates convexity:

## $\frac{\partial F}{\partial x}, \frac{\partial f}{\partial x}$ monotonically non-increasing

direct consequence of convexity:



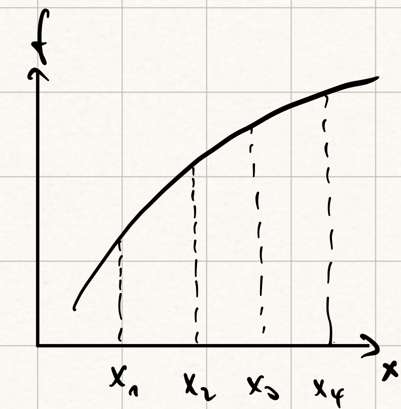




## f is differentiable almost everywhere

convexity implies:

$$\frac{f(x_2) - f(x_1)}{x_2 - x_1} \geq \frac{f(x_4) - f(x_3)}{x_4 - x_3}$$

i.e.: $f'_-(x) \geq f'_+(x) \geq f'_-(y) \geq f'_+(y)$, for $x < y$




for every point x where $f'_-(x) > f'_+(x)$

pick rational number $q_i$ with $f'_-(x) < q_i < f'_+(x)$

all $q_i$ have to be distinct $\Rightarrow$ countable non-analytic points