Review of previous lecture (May 02)

$$\mathcal{F}(V) = V \cdot f_b(V) + S f_s(S) + O(L^{d-2}) + \dots$$

f_b: bulk free energy per unit volume

f_s: surface free energy per unit area

thermodynamic limit: $$f_b = \lim_{V\to\infty,\, n=\frac{N}{V}=\text{const}} \frac{\mathcal{F}(V)}{V}$$

phases are regions in which $f_b[k]$ is analytic $(k = \{T, B, J, \dots\})$

phase boundaries are points, lines, planes of non-analyticities of $f_b(\{k\})$ as a function of k_i

classification of phase transitions (Ehrenfest):

a) at least one $\frac{\partial f_b[k]}{\partial k_i}$ is discontinuous (first order)

b) all $\frac{\partial f_b[k]}{\partial k_i}$ are continuous

(continuous or 2nd order phase transition)

Phases are generally only defined in thermodynamic limit.

For finite N and T $f_b[k]$ is generally analytic.

Central question in statistical physics:
How can the phase diagram of a system be computed as a function of the parameters k_i including the nature of the phase transitions.

Phase transitions at $T=0$ and the Ising model

Consider Ising model with a constant external magnetic field B and a constant two-spin interaction J that couples nearest neighbors

$$H = -B \sum_{i=1}^{N} \sigma_i - J \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$

free energy: $F(T,B,J) = -k_B T \log \operatorname{Tr} e^{-\beta H}$

$$\hookrightarrow \sum_{\sigma_1=\pm 1} \sum_{\sigma_2=\pm 1} \cdots \sum_{\sigma_N=\pm 1}$$

magnetization (per site):
$$m = \frac{1}{N} \sum_{i=1}^{N} \langle \sigma_i \rangle$$
$$= \frac{1}{N} \sum_{i=1}^{N} \operatorname{Tr}(\rho \sigma_i)$$
$$= \frac{1}{N} \sum_{i=1}^{N} \frac{\operatorname{Tr}(\sigma_i e^{-\beta H})}{\operatorname{Tr} e^{-\beta H}}$$
$$= -\frac{1}{N} \frac{\operatorname{Tr}\left(\frac{\partial H}{\partial B} e^{-\beta H}\right)}{\operatorname{Tr} e^{-\beta H}}$$
$$= -\frac{1}{N} \frac{\partial F}{\partial B} = -\frac{\partial f}{\partial B}$$

at zero temperature M of the ground state can be determined by simple inspection (assume $J>0$):

- $-J\sum_{\langle i,j\rangle}\sigma_i\sigma_j$ can be minimized for $\sigma_i=\sigma_j$
- $-B\sum_i \sigma_i$ can be minimized by $\sigma_j = \begin{cases} +1 & B>0 \\ -1 & B<0 \end{cases}$

$\Rightarrow$ ground state configuration:

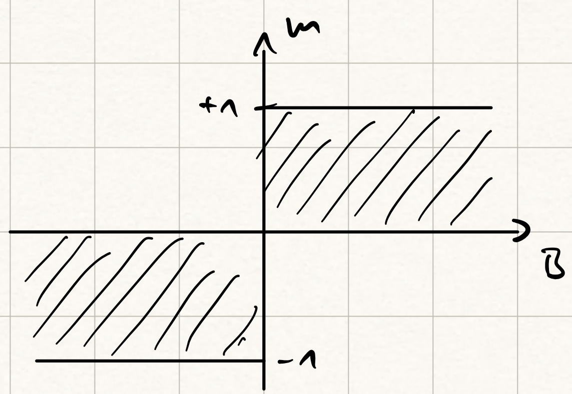
$$\sigma_i = \begin{cases} +1, & B>0,\ J>0 \\ -1, & B<0,\ J>0 \end{cases}$$

$$\Rightarrow m = \frac{1}{N}\sum_{i=1}^{N}\langle\sigma_i\rangle = \begin{cases} +1 & B>0 \\ -1 & B<0 \end{cases}$$

$\rightarrow$ $m = -\dfrac{\partial f}{\partial B}$ is discontinuous at $B=0$

↳ phase transition

Note that in the present case the phase transition happens at finite N
(no thermodynamic limit needed!)



non-analytic behaviour results from $\underline{\beta\to\infty}$, not $N\to\infty$ in

$$e^{-\beta F} = \mathrm{Tr}\, e^{-\beta H}$$

Phase transitions at $T>0$ in 1d (short-range int)

consider a spin chain in 1 dimension at $T>0$, $B=0$ and $J>0$ (see previous section)

- ground state at $T=0$ takes the form (see above)

$$\uparrow\uparrow\uparrow\uparrow\uparrow\ldots \quad \text{or} \quad \downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\ldots$$

  the energy is $E=-N\cdot J$
  and the free energy $F=E-TS=E$

- increasing the temperature leads to brownian motion and random spin flips

$$\uparrow\uparrow\uparrow\uparrow\downarrow\uparrow\uparrow\downarrow\ldots$$

Question: Do these spin flips destroy the long-range order?

consider system at $T>0$ with 2 domains:

what is the energy of the system?

$$\ldots\uparrow\uparrow\uparrow\uparrow \,\vdots\, \downarrow\downarrow\downarrow\downarrow\ldots$$

$$E=-\underbrace{(N-1)J}_{N-1\text{ parallel spin pairs}}+\underbrace{J}_{1\text{ antiparallel spin pair}}=-N\cdot J+2J$$

for the free energy F we need the entropy contribution $T\cdot S$

for the determination of the entropy S, note that the domain boundary can be at any of the N lattice sites:

$\Rightarrow$ $S = k_B \cdot \log N$ (since we consider a state with fixed energy we compute the microcanonical entropy)

$\Rightarrow$ free energy difference between 1-domain and 2-domain state is:

$$F^{(2)} - F^{(1)} = 2J - k_B \cdot T \cdot \log N$$

$\Rightarrow$ for $N \to \infty$ we can lower the free energy by creating a domain wall

- argument can be repeated, i.e. free energy can be further lowered by creating additional domain walls until all long-range order is destroyed

$\Rightarrow$ long-range order is unstable against thermal fluctuations at $T>0$, i.e.

$$m(B=0) = 0 \quad \text{for} \quad T>0$$

remarks:

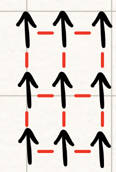
- valid for all interactions with

$$J_{ij} = \frac{J}{|i-j|^{\sigma}} \quad \text{with } \sigma > 2$$

- for $1 \leq \sigma \leq 2$ long-range order might persist for $0 < T < T_c$

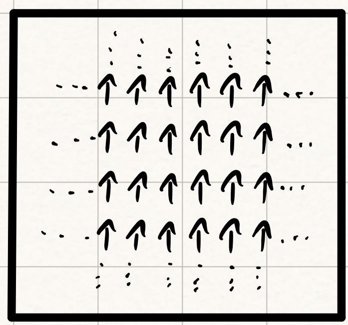
Phase transitions at $T>0$ in 2d

now we extend the arguments of previous section to two dimensions (again nearest-neighbour interaction, $B=0$)



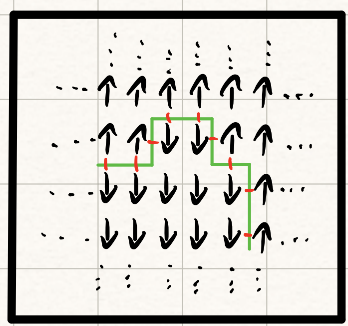
this discussion highlights the key role of the <u>dimensionality</u> of the system for phase transitions!

also in 2d the ground state at $T=0$ has zero entropy $S=0$ (all spins pointing up or down)



consider state consisting of 2 domains, domain boundary contains n bonds

energy difference: $E^{(2)} - E^{(1)} = 2 \cdot J \cdot n$



$(n=9)$

now determine entropy for 2-domain state, give <u>upper estimate</u>:

How many ways are there to form a boundary with n bonds?

- choose a lattice point as starting point
- for a square lattice there are 4 adjacent lattice points
- we need to take n steps to form a boundary with n bonds, in order to avoid backtracking we effectively only have up to 3 choices at each lattice point

- hence an upper boundary for the entropy is:

$$S_{max} \sim k_B \cdot \log(\underbrace{N}_{\text{N possible starting points}} \cdot \underbrace{3^n}_{\text{upper limit for number of paths}}) \sim k_B\, n \cdot \log 3$$

- we are interested in domain walls that contain a macroscopically large number of spins, hence consider the thermodynamical limit $n \to \infty$

$$\Delta F = F^{(2)} - F^{(1)} = 2Jn - k_B T n \log 3$$
$$= n(2J - k_B T \log 3)$$

$\Rightarrow$ for $T > T_c = \frac{2J}{k_B \cdot \log 3}$ we have $\Delta F \to -\infty$ for $n \to \infty$

that means the system is unstable against formation of domain walls, no long-range order for $T > T_c$

$\Rightarrow$ for $T < T_c$, however, long-range order is stable and ground state has a nonvanishing net magnetization!

$$m(B=0, T<T_c) \neq 0$$

The results above apply to all Hamiltonians with a discrete symmetry and short-range interactions!

$\hookrightarrow$ here: $H(\{\sigma_i\}) = H(\{-\sigma_i\})$.