Review of previous lecture (May 16)

mean field theory (nearest-neighbor Ising model, 1d)

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

no interaction: $H = -\sum_i B_i \sigma_i$, each spin only feels the external field B_i

$\Rightarrow$ partion function separates into product of single-particle partition functions $Z_c = \prod_{i=1}^{N} Z_c^i = \prod_{i=1}^{N} 2\cosh(\beta B_i)$

$$\boxed{B_i = B} \Rightarrow m = -\frac{\partial f}{\partial B} = \tanh(B)$$

mean-field approximation of interacting system:
transform H to a non-interacting form $H = -\sum_i B_i^{\text{eff}} \sigma_i$,
B_i^{eff} contains contributions from external B_i and averaged interactions with other spins:

$$\begin{aligned} B_{\text{eff}}^i &= B_i + \sum_{j=i\pm1} J_{ij} \sigma_j \\ &= B_i + \sum_{j=i\pm1} J_{ij} \langle \sigma_j \rangle + \cancel{\sum_{j=i\pm1} \left(\sigma_j - \langle \sigma_j \rangle \right)} \end{aligned}$$

$$\begin{pmatrix} B_i = B \\ J_{ij} = J \end{pmatrix} \rightarrow B + 2Jm$$

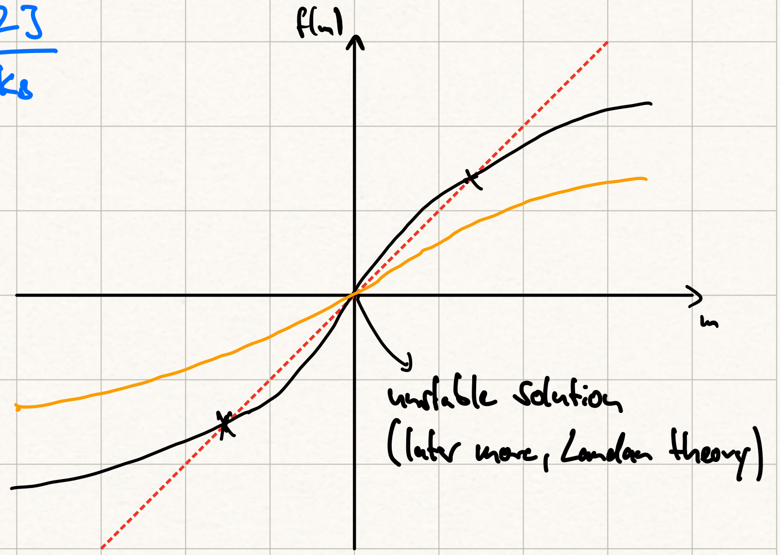
study spontaneous magnetization $(B=0)$: $m = \tanh(2\beta J m)$

for solutions $m \neq 0$ we need

$$\tanh(2\beta J m) > m \quad \left(\text{for small } m: \tanh x \sim x - \frac{x^3}{3} + \dots\right)$$

critical value of T for a nontrivial solution:

$$m = \frac{2J\,m}{k_B \cdot T_c} \Rightarrow T_c = \frac{2J}{k_B}$$



phase transition
(in contrast to exact solution!)

determine critical exponents:

$$m \sim |T - T_c|^{\beta}$$

$$B \sim m^{\delta} \quad (\text{at } T = T_c)$$

$$\chi_T = \left.\frac{\partial m}{\partial B}\right|_T \sim |T - T_c|^{-\gamma}$$

expand equation of state around $T = T_c$:

$$m = \tanh(\beta(B + 2Jm))$$

$$= \tanh\left(\frac{B}{k_B T} + m \cdot \tau\right) \quad \text{with} \quad \tau = \frac{T_c}{T} = \frac{2J}{k_B T}$$

$$\sim \left(\frac{B}{k_B T} + m\tau\right) - \frac{1}{3}\left(\frac{B}{k_B T} + m\tau\right)^3 + \dots$$

small B and m

for $B=0$ we obtain: $m(1-\tau) = -\frac{1}{3} m^3 \tau^3$

$$\Rightarrow m^2 = -\frac{3(1-\tau)}{\tau^3} \sim (T-T_c) \quad \Rightarrow \underline{\beta = \tfrac{1}{2}}$$

<u>for δ</u>: $\underset{\substack{\downarrow \\ 0}}{m(1-\tau)} = \frac{B}{k_B \cdot T} - \frac{1}{3}\left(\frac{B}{k_B T} + m\tau\right)^3$

$$= \frac{B}{k_B \cdot T} - \frac{1}{3} m^3 \tau^3 \underbrace{\cancel{- \frac{1}{3} \frac{B^3}{(k_B T)^3} - \frac{B}{k_B \cdot T} m^2 \tau^2}}_{\text{higher order terms in powers of } B}$$

$$\Rightarrow \frac{B}{k_B T} \sim m^3 \quad \Rightarrow \underline{\delta = 3}$$

justify a posteriori → higher order terms in powers of B

for γ: $\left.\frac{\partial m}{\partial B}\right|_T = \chi_T = \frac{1}{k_B \cdot T} + \chi_T \cdot \tau + m^2$

$$\Rightarrow \chi_T (1-\tau) = \frac{1}{k_B T} \quad \Rightarrow \chi_T \sim \frac{1}{T-T_c} \, , \quad \underline{\gamma = 1}$$

liquid-gas transition, van-der-Waals equation of state

no phase transition for a free non-interacting gas

<u>basic idea:</u> modify ideal gas equation of state,

$$p \cdot V = N \cdot k_B \cdot T$$

so that a <u>finite volume</u> and an <u>averaged interaction</u> is taken into account consider semiclassical partition function of a free gas:

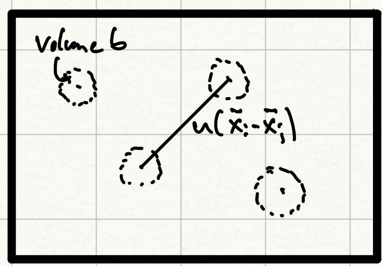
$$Z_c = Z_0 = \frac{V^N}{N!\,\lambda^{3N}} \quad \text{with thermal wavelength:} \quad \lambda = \frac{h}{\sqrt{2\pi m k_B T}}$$

(see exercise)

now consider system with particle interactions $u(\vec{x}_i - \vec{x}_j)$ and particle volume b

$$\Rightarrow \quad Z_c = \frac{1}{N!\,\lambda^{3N}} \int d^3x_1 \dots \int d^3x_N \; e^{-\beta \sum_{i<j} u(\vec{x}_i - \vec{x}_j)}$$

apply mean-field approximation for interaction term:



$$-\beta \sum_{i<j} u(\vec{x}_i - \vec{x}_j) = -\frac{\beta}{2} \sum_{i \neq j} u(\vec{x}_i - \vec{x}_j)$$

$$= -\frac{\beta}{2} \int d^3x \int d^3x' \, \rho(\vec{x})\, u(\vec{x} - \vec{x}')\, \rho(\vec{x}')$$

$$\xrightarrow{\text{mean field approx.}} -\frac{\beta}{2} \int d^3x \int d^3x' \, \langle \rho \rangle^2 \, u(\vec{x} - \vec{x}')$$

$$\left[\rho(\vec{x}) = \sum_i \delta(\vec{x} - \vec{x}_i), \quad \langle \rho \rangle = \frac{1}{V} \int d^3x \, \rho(\vec{x}) = \frac{N}{V} \right]$$

$$= -\frac{\beta}{2} \frac{N^2}{V^2} \underbrace{\int d^3(\vec{x} - \vec{x}')\, u(\vec{x} - \vec{x}')}_{= -2a} \underbrace{\int d^3(\vec{x} + \vec{x}')}_{\to V}$$

$$= \beta \frac{N^2}{V} a$$

$$\Rightarrow \quad Z_c = \frac{1}{N!\,\lambda^{3N}} \int d^3x_1 \int d^3x_2 \cdots \int d^3x_N \; e^{\beta \frac{N^2}{V} a}$$

$$= \frac{(V-bN)^N}{N!\,\lambda^{3N}} \, e^{\beta \frac{N^2}{V} a}$$

$\rightarrow$ exercise

$$F = -k_B \cdot T \log Z_c$$

$$\sim -N k_B T \log \frac{(V-bN)}{N\lambda^3} - k_B T \beta \frac{N^2}{V} a$$

$$p = -\frac{\partial F}{\partial V}\Big|_{T,N} = \frac{N k_B T}{V-Nb} - \frac{N^2}{V^2} a$$

$\rightarrow$ exercise

critical behaviour of Van-der-Waals liquids

Ising model

$$m \sim |T-T_c|^\beta$$

$$B \sim m^\delta$$

$$\chi_T = \frac{\partial m}{\partial B}\Big|_T \sim |T-T_c|^{-\gamma}$$

in mean-field approx. we found

$$\beta = \frac{1}{2}, \quad \delta = 3, \quad \gamma = 1$$

Van-der Waals liquid

$$V_g - V_e \sim |T-T_c|^\beta$$

$$|p-p_c| \sim |V-V_c|^\delta$$

$$\kappa_T = -\frac{1}{V}\frac{\partial V}{\partial p}\Big|_T \sim |T-T_c|^{-\gamma}$$

here we find the same critical exponents

$\hookrightarrow$ exercise

universality