

Reminder

Importance-sampling Monte Carlo determines/uses Boltzmann weights in partition function Z only up to unknown prefactor

→ Z cannot be measured with (imp. samp.) MC

→ F " " " " " "

→ S " " " " " "

↑
 E measurable, $F = E - TS$

Mean-field solution of the Ising model

Mean-field approximation: correlations of the form $\langle (\sigma_i - \langle \sigma_i \rangle)(\sigma_j - \langle \sigma_j \rangle) \rangle$ are neglected.

For homogeneous case ($\langle \sigma_i \rangle = \langle \sigma_j \rangle \equiv \langle \sigma \rangle = M$)

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - B \sum_i \sigma_i \quad \text{here: } (\mu_B = 1)$$

$$\approx \mathcal{H}_{MF} = -J \sum_i \sigma_i \sum_{\substack{j \\ \text{of } i}} \langle \sigma \rangle - B \sum_i \sigma_i$$

$$= - \underbrace{(B + qJ \langle \sigma \rangle)}_{B_{eff}} \sum_i \sigma_i$$

q : coordination number (# of nearest neighbors)

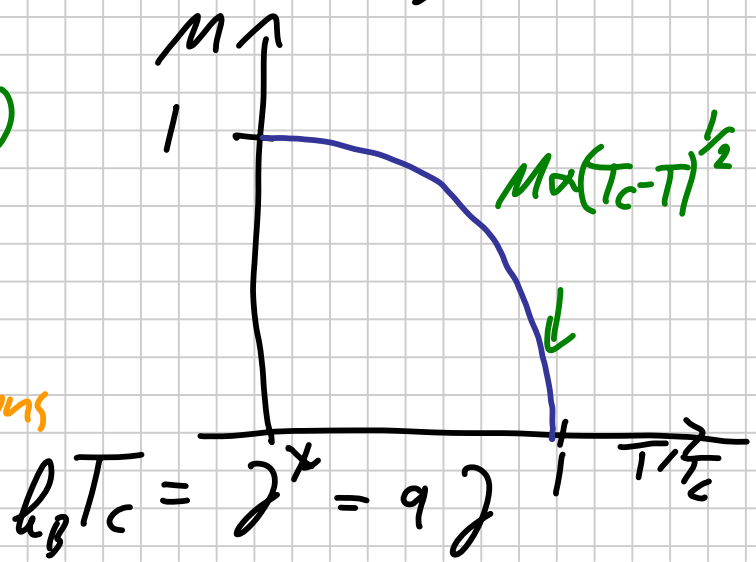
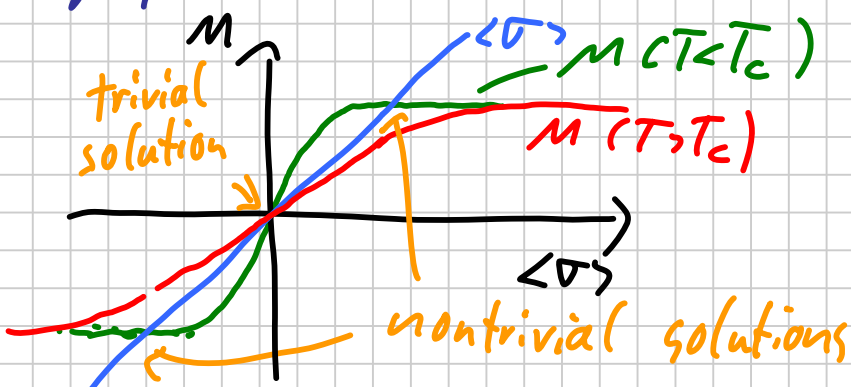
effective single-spin Hamiltonian with self-consistency condition

$$\Rightarrow \text{partition function} \quad Z = \left(\sum_{\sigma_i = \pm 1} \exp\left(\sigma_i \frac{B + qJ \langle \sigma \rangle}{k_B T}\right) \right)^N$$

$$= \left(2 \cosh \frac{B + qJ \langle \sigma \rangle}{k_B T} \right)^N$$

$$\Rightarrow \text{magnetization} \quad M = \langle \sigma \rangle = \tanh \frac{B + qJ \langle \sigma \rangle}{k_B T}$$

graphical solution:



Ising model: solution in 1 dimension

(i) simple case: open chain, no magnetic field

$$\mathcal{H} = -J \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1} = -J \sum_{i=2}^N \sigma_{i-1} \sigma_i$$

$$Z = \sum_{\sigma_1=\pm} \sum_{\sigma_2=\pm} \dots \sum_{\sigma_N=\pm} e^{-\beta \mathcal{H} \{\sigma_i\}}$$

Trick: introduce new variables $\{s_i\}$ with

$$s_1 = \sigma_1; \quad s_i = \sigma_i \sigma_{i-1} \text{ for } i \geq 2 \quad (\Rightarrow) \quad \sigma_i = \prod_{j=1}^i s_j$$

$$\Rightarrow \mathcal{H} = -J \sum_{i=2}^N s_i$$

$$Z = \left(\sum_{s_1=\pm} \right) \left(\sum_{s_2=\pm} e^{-\beta J s_2} \right) \left(\sum_{s_3=\pm} e^{-\beta J s_3} \right) \dots \left(\sum_{s_N=\pm} e^{-\beta J s_N} \right)$$

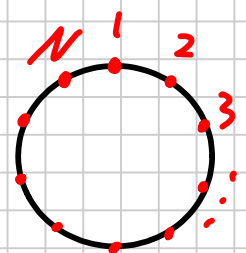
$$= 2 (2 \cosh(\beta J))^{N-1} = 2^N [\cosh(\beta J)]^{N-1}$$

$$\Rightarrow E(\beta) = -\frac{\partial \ln Z}{\partial \beta} = -(N-1) \tanh(\beta J)$$

$$E(T) = -(N-1) J \tanh(J/k_B T)$$

∞ often differentiable for all $0 < T < \infty \rightarrow$ no finite- T phase trans.

(ii) more relevant case: periodic boundary conditions (+ magnetic field)



$$\mathcal{H} = -J \sum_{i=1}^N \sigma_i \sigma_{i+1} - \mu_B B \sum_{i=1}^N \sigma_i \quad (\sigma_{N+1} \equiv \sigma_1)$$

Treat using bond transfer matrices (2x2), see

<http://komet337.physik.uni-mainz.de/Bluemer/Scripts/comp-sim-ws0607-v10.pdf>

$$\Rightarrow Z = (p^+)^N + (p^-)^N \quad \text{where}$$

$$p_{\pm} = e^{\beta J} \cosh(\beta \mu_B B) \pm \sqrt{e^{2\beta J} \sinh^2(\beta \mu_B B) + e^{-2\beta J}}$$

magnetization (in thermodynamic limit):

$$M = \frac{\sinh(\beta \mu_B B)}{\sqrt{\sinh^2(\beta \mu_B B) + e^{-4\beta J}}}; \quad m = N \mu_B M$$

no finite-temperature magnetism: $m \xrightarrow{B \rightarrow 0} 0$ for $T > 0$
(but ground state fully polarized: $m = \pm N \mu_B$ for $T = 0$)

On the basis of these results, Ising and Lenz discarded the model as irrelevant for (finite T) magnetism.

Ising model on the 2d square lattice

Combination of high- and low-temperature expansions (Kramers, Wannier, 1941) using duality

$$\Rightarrow \frac{J}{k_B T_c} = \frac{1}{2} \operatorname{arcsinh}(1) = \frac{1}{2} \ln(\sqrt{2} + 1) \approx 0.4407$$

$$T_c \approx 2.2692 \frac{J}{k_B}$$

Critical exponents: $\alpha = 0$, $\beta = \frac{1}{8}$, $\gamma = \frac{7}{4}$, $\delta = 15$

For details, see Thermodynamics script by P. van Dongen and

<http://komet337.physik.uni-mainz.de/Bluemer/Scripts/comp-sim-ws0607-v10.pdf>

Ising-Model (NN interactions) - critical temperatures

dim	lattice	q	$k_B T_c / J$	$k_B T_c / J q$
1	chain/ring	2	0	0
2	honeycomb	3	~ 1.52	~ 0.5
	square	4	2.269	0.57
	triangular	6	~ 3.64	~ 0.61
3	diamond	4	~ 2.704	~ 0.68
	cubic	6	~ 4.512	~ 0.75
	bcc	8	~ 6.35	~ 0.79
	fcc	12	~ 9.79	~ 0.82
4	hypercubic	8	~ 6.68	~ 0.84
∞		∞	∞	1.0

Most values taken from Peter Meyer, PhD thesis, University of Derby (2000) <http://www.hermetic.ch/compsci/thesis/chap7.htm>

Note:

- phase transition for all lattices in $d > 1$
- $T_c \xrightarrow{q \rightarrow \infty} Jq/k_B$ (coordination number q)

Ising critical exponents in $d=3$ dimensions

$$\alpha = 0.110(1); \quad \beta = 0.3265(3); \quad \gamma = 1.2372(5);$$

$$\delta = 4.789(2); \quad \nu = 0.6301(4); \quad \eta = 0.0364(5); \quad \omega = 0.84(4)$$

Pelissetto, Vicari, Physics Reports 368, 549 (2002) <http://arxiv.org/abs/cond-mat/0012164>
[http://dx.doi.org/10.1016/S0370-1573\(02\)00219-3](http://dx.doi.org/10.1016/S0370-1573(02)00219-3)

(for comparison: $d=2$: $\alpha=0, \beta=\frac{1}{8}, \gamma=\frac{7}{4}, \delta=15, \nu=1$)
 mean field, i.e. $d \geq 4$: $\alpha=0, \beta=\frac{1}{2}, \gamma=1, \delta=2, \nu=\frac{1}{2}$)