Addendum to last lecture:

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

$\rightsquigarrow$ $Z$ cannot be measured with (imp. samp.) MC

$\rightsquigarrow$ $F$ " " " " " "

$\rightsquigarrow$ $S$ " " " " " "

$E$ 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 $(\langle\sigma_i\rangle = \langle\sigma_j\rangle \equiv \langle\sigma\rangle = M)$

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - B \sum_i \sigma_i$$

here: $(\mu_B \equiv 1)$

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

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

$q$: coordination number (# of nearest neighbors)

effective single-spin Hamiltonian with self-consistency condition

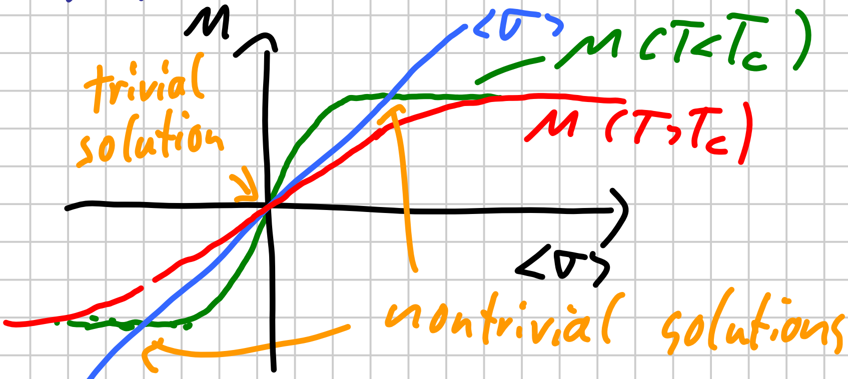
$\Rightarrow$ partition function

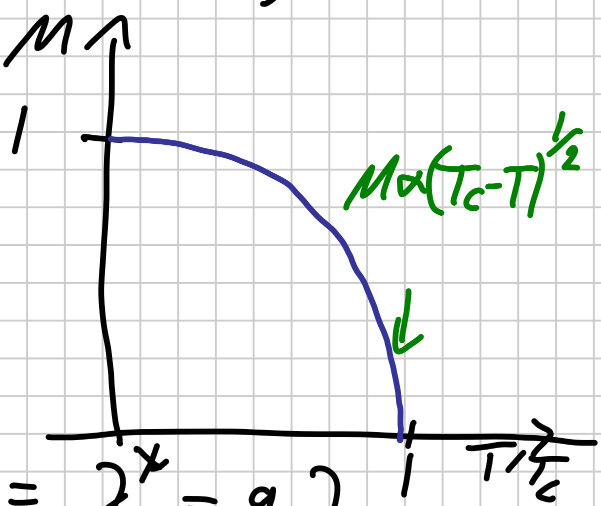
$$Z = \left( \sum_{\sigma_i = \pm 1} \exp\left(\sigma_i \frac{B + qJ\langle\sigma\rangle}{k_B T}\right) \right)^N$$

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

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

graphical solution:




$$k_B T_c = J^* = qJ$$

# Ising model: solution in 1 dimension

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

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

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

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

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

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

$$Z = \left(\sum_{s_1=\pm}\right)\left(\sum_{s_2=\pm} e^{-\beta J s_2}\right)\left(\sum_{s_3=\pm} e^{-\beta J s_3}\right)\cdots\left(\sum_{s_N=\pm 1} e^{-\beta J s_N}\right)$$

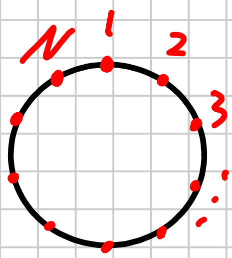
$$= 2\left(2\cosh(\beta J)\right)^{N-1} = 2^N\left[\cosh(\beta J)\right]^{N-1}$$

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

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

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

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




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

Treat using bond transfer matrices (2x2), see

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

$$\boxed{\Rightarrow \; Z = (p^+)^N + (p^-)^N \quad \text{where} \quad p_\pm = e^{\beta J}\cosh(\beta\mu_B B) \pm \sqrt{e^{2\beta J}\sinh^2(\beta\mu_B B) + e^{-2\beta J}}}$$

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: $m \xrightarrow{B\to 0} 0$ 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

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

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

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/Scrips/comp-sim-ws0607-v10.pdf

# Ising-Model (NN interactions) – critical temperatures

| dim | lattice | $q$ | $k_B T_c / J$ | $k_B T_c / Jq$ |
|---|---|---|---|---|
| 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 |
| $\infty$ | " | $\infty$ | $\infty$ | 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 $d > 1$
- $T_c \xrightarrow{q \to \infty} Jq/k_B$ (coordination number $q$)

# Ising critical exponents in $d=3$ dimensions

$\alpha = 0.110(1)$; $\beta = 0.3265(3)$; $\gamma = 1.2372(5)$;
$\delta = 4.789(2)$; $\nu = 0.6301(4)$; $\eta = 0.0364(5)$; $\omega = 0.84(4)$

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

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

# Finite-size scaling

Goal of finite-size scaling (FSS) is the extrapolation of critical behavior in the thermodynamic limit from the (non-singular) properties of finite systems.

Fundamental hypothesis: close to $2^{nd}$ order phase transitions the relevant length scale for the singular part of the free energy is the correlation length $\xi$, not a microscopic length scale ((lattice spacing, average particle distance etc).

$\rightsquigarrow$ Size of cubic system with volume $V = L^d$ is characterized by ratio $L/\xi$; the singular part of the free energy density is to leading order:

$$f^{(s)}(L,T) = \frac{1}{V} F^{(s)}(L,T) \approx \frac{1}{V} \tilde{Y}\left(\frac{L}{\xi(T)}\right), \text{ where}$$

$$\xi(T) = \xi_0 \, \varepsilon^{-\nu}; \qquad \varepsilon = \left|1 - \frac{T}{T_c}\right|$$

$\Rightarrow$ dimensionless length: $\frac{L}{\xi} = \xi_0^{-1} \varepsilon^{\nu} L$

rescaling: $$\left(\frac{L}{\xi} \frac{\xi_0}{L_0}\right)^{1/\nu} = \varepsilon \left(\frac{L}{L_0}\right)^{\frac{1}{\nu}}$$

microscopic length scale
often: $L_0 \equiv 1$

nonuniversal

$$f^{(s)}(L,T) \approx L^{-d} \, Y(C_1 \varepsilon L^{1/\nu}, 0)$$

universal function

For the coupling to a magnetic field, one assumes that the effect of $B$ is amplified by a power of $\xi$, since (for ferromagnetic models) areas of radius $\xi$ are approximately parallel:

$$\Rightarrow \boxed{f^{(s)}(L,T,B) = L^{-d}\, Y\left[C_1 \varepsilon L^{1/\nu},\, C_2 B L^{\frac{\beta+\gamma}{\nu}}\right]}$$

V. Privman, M. E. Fisher, PRB 30, 322 (1984) http://prola.aps.org/abstract/PRB/v30/i1/p322_1

Here, all exponents and the function $Y$ depend only on the universality class (in particular on the dimensions of space and order parameter).

One can derive scaling equations for observables, e.g.:

$$M(L,T) = \tilde{M}(\varepsilon L^{1/\nu})\, L^{-\beta/\nu}$$

$$\chi(L,T) = \tilde{\chi}(\varepsilon L^{1/\nu})\, L^{\gamma/\nu}$$

$$C(L,T) = \tilde{C}(\varepsilon L^{1/\nu})\, L^{\alpha/\nu}$$

Here, we have used scaling relations between the exponents:

$\alpha + 2\beta + \gamma = 2$ Rushbrooke $\qquad \gamma = \beta(\delta - 1)$ Widom

$d\nu = 2 - \alpha$ Josephson $\qquad \gamma = \nu(2-\eta)$ Fisher

The functions $\tilde{M}, \tilde{\chi}, \tilde{C}$ etc. can be expressed by derivatives of the universal function $Y$ and the nonuniversal coefficients $C_1, C_2$.