I.4 Das Ising-Modell

Vorübergehend englischsprachige Notizen, übernommen von der Vorlesung "Computer Simulations in Statistical Physics": http://komet337.physik.uni-mainz.de/Bluemer/lectures_WS2006

Model of interacting quantum spins in a magnetic field, introduced as model for ferromagnetism by Wilhelm Lenz (~ Runge-Lenz vector) and Ernst Ising in Ising's PhD thesis (Hamburg, 1924).
(10.5.1900 - 11.5.1998)

[Ising later became teacher, emigrated via Luxemburg to the USA. After Onsager's solution (1944) he became professor at Bradley university, Peoria, Illinois, but never published another journal article.]

Hamiltonian of general Ising model (N lattice sites): *

$$\mathcal{H} = -\frac{1}{2}\sum_{i,j=1}^{N} J_{ij}\,\sigma_i\sigma_j - \mu_B B\sum_{i=1}^{N}\sigma_i \qquad \sigma_i \in \{+1,-1\}$$

specifically for translation-invariant, isotropic nearest-neighbor interaction:

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

sum over NN pairs, each pair counted once

- important special case: $B=0$
- trivial single-spin (noninteracting) limit: $J=0$

- ferromagnetic/antiferromagnetic coupling for $J \gtrless 0$
- properties strongly dependent on lattice (i.e. also on dimensionality)

* more general spin Hamiltonian:

$$\mathcal{H} = -\frac{1}{2} \sum_{ij} \vec{S}_i \cdot \overleftrightarrow{I}_{ij} \cdot \vec{S}_j$$

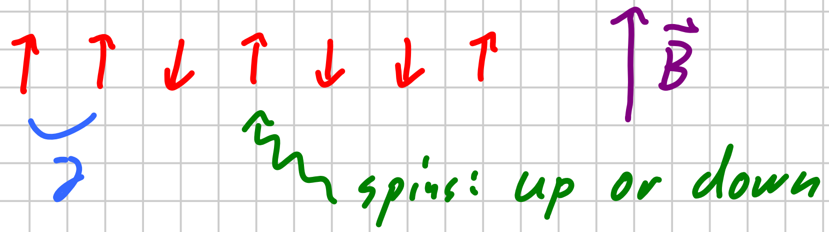
Eigenvalues $\pm \frac{1}{2}\hbar$

(isotropic) Heisenberg model: $\overleftrightarrow{I}_{ij} = I_{ij} \mathbb{1}$

Ising model: $(I_{ij})_{\mu\nu} = I_{ij}\, \delta_{\mu 3} \delta_{\nu 3}$

use scaled interactions $J_{ij} = \left(\frac{1}{2}\hbar\right)^2 I_{ij}$

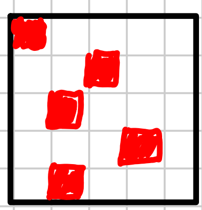
possible visualization:



$$\sigma_i = \frac{2}{\hbar} S_i^z \quad (\vec{S}_i : \text{spin vector})$$

alternative visualizations:

+	−	−	+	+
−	+	−	+	−
−	+	+	−	+
+	−	−	+	−
+	+	−	+	+



closely related: lattice gas model (lattice sites occupied/empty):

$$\mathcal{H}_{LGM} = U_{NN} \sum_{\langle ij \rangle} n_i n_j - \mu \sum_i n_i \; ; \quad n_i \in \{0, 1\}$$

μ: chem. potential (in grand canonical ensemble)

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

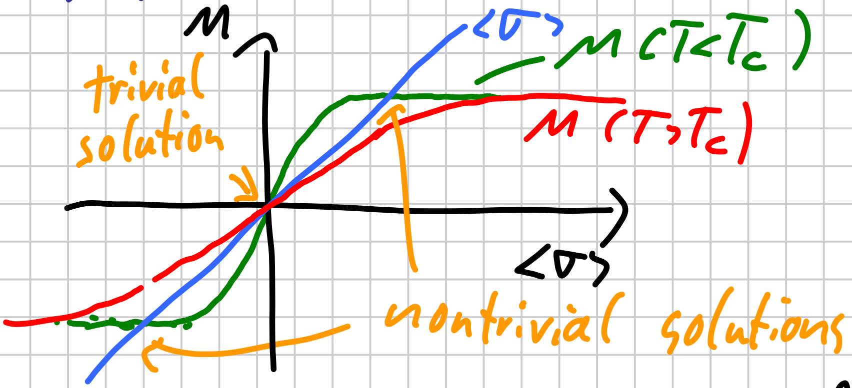
$\Rightarrow$ partition function

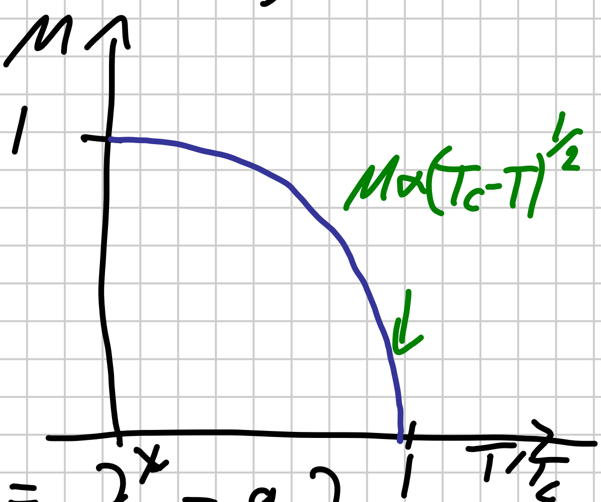
$$Z = \left(\sum_{\sigma_i=\pm 1}\exp\left(\sigma_i\,\frac{B+qJ\langle\sigma\rangle}{k_BT}\right)\right)^N$$

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

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

graphical solution:





$$k_BT_c = J^* = qJ$$

Ising model: solution in 1 dimension

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

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

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

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

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

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

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

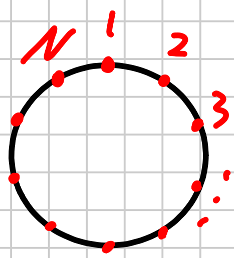
$$= 2\,(2\cosh(\beta J))^{N-1} = 2^N[\cosh(\beta J)]^{N-1}$$

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

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

∞ often differentiable for all $0<T<\infty$ $\rightsquigarrow$ 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 (2×2), see

http://komet337.physik.uni-mainz.de/Bluemer/Scrips/comp-sim-ws0607-v08.pdf

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

magnetization (in thermodynamic limit):

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

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

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

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

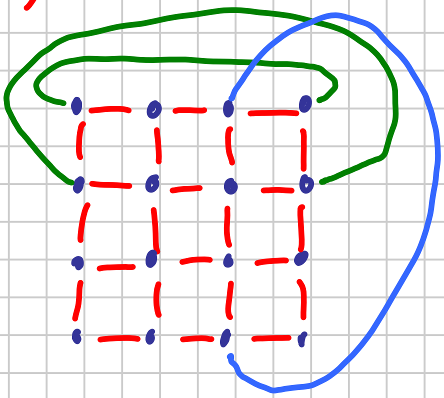
Critical exponents: $\alpha = 0$, $\beta = \frac{1}{8}$, $\gamma = \frac{7}{4}$, $\delta = 15$

For details, see Thermodynamics script by P. van Dongen and http://komet337.physik.uni-mainz.de/Bluemer/Scrips/comp-sim-ws0607-v10.pdf

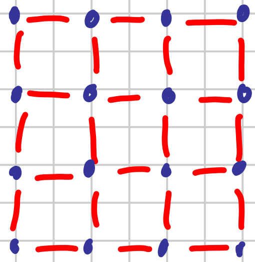
Ising model: simulation

1^{st} consideration: Hamiltonian for finite-size system, i.e. boundary conditions

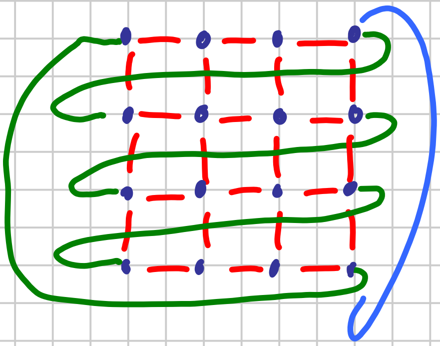
(i) conventional choice: periodic boundary conditions
$\Rightarrow$ all sites equivalent



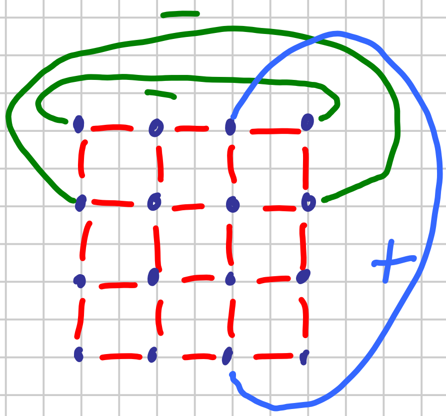
(ii) other extreme: open/free edge boundary conditions
$\Rightarrow$ inner + surface sites



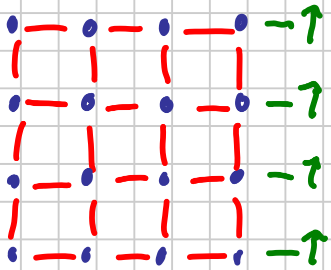
(iii) screw periodic boundary cond.
easy to implement on 1d vector $\Rightarrow$ introduces seam



(iv) antiperiodic boundary conditions:
flip sign of interaction along some boundaries
$\Rightarrow$ generate odd number of domain walls (e.g. 1) at $T \to 0$



(v) fixed or mean-field boundary conditions: boundary sites couple to external medium



Possibilities can be combined/mixed ...

Metropolis importance sampling Monte Carlo scheme

(i) choose initial spin configuration

(ii) select site i

(iii) calculate $\Delta E = E\{\sigma_\ell;\ \sigma_i \to -\sigma_i\} - E\{\sigma_\ell\}$

(iv) Metropolis step:

- if $\Delta E < 0$: accept move
- else generate random number $r \in [0,1)$
  - if $r < \exp[-\Delta E / k_B T]$: flip spin ($\sigma_i \to -\sigma_i$)
  - else: keep state

(v) after warm-up: measure

$$\left.\begin{aligned} &nsum \mathrel{+}= 1 \\ &msum \mathrel{+}= mag\{\sigma_\ell\} \\ &Esum \mathrel{+}= E\{\sigma_\ell\} \\ &\quad\vdots \end{aligned}\right\}$$

compute internally or print for external analysis

(vi) enough sweeps ($N = L^d$ attempted spin flips)?

- yes: compute averages + error bars (if done internally)
- no: → go back to (ii)

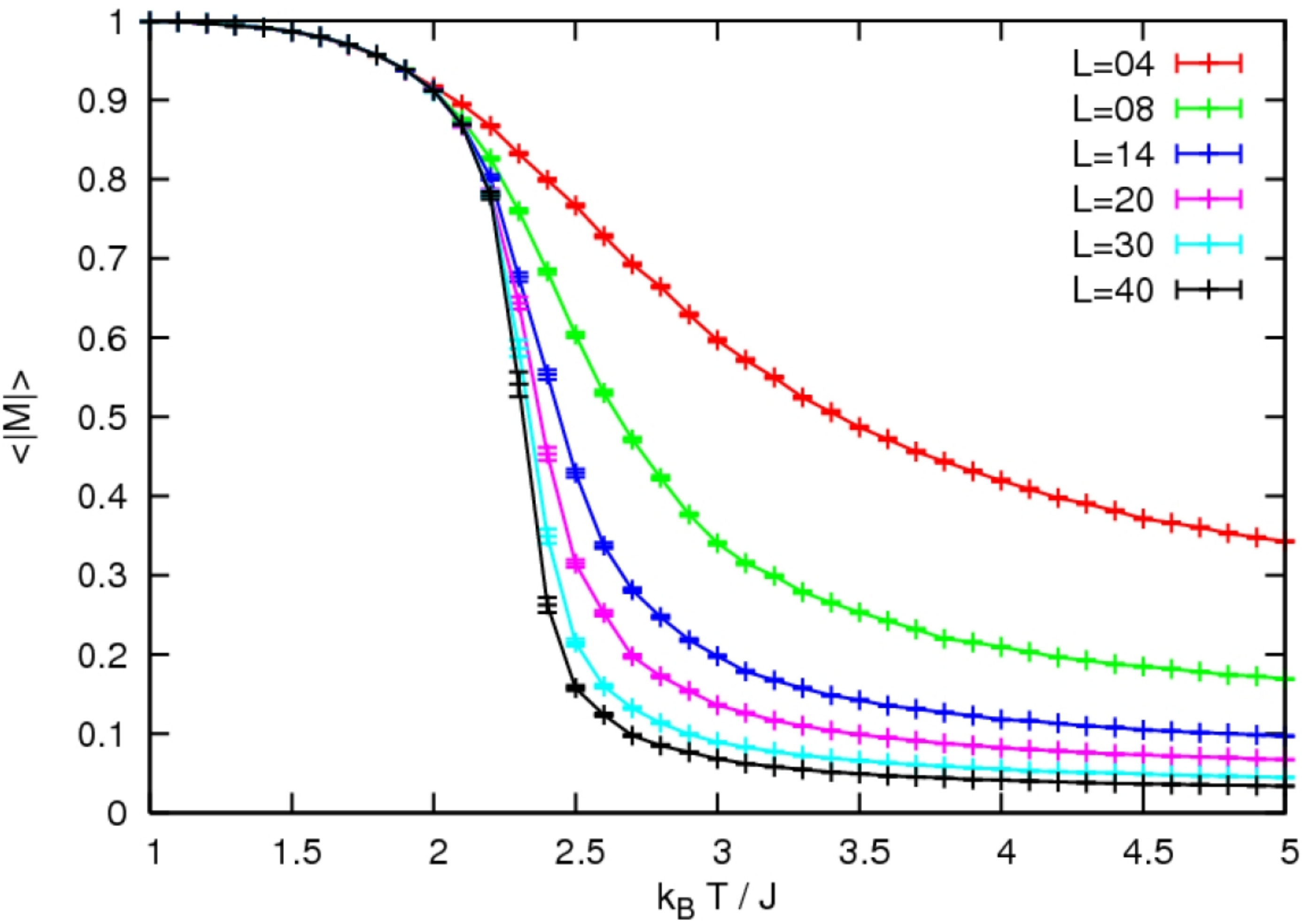
<u>note:</u> ΔE depends only on nearest neighbors of site i, specifically only on number of up spins in neighborhood (and σ_i)
⇝ look-up table possible

Hausaufgabe (siehe Kursseite)

- 14.05.2007 **Monte-Carlo-Simulation des 2D-Ising-Modells** (Abgabetermin: 24.05.2007)
  - Schreiben Sie ein Metropolis-Monte-Carlo-Programm zur Berechnung von Energie und Magnetisierung des Ising-Modells in 2 Raumdimensionen. Dabei dürfen Sie das unten verlinkte Templat benutzen.
  - Berechnen Sie Mittelwerte E(T) und |M(T)| (mit Fehlerbalken) in einem sinnvollen Temperaturbereich für Gitter mit linearer Ausdehnung zwischen 4 und etwa 20-40.
  - Tragen Sie die Binder-Kumulante $U_4(T)=1-\langle m^4\rangle/(3\langle m^2\rangle^2)$ für verschiedene Gittergrößen auf und bestimmen Sie aus dem asymptotischen Schnittpunkt die kritische Temperatur T_c.
  - Optional: Bestimmen Sie die spezifische Wärme und die magnetische Suszeptibilität bei ausgewählten Temperaturen.

Beispiel:

Magnetization (10^5 sweeps)



http://komet337.physik.uni-mainz.de/Bluemer/Scripts/num-meth-ss07-v05.pdf