Phase transition – Ising model

Description of phase transitions with partition function (?)

First-order phase transition:
• discontinuity in the first derivative of A
Second-order phase transition :
• discontinuity in the second derivative of A
(Ehrenfest's classification based on free energy

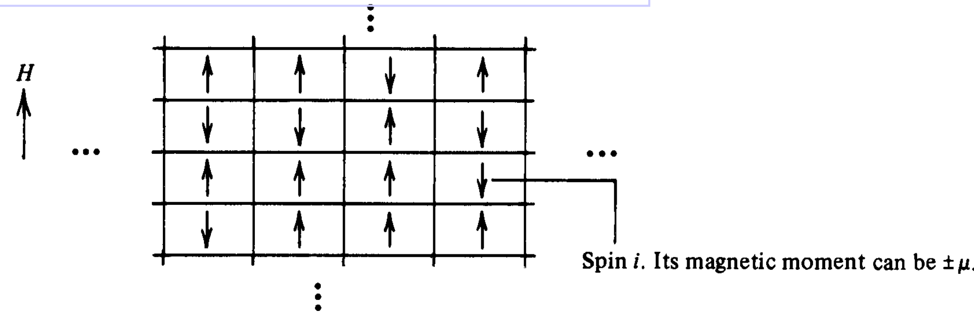


Fig. 5.1. Spins on a lattice.

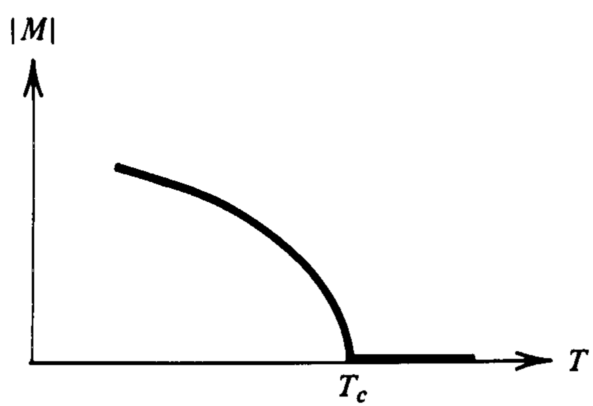
$$E_\nu = -\sum_{i=1}^{N} H\mu s_i + \text{(energy due to interactions between spins)}$$

$$s_i = \pm 1 \qquad\qquad -J\sum_{ij}{}' s_i s_j$$

Lattice topology and dimensionality
Cubic lattice: E_0=-DNJ

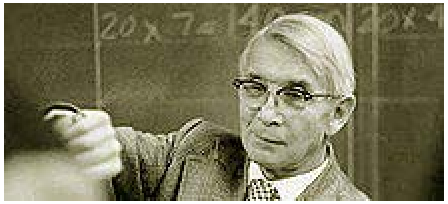
$$\langle M \rangle = \sum_{i=1}^{N} \mu s_i$$

J > 0: Spontaneous magnetization - „long ranged correlation“, „long ranged order“



T_c – critical (Curie) temperature

Macroscopic properties of Ising (magnetic lattice) – partition function



$$Q(\beta, N, H) = \sum_{\nu} e^{-\beta E_\nu} = \sum_{s_1}\sum_{s_2}\ldots\sum_{s_N} e^{\left[\beta\mu H \sum_{i=1}^{N} s_i + \beta J \sum_{ij}{}' s_i s_j\right]}$$

<u>One-dimmensional lattice</u> $-J\sum_{i=1}^{N} s_i s_{i+1}$

No spontaneous magnetization

(periodic boundary conditions)

$$\begin{array}{ccccccccc} \uparrow & \uparrow & \downarrow & \cdots & \uparrow & \downarrow & \downarrow & \cdots & \uparrow \\ 1 & 2 & 3 & & i-1 & i & i+1 & & N \end{array}$$

$$Q(\beta, N, 0) = [2\cosh(\beta J)]^N$$

$$\begin{array}{ccccccccc} \uparrow & \uparrow & \uparrow & \cdots & \uparrow & \uparrow & \cdots & \uparrow \\ 1 & 2 & & & \frac{N}{2} & & & N \end{array}$$

$$E = -NJ$$

$$\Delta E = 4J$$

$$\begin{array}{ccccccccc} \uparrow & \uparrow & \uparrow & \cdots & \uparrow & \downarrow & \cdots & \downarrow \\ 1 & 2 & & & \frac{N}{2} & & & N \end{array}$$

$$E = (-N+4)J$$

Too small difference for macroscopic system

$$T_c \approx \frac{J}{Nk} \to 0$$

2-D lattice:

$$
\begin{array}{ccccccc}
\cdots & \uparrow & \uparrow & \uparrow & \uparrow & \uparrow & \cdots \\
 & \uparrow & \uparrow & \uparrow & \uparrow & \uparrow & \\
\cdots & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \cdots \\
 & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow &
\end{array}
$$

$$\boxed{\Delta E = 4J\sqrt{N}}$$

Analytical solution (Onsager):

$$\boxed{Q(\beta, N, 0) = [2\cosh(\beta J)e^{I}]^{N}}$$

$$I = (2\pi)^{-1}\int_0^{\pi} d\phi \, \ln\{\tfrac{1}{2}[1 + (1 - \kappa^2 \sin^2 \phi)^{1/2}]\}$$

$$\kappa = 2\sinh(2\beta J)/\cosh^2(2\beta J)$$

$$\downarrow$$

$$\boxed{T_c = 2.269 J/k_B}$$

Heat capacity – singularity

$$\boxed{(C/N) \sim (8k_B/\pi)(\beta J)^2 \ln|1/(T - T_c)|}$$

Magnetization

$$(M/N) \sim (\text{constant})(T_c - T)^{\beta}, \qquad T < T_c, \qquad \beta = 1/8$$

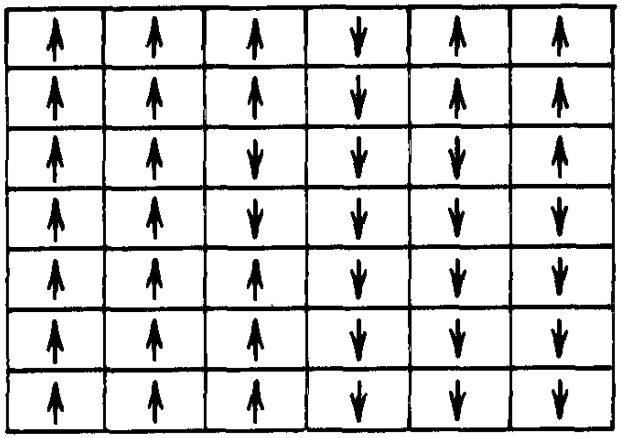
3-D lattice:

No analytical solution, numerical approach: $\boxed{(C/N) \propto |T - T_c|^{-\alpha}}$

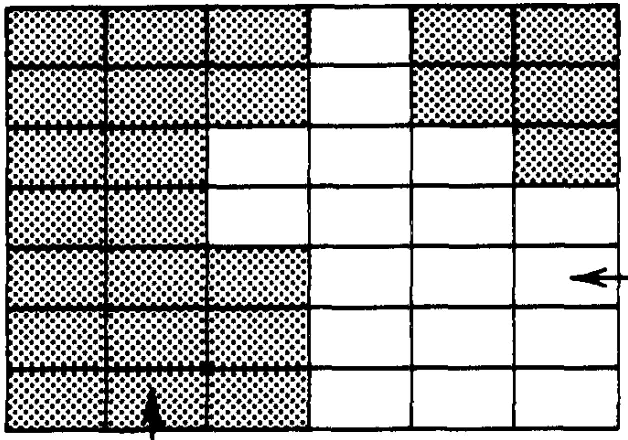
$$\boxed{(M/N) \propto (T_c - T)^{\beta}, \qquad T < T_c,}$$

$$\alpha \approx 0.125, \qquad \beta \approx 0.313$$

„Lattice Gas“



Ising magnet



Lattice gas

$S_i = -1, 1$

$-J \sum_{ij}' s_i s_j$

$n_i = 0, 1$

$-\varepsilon \sum_{i,j}' n_i n_j$

$s_i = 2n_i - 1$

$J = \varepsilon/4$

$$\Xi = \sum_{\substack{n_1,\ldots,n_N \\ =0,1}} \exp\left\{\beta\mu \sum_{i=1}^{N} n_i + \beta\varepsilon \sum_{ij}' n_i n_j\right\}$$

Ising magnet– broken symmetry

Magnetization: $$\langle M \rangle = Q^{-1} \sum_{\nu} \left(\sum_{i=1}^{N} \mu s_i \right) e^{-\beta E_\nu}$$

No external field – should go to 0 $\boxed{P_{M_\nu} = P_{-M_\nu}}$

$$Q(\beta, N, H) = \sum_{\nu} e^{-\beta E_\nu} = \sum_{M} \tilde{Q}(M)$$

$M = M_\nu$ => 1, otherwise 0

Summing for particular magnetization M

$$\tilde{Q}(M) = \sum_{\nu} \Delta(M - M_\nu) e^{-\beta E_\nu}$$

$$\boxed{A(N, H, T) = -kT \ln Q}$$

$$\downarrow$$

$$\boxed{\tilde{A}(M) = -kT \ln \tilde{Q}(M)}$$

Free energy – reverzible work required to change magnetization of the system

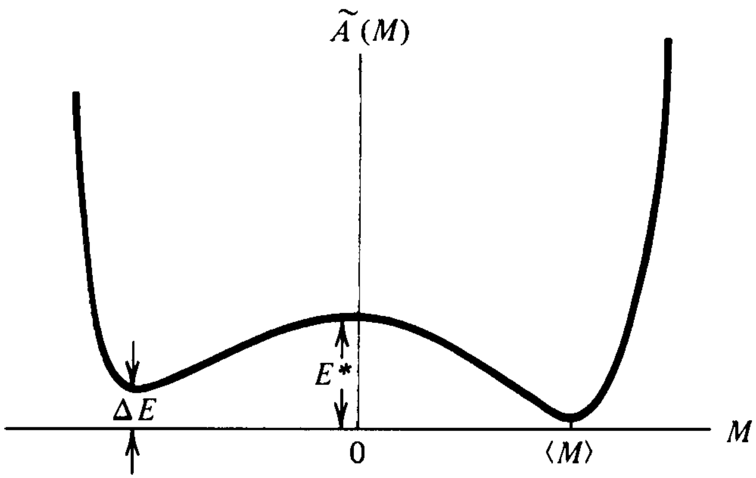


Fig. 5.4. Reversible work function for the magnetization.

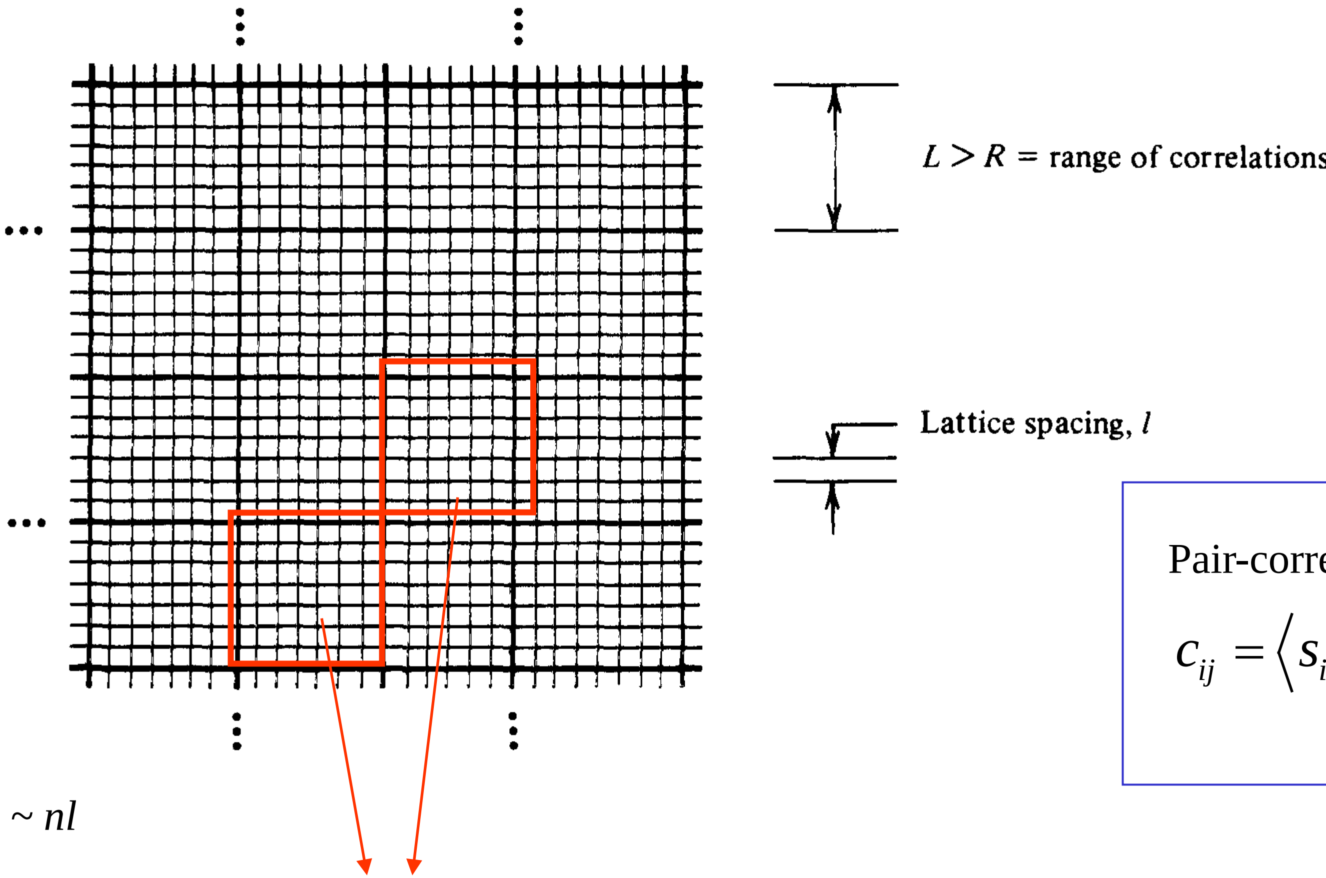
Change of magnetization requires fluctuation
With energy of the size of E^*

- Half of the spins must be reversed

$2D \sim N^{1/2}$

$3D \sim N^{2/3}$

Phase transitions are related to the range of correlation
„Range of correlation“ – R – fluctuations are correlated
for points outside this range – fluctuations are not correlated



Pair-correlation function:

$$c_{ij} = \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle$$

$R \sim nl$

No correlation – average magnetization is zero.

$R \sim$ macroscopic – magnetization may exist

Phase transitions

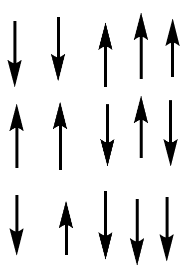
(approximations required)

Methods

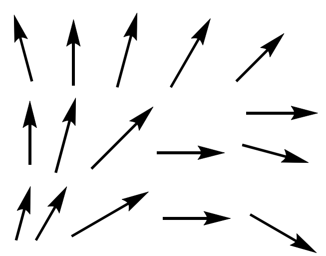
- Mean Field Theory
- Renormalization group
- Monte Carlo

Models

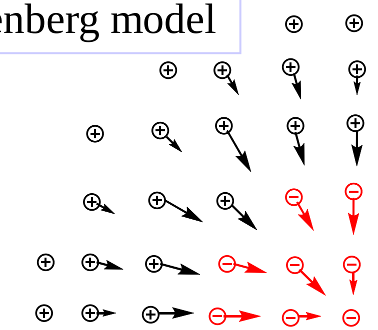
- Ising model



- Potts model

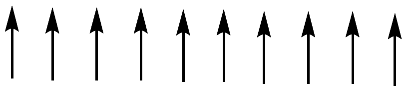
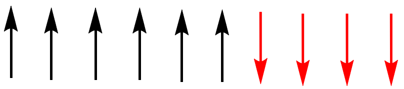
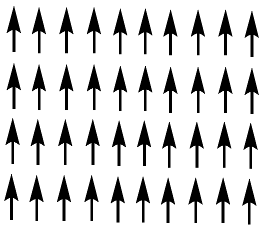
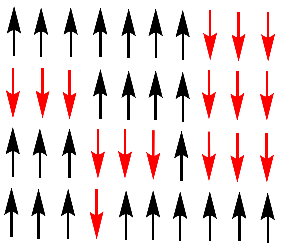
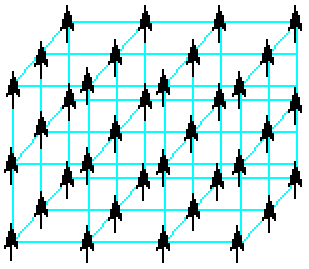
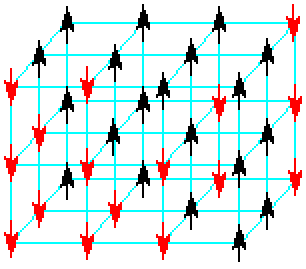


- Heisenberg model



Arbitrary dimensionality of the model – analytic solution for lower dimenesionality

Ising Model

	Low T	High T	Solved
1-D			**Ising – 1925**
2-D			**Onsager – 1944**
3-D			**Proven computationally intractable - 2000**

As T increases, S increases but net magnetization decreases

Mean Field Theory (1970)

Individual particals (spin) feels average potential of environment.
Fluctuations are not explicitely considered.
Reduction of manyparticle problem to a one-particle problem.
Approximate solutions – not too good in the vicinity of critical point
advantage – can be obtained for any dimmensionality

Energy for Ising model
$$E_\nu = -\mu H \sum_i s_i - \tfrac{1}{2} \sum_{i,j} J_{ij} s_i s_j$$
J_{ij} nonzero only for neighbors

Force exerted on s_i
$$-(\partial E_\nu / \partial s_i) = \mu H + \sum_j J_{ij} s_j$$

Instatntenous field impinging on s_i
$$\mu H_i = \mu H + \sum_j J_{ij} s_j$$

Fluctuation due to its neighbors
$$\langle H_i \rangle = H + \sum_j J_{ij} \langle s_j \rangle / \mu = H + Jz \langle s_i \rangle / \mu$$

Mean valeu of s_i is the same For all spins.

Number of neighbors considered

=> H_i does not depend on the orientation but only on the mean value of s_i.

Average spin

$$\langle s_1 \rangle \approx \sum_{s_1=\pm 1} s_1 \exp\left[\beta\mu(H+\Delta H)s_1\right] \Big/ \sum_{s=\pm 1} \exp\left[\beta\mu(H+\Delta H)s\right]$$

$$\Delta H = Jz\langle s_j \rangle / \mu$$

Magnetization per particle

$$m = \langle M \rangle / N\mu = \left\langle \sum_{i=1}^{N} \mu s_i \right\rangle / N\mu$$

$$m = \tanh\left(\beta\mu H + \beta z J m\right)$$

s_i depens on H_i → SCF solution

$$T_c = 2DJ / k_B$$

MFT predicts phase transion even for 1-D model ($2J/k_B$) !!

MFT gives $T_c = 4J/k_B$ for 2-D model (Onsager 2.3)

Model can be improved in number of ways within MFT.

Renormalization group theory (1971)

Metoda for the investigation of phase transitions and other phenomena
Kenneth Wilson – 1982 Nobel prize