

Chapter 3

The Ising Model

3.1 Introduction

3.1.1 Definition of the Ising model

Given some regular lattice in d dimensions ($d=1,2,3,\dots$)
(e.g., in 3 dimensions, cubic, fcc, bcc, ...)

Ingredients:

- (i) Each lattice site carries a "Spin" $S_i = \pm 1$, i.e., a variable that can take one out of two values (not a quantum mechanical spin)
 - (ii) Cooperativity: The value of one spin influences the neighbor spins
 - (iii) Possibly an external "field" H that favors a certain value of S_i
- No kinetic degrees of freedom (momentum etc.)

$\Rightarrow$ Energy function
("Hamiltonian")

$$\mathcal{H}[\{S_i\}] = -J \sum_{\substack{\langle ij \rangle \\ \text{nearest neighbors}}} S_i S_j - H \sum_i S_i$$

Cooperativity (ii) Field (iii)

The most common choice is $J > 0$ ("ferromagnetic"),
but $J < 0$ is also possible ("antiferromagnetic").

Based on the energy function, one calculates

- The partition function $\mathcal{Z} = \sum_{\{S_i=\pm 1\}} e^{-\beta \mathcal{H}[\{S_i\}]}$
 - The free energy $F = -k_B T \ln \mathcal{Z}$
- etc.

Extensions and generalizations are possible and have been studied,

e.g., additional interactions between spins that are further apart,
anisotropic or spatially varying interactions J_{ij} or fields H_i ,
Ising models on irregular lattices or other graphs, etc.

3.1.2 Motivation

- Original motivation: Designed as simple model for magnetism, therefore "magnetic" language (spins, field, etc.)
However, the Ising model is actually not a good model for a magnetic system, since magnetic moments ("Spins") are quantum objects and three dimensional vectors ($\vec{S}$)
- Can be a good model for certain binary alloys in the context of order-disorder transitions (a "spin" $S = \pm 1$ then indicates the occupation of a lattice site with an atom of type A or B).
- The Ising model at $H = 0$ is one of the simplest model systems that exhibits a phase transition
 $\leadsto$ used to study fundamental properties of phase transitions
- Universality: Many practically important phase transitions are in the so-called "Ising universality class", e.g., the liquid-gas transition, binary mixtures, ... ($\rightarrow$ see sections ?? and ??)
- (• Historically: Has been studied extensively. Many techniques and arguments that were developed in this context are simply fun!
First case, where a non-trivial phase transition has been calculated exactly from first principles, i.e., starting from the partition function of a microscopic model)

3.1.3 History

- 1925: Introduction by Ising (in his PhD thesis, supervised by Lenz)
Model for magnetism
Exact solution in one dimension, unfortunately no phase transition :-(
(Ising believed/argued, that there would be no phase transition in higher dimensions either)
- 1934, 35: Bragg, Williams, Bethe
Took interest in Ising model as model for binary mixtures
 $\rightarrow$ Developed approximate solution methods ("mean-field approximations") that gave a phase transition
- 1936: Bethe
Argument, why there should be a phase transition in 2 dimensions
(not entirely accurate, later completed in 1964 by Griffiths)
- 1941: Kramers, Wannier
Symmetry considerations $\rightarrow$ exact expression for T_c in two dimensions
- 1944: Onsager
Exact solution in two dimensions for the case $H = 0$
(Solutions for $H \neq 0$ also became available later.)

3.1.4 Remark: Identifying phase transitions in the Ising model

Problem: For symmetry reasons, one always has $M = \langle \sum_i S_i \rangle = 0$ at $H = 0$.

→ How can one identify a phase transition then?

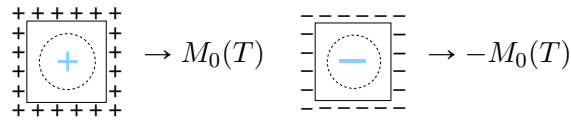
Possible approaches:

(i) Calculate free energy F and search for singularities

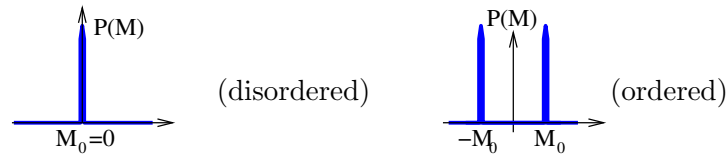
(ii) Introduce a symmetry breaking infinitesimal field $H \rightarrow 0^\pm$

Symmetry breaking phase transition: $\lim_{H \rightarrow 0^+} M(T, H) \neq \lim_{H \rightarrow 0^-} M(T, H)$

(iii) Symmetry breaking boundary conditions



(iv) Analyze histogram of M



3.2 One-Dimensional Ising Model

We first consider the one dimensional Ising chain:

$$\begin{array}{cccccccc} + & - & - & + & - & + & + & - \\ 1 & & & & & & & N \end{array} \quad \mathcal{H} = -J \sum_{i=1}^{N-1} S_i S_{i+1}$$

3.2.1 Why there cannot be a phase transition

- "Ground state" (State with lowest energy)

All Spins have the same sign, e.g., $++++++$
 Energy: $E = -J(N-1) =: E_0$

- Lowest excitation:

One "kink": $++++|- - -$

Energy: $E = -J(N-2) + J = E_0 + 2J$

$\leadsto$ Energy costs compared to ground state: $\Delta E = 2J$

$\leadsto$ Boltzmann probability of such a kink

$$P_{\text{kink}} \propto e^{-\beta \Delta E} = e^{-2\beta J}: \text{Finite number } (0 < P_{\text{kink}} < 1).$$

But: Every kink destroys the order

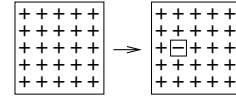
Probability, that no kink is present (i.e., order persists):

$$P_{\text{no kink}} \propto (1 - P_{\text{kink}})^{N-1} \xrightarrow{N \rightarrow \infty} 0$$

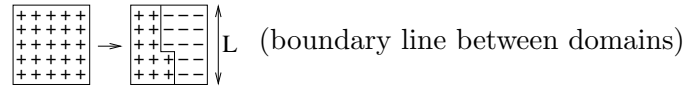
$\downarrow$
possible positions of kinks

$\Rightarrow$ Ising chain is always disordered !

NB: Argument does not work in two dimensions,
 since lowest excitation (one flipped spin)
 does not yet destroy global order



Global order is destroyed by an excitation of the form



However, the energy costs of this excitation are: $\Delta E \geq 2JL$

$$\Rightarrow P \propto e^{-2\beta LJ} \rightarrow 0 \text{ for } L \rightarrow \infty$$

3.2.2 Solution of the one-dimensional Ising model

Consider one dimensional Ising chain $\mathcal{H} = -J \sum_{i=1}^N S_i S_{i+1} - H \sum_i S_i$
with periodic boundary conditions: $S_{N+1} := S_1$

★ Free energy: Exact calculation *via* transfer matrix method

$$\begin{aligned}
 & \text{Starting point: Partition function } \mathcal{Z} = \sum_{\{S_i\}} e^{-\beta \mathcal{H}[\{S_i\}]} \\
 & \text{Notation (motivated by quantum mechanical bras and kets):} \\
 & S \triangleq |S\rangle \text{ with } S = +1 \triangleq \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad S = -1 \triangleq \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\
 & \Rightarrow e^{-\beta \mathcal{H}} = \underbrace{e^{\beta J S_1 S_2 + \beta \frac{H}{2} (S_1 + S_2)}}_{\triangleq \langle S_1 | V | S_2 \rangle} \underbrace{e^{\beta J S_2 S_3 + \beta \frac{H}{2} (S_2 + S_3)}}_{\triangleq \langle S_2 | V | S_3 \rangle} \dots \\
 & \text{with } V = \begin{pmatrix} e^{\beta J + \beta H} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J - \beta H} \end{pmatrix} \quad (\text{check by inserting!}) \\
 & \Rightarrow \mathcal{Z} = \sum_{S_1 \dots S_N} \langle S_1 | V | S_2 \rangle \dots \langle S_N | V | S_1 \rangle = \sum_{S_1} \langle S_1 | V^N | S_1 \rangle = \text{Tr}(V^N) \\
 & = \underbrace{(\lambda_1^N + \lambda_2^N)}_{\substack{\text{Eigenvalues, } \lambda_1 > \lambda_2}} = \lambda_1^N (1 + (\lambda_2/\lambda_1)^N) \xrightarrow{N \rightarrow \infty} \lambda_1^N \\
 & \Rightarrow F = -k_B T \ln \mathcal{Z} = -k_B T N \ln \lambda_1 \\
 & \text{Specifically: Eigenvalues of } V \text{ are given by} \\
 & \lambda_{1,2} = e^{\beta J} \cosh(\beta H) \pm \sqrt{e^{2\beta J} \sinh^2(\beta H) + e^{-2\beta J}} \\
 & (\text{at } H = 0: \lambda_{1,2} = e^{\beta J} \pm e^{-\beta J})
 \end{aligned}$$

$$\Rightarrow F = -k_B T N \ln \left[e^{\beta J} \cosh(\beta H) + \sqrt{e^{2\beta J} \sinh^2(\beta H) + e^{-2\beta J}} \right]$$

In particular, at $H = 0$: $F = -k_B T N \ln [2 \cosh(\beta J)]$

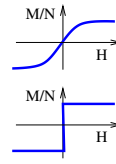
Analytical function for all temperatures $\leadsto$ No phase transition!

★ "Magnetization": $M = \langle \sum_i S_i \rangle = -\frac{\partial F}{\partial H}$

$$\begin{aligned}
 & (\text{Since: } F = -k_B T \ln \sum e^{-\beta \mathcal{H}} = -k_B T \ln (\sum e^{\beta J \sum S_i S_j + \beta H \sum S_i}) \\
 & \Rightarrow \frac{\partial F}{\partial H} = -k_B T \frac{\sum e^{-\beta \mathcal{H}} \beta \sum S_i}{\sum e^{-\beta \mathcal{H}}} = -\langle \sum S_i \rangle \checkmark)
 \end{aligned}$$

$$\Rightarrow M = \dots = N \sinh(\beta H) / \sqrt{\cosh^2(\beta H) - 1 + e^{-2\beta J}}$$

$$\left| \begin{array}{ll} \beta J \rightarrow 0 & : \quad M/N \approx \tanh(\beta H) \\ \beta J \rightarrow \infty & : \quad M/N \approx \frac{\sinh(\beta H)}{\sqrt{\sinh^2(\beta H) - \text{sign}(\beta J)}} \end{array} \right.$$



step function

$\leadsto$ "Phase transition" at $T = 0$?

★ Correlations: $G_{ij} = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle$

Specifically $H = 0 \leadsto \langle S_i \rangle = \langle S_j \rangle = 0$

$$\text{Longer calculation (homework)} \Rightarrow \boxed{G_{ij} \propto e^{-|i-j|/\xi}}$$

$$\text{with } \xi(H = 0, T) = \frac{1}{-\ln(\tanh(\beta J))} \sim e^{2\beta J} \rightarrow \infty \text{ for } \beta \rightarrow \infty$$

$\leadsto$ Correlation length ξ diverges at $T \rightarrow 0$

$\leadsto$ Characteristic feature of critical behavior

3.3 Two-Dimensional Ising Model: Exact Results

Now we discuss the two dimension Ising model at $H = 0$,

$$\mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j \quad (\text{with } \langle ij \rangle: \text{nearest neighbors})$$

In this section we will restrict ourselves to the square lattice. (Generalizations of the arguments below to other lattices are sometimes possible, but not always.)

3.3.1 Peierl's argument for the existence of a phase transition

(Peierls 1936, Griffiths 1964, Dobrushin 1965)

Idea of the argument:

- Consider Ising system $\hat{\Omega}$
with fixed boundary condition:
Surrounded by spins $S = +1$.
- Show, that for sufficiently low temperatures, there exists an $\alpha > 0$ such that, at $H = 0$, the magnetization per spin $M_{\hat{\Omega}}/N = \frac{1}{N} \langle \sum_i S_i \rangle$ is always larger than α , $M_{\hat{\Omega}}/N \geq \alpha$, independent of system size (i.e., this system has positive magnetization).
- At these temperatures, $\lim_{N \rightarrow \infty, H \rightarrow 0^+} M/N \geq \alpha$ holds generally, independent of the boundary condition. ($H \rightarrow 0^+$ is introduced to break the $S = \pm 1$ symmetry in the absence of the boundary condition.)

(Reason: Free energy $F(T, H)$)

$$\text{Magnetization at } H \rightarrow 0^+ : M = - \left(\frac{\partial F}{\partial H} \right)_{H \rightarrow 0^+}$$

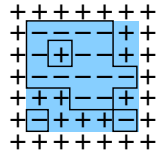
But: F is extensive (additive) at $L \rightarrow \infty$

$$\leadsto \text{Boundary only contributes with surface term to } F, F_{\text{surf}} \propto L \propto \sqrt{N}$$

$$\leadsto F_{\text{general}} = F_{\hat{\Omega}} + \mathcal{O}(L) \Rightarrow \lim_{H \rightarrow 0^+} M_{\hat{\Omega}} = \lim_{H \rightarrow 0^+} M_{\text{general}} + \mathcal{O}(L)$$

Goal therefore: Search for lower bound for $\frac{M_{\hat{\Omega}}}{N} = 1 - 2 \frac{\langle N_- \rangle}{N}$ in the system $\hat{\Omega}$ where N_- : Number of sites with $S_i = -1$

- ★ Consider some (arbitrary) configuration $\mathcal{C}$



Draw domain wall lines between spins of different sign

$\leadsto$ Lines form closed polygons

$\leadsto$ Every spin $S = -1$ lies inside at least one polygon

Label all possible polygons ($\rightarrow$ label p)

Define variables $X_p = \begin{cases} 1 & : \text{polygon } p \text{ appears in configuration } \mathcal{C} \\ 0 & : \text{otherwise} \end{cases}$

$$l_p := \text{contour length of polygon } p$$

Polygon p contains at most $(l_p/4)^2$ spins

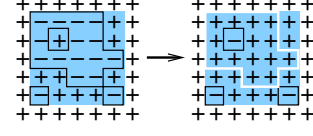
$$\Rightarrow \text{Estimate: } N_- \leq \sum_p X_p \left(\frac{l_p}{4} \right)^2$$

- ★ Also holds in the thermal average $\Rightarrow \langle N_- \rangle \leq \sum_p \langle X_p \rangle \left(\frac{l_p}{4} \right)^2$

$$\text{with } \langle X_p \rangle = \frac{\sum' e^{-\beta \mathcal{H}}}{\sum e^{-\beta \mathcal{H}}} \quad \begin{array}{l} \text{configurations } \mathcal{C} \text{ that contain polygon } p \\ \text{all configurations} \end{array}$$

- ★ Upper bound for $\langle X_p \rangle$ and $\langle N_- \rangle$

Trick: For each configuration $\mathcal{C}$ (in Σ') that contains polygon p , construct a partner configuration $\mathcal{C}^*$ by inverting all spins inside the polygon.



$$\begin{aligned} & \leadsto \text{Energy difference: } \mathcal{H}(\mathcal{C}^*) = \mathcal{H}(\mathcal{C}) - 2l_p J \\ \Rightarrow \text{Estimate: } & \sum_{\text{all confs}} e^{-\beta \mathcal{H}} \geq \sum_{\mathcal{C}^*} e^{-\beta \mathcal{H}} = e^{2l_p \beta J} \sum_{\mathcal{C}} e^{-\beta \mathcal{H}} = e^{2l_p \beta J} \sum' e^{-\beta \mathcal{H}} \\ \Rightarrow \langle X_p \rangle = & \frac{\sum' e^{-\beta \mathcal{H}}}{\sum e^{-\beta \mathcal{H}}} \leq e^{-2l_p \beta J} \end{aligned}$$

$$\Rightarrow \langle N_- \rangle \leq \sum_p e^{-2l_p \beta J} \left(\frac{l_p}{4}\right)^2 = \sum_l e^{-2l \beta J} \left(\frac{l}{4}\right)^2 \overbrace{n(l)}^{\text{number of polygons of length } l}$$

- ★ Upper bound for $n(l)$ (number of polygons of length l)

Construction of a polygon:

$$\left. \begin{array}{l} \text{First line: } 2N \text{ possibilities (+ border)} \\ \text{Second line: At most 3 possibilities} \end{array} \right\} \Rightarrow n(l) \leq 2N 3^{l-1}$$

- ★ Combine everything:

$$\begin{aligned} \langle N_- \rangle & \leq \sum_l e^{-2l \beta J} \left(\frac{l}{4}\right)^2 2N 3^{l-1} = \frac{N}{24} \sum_{l=0}^{\infty} (3e^{-2\beta J})^l l^2 = \frac{N}{24} f(3e^{-2\beta J}) \\ \text{with } f(x) = & \frac{x(1+x)}{(1-x)^3} \text{ (since: } \sum_l x^l l^2 = \frac{d^2}{d\alpha^2} \sum_l (xe^\alpha)^l \Big|_{\alpha=0} = \dots = \frac{x(1+x)}{(1-x)^3} \text{)} \\ f(x) & \text{ becomes arbitrarily small at } x \rightarrow 0: \end{aligned}$$

$$\text{For example, choose } \beta \text{ large enough } f(3e^{-2\beta J}) \leq \frac{1}{2} \Rightarrow \langle N_- \rangle \leq \frac{N}{48}$$

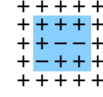
$$\Rightarrow \frac{M_{\hat{O}}}{N} = 1 - \frac{2\langle N_- \rangle}{N} \geq 1 - \frac{1}{24} \text{ independent of system size } \checkmark$$

3.3.2 Kramers-Wannier method to determine T_c

Consider Ising model, square lattice, $H = 0$:

Number of sites: N

Number of edges ("bonds"): K



This subsection: Exact method to determine T_c (under certain assumptions) based on a comparison of different series expansions of the partition function

$\leadsto$ Smart approach (fun), will also teach us about series expansions

(a) **Series Expansions** of the partition function: Two approaches

(i) Low temperature expansion

$$\star T = 0: \quad \mathcal{Z}_N = \sum_{\{S_i\}} e^{\beta J \sum_{\langle ij \rangle} S_i S_j} = e^{\beta J K}$$

$$\star T \text{ finite: } \quad \leadsto \text{Polygons } P \text{ with total contour length } l$$

$$\text{Costs: } \Delta \mathcal{H} = 2\beta J l$$

$$\mathcal{Z}_N = \sum_{\{S_i\}} e^{\beta J \sum_{\langle ij \rangle} S_i S_j} = e^{\beta J K} \sum_P e^{-2\beta J l(P)} \quad \begin{array}{l} \text{all polygon} \\ \text{configurations} \end{array} \quad \begin{array}{l} \text{summed over all polygons} \end{array}$$

(NB: Uniqueness: Polygons do not cross each other: $\square \neq \square$)

- ★ At low temperatures, the dominant contributions correspond to polygons with short contour lengths.

$$\Rightarrow \text{"Low temperature expansion": Expansion in powers of } \boxed{e^{-2\beta J}}$$

★ Construction of the coefficients (lowest order terms)

$l = 4$: $+\square+$ $\rightarrow N$ possibilities

$l = 6$: $\square\square$ $\rightarrow \frac{1}{2}N \cdot 4$ possibilities

$l = 8$: $\begin{array}{c} \square \square \\ \square\square \\ \square\square \end{array}, \begin{array}{c} \square \\ \square\square \end{array} \rightarrow \left. \begin{array}{l} \frac{1}{2}N(N-5) \\ +6N \\ +N \end{array} \right\} = \frac{1}{2}N(N+9) \text{ possibilities}$

$$\leadsto \mathcal{Z}_N = e^{\beta JK} (1 + Ne^{-2\beta J \cdot 4} + 2Ne^{-2\beta J \cdot 6} + \frac{1}{2}N(N+9)e^{-2\beta J \cdot 8} + \dots)$$

$$\Rightarrow \text{General result: } \boxed{\mathcal{Z}_N = e^{\beta JK} \sum_l \sum_{\{P\}_l} e^{-2\beta J l}}$$

Possible polygon configurations made of boundary lines
with total contour length l (all polygons)

NB: Expansion is finite ($l \leq 2N$) for finite systems

Infinite series at $N \rightarrow \infty$, possibly with convergence radius

(ii) High temperature expansion

★ $T \rightarrow \infty$ or $\beta = 0 \Rightarrow \mathcal{Z}_N = \sum_{\{S_i\}} 1 = 2^N =: \mathcal{Z}_{N,0}$

$$\begin{aligned} \star T \text{ finite: } \mathcal{Z}_N &= \sum_{\{S_i\}} e^{\beta J \sum_{\langle ij \rangle} S_i S_j} = \mathcal{Z}_{N,0} \frac{\sum_{\{S_i\}} e^{\beta J \sum_{\langle ij \rangle} S_i S_j}}{\sum_{\{S_i\}} 1} \\ &= \mathcal{Z}_{N,0} \langle e^{\beta J \sum_{\langle ij \rangle} S_i S_j} \rangle_{0\text{-average at } \beta=0} \\ &\quad \left| \begin{array}{l} e^{\beta J S_i S_j} = \cosh(\beta J) + S_i S_j \sinh(\beta J) \end{array} \right. \\ &= \mathcal{Z}_{N,0} (\cosh(\beta J))^K \langle \prod_{\langle ij \rangle} (1 + v S_i S_j) \rangle_0 \end{aligned}$$

with $v = \tanh(\beta J)$

★ At high temperatures, the dominant contributions correspond to terms of low order in $v = \tanh(\beta J)$.

$\Rightarrow$ "High temperature expansion": Expansion in powers of v

★ Construction of the coefficients: Graphical approach

Every term " $v S_i S_j$ " corresponds to a line $i-j$ along the edge $\langle ij \rangle$.

$\leadsto$ First Order: $-$; Second order: $- - + \perp$ etc.

◇ For unequal indices i, j , one has $\langle S_i^{n_1} S_j^{n_2} \rangle_0 = \langle S_i^{n_1} \rangle_0 \langle S_j^{n_2} \rangle_0$
For odd powers n , one has $\langle S_i^n \rangle_0 = 0$

$\leadsto$ Graphs with free line ends or graphs, where an odd number of lines meet at one vertex, do not contribute (e.g., first order terms: $- \triangleq \langle S_i S_j \rangle_0 = \langle S_i \rangle_0 \langle S_j \rangle_0 = 0$).

$\leadsto$ Only graphs consisting of closed polygons contribute.

◇ Lowest nonvanishing order: v^4 ($\square$)

Next orders: v^6 ($\square\square$)

v^8 ($\square\square\square + \square\square\square + \square\square\square$)

$$\Rightarrow \text{General result: } \boxed{\mathcal{Z}_N = 2^N (\cosh(\beta J))^K \sum_l \sum_{\{P\}_l} (\tanh(\beta J))^l}$$

Possible polygon configurations made of edges
with total length l (all polygons)

(b) Duality

Compare (i) and (ii): Very similar expressions

$\mathcal{Z} \triangleq$ in both cases a sum over polygon configurations,
however, different alignment with the underlying lattice

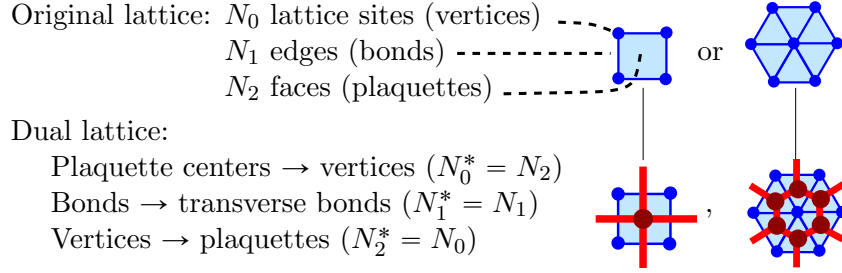
(i) Low temperature expansion

 Polygon lines perpendicular to bonds between lattice sites

(ii) High temperature expansion

 Polygon lines lie on to bonds between lattice sites

Formal relation: Dual lattice



Euler relation: $N_0 - N_1 + N_2 = N_0^* - N_1^* + N_2^* = 2$
 (NB: The outside of the graph counts as one face.)

Consequence for partition function

High temperature expansion: Polygon expansion on original lattice:

$$\mathcal{Z}_{N_0, \text{HT}}(\beta) / 2^{N_0} (\cosh(\beta J))^{N_1} = \sum_l \sum_{\{P\}_l} (\tanh(\beta J))^l$$

Low temperature expansion: Polygon expansion on dual lattice:

$$\mathcal{Z}_{N_2^*, \text{LT}}(\beta) / e^{2\beta J N_1^*} = \sum_l \sum_{\{P\}_l} (e^{-2\beta J})^l$$

$\leadsto$ Consider now an Ising model on the dual lattice with partition function $\mathcal{Z}_{N_0^*}^*$. Then the expansions of $\mathcal{Z}$, $\mathcal{Z}^*$ can be mapped onto each other: $\mathcal{Z}_{N_0^*, \text{HT}}^*(\beta^*) \propto \mathcal{Z}_{N_2^*, \text{LT}}(\beta)$

$$\text{with } \tanh(\beta^* J) = e^{-2\beta J} \Leftrightarrow \boxed{\sinh(2\beta J) \sinh(2\beta^* J) = 1}$$

$\leadsto$ Duality relation: High temperatures map onto low temperatures
 Specifically, the square lattice is self dual: $\mathcal{Z}^*(\beta^*) = \mathcal{Z}(\beta^*)$

Consequence for phase transition

Phase transition $\leftrightarrow$ Singularity of $F = -k_B T \ln \mathcal{Z}$ at $N \rightarrow \infty$

Here: $F(\beta) = -k_B T \ln \left(\sum_l \sum_{\{P\}_l} (e^{-2\beta J})^l \right) + N \cdot \text{analytic terms}$

$$F^*(\beta^*) = -k_B T \ln \left(\sum_l \sum_{\{P\}_l} (\tanh(\beta^* J))^l \right) + N \cdot \text{analytic terms}$$

$\Rightarrow$ If $F(\beta)$ is nonanalytic at β_c , then $F^*(\beta^*)$ is nonanalytic at β_c^*

Self dual lattice: $F^*(\beta^*) = F(\beta^*)$

$\Rightarrow F(\beta)$ is also nonanalytic at β_c^* , singularities come in pairs

Assume only one singularity $\Rightarrow \beta_c = \beta_c^* \Rightarrow (\sinh(2\beta_c J))^2 = 1$

$$\Rightarrow \boxed{\beta_c J = \frac{1}{2} \text{arsinh}(1) = \frac{1}{2} \ln(1 + \sqrt{2}) = 0.4407}$$

Summary and Conclusions

- We have used symmetry considerations to determine T_c without actually "solving" the Ising model (i.e., calculating the partition function)
- On this occasion, we also introduced the method of series expansions for $\beta \rightarrow 0$ and $\beta \rightarrow \infty$. They generally play an important role independent of this argument here.

Remarks

- Duality trick does not work in three dimensions, since the lattice and the dual lattice are too different
- The trick can also be used for the triangular lattice / honeycomb lattice $\leadsto$ "star-triangle transformation"

$$\text{Result: } (\tanh(\beta_c J))^{-1} = \begin{cases} 2 + \sqrt{3} & : \text{triangular lattice} \\ \sqrt{3} & : \text{honeycomb lattice} \end{cases}$$

3.3.3 Exact solution of the Ising model on the square lattice

In his original solution of the 2D Ising model, Onsager (1944) used the transfer matrix method (see Sec. 3.2.2).

Here, we present an alternative approach due to Samuel (1980), which is based on the high temperature expansion (Sec. 3.3.2) and the mathematical framework of "Grassmann variables".

For a more detailed discussion see also the book by F. Wegner:
"Supermathematics and its Applications to Statistical Physics"

We consider an Ising model with $N = L_x \times L_y$ spins on a square lattice

(1) General properties of Grassmann variables

- Symbols ξ with $\xi_i \xi_j = -\xi_j \xi_i$ ($\Rightarrow \xi_i^2 = 0$)
Application example: $\exp(\xi_i) = 1 + \xi_i$
- Generate so-called "Grassmann algebra"
with elements $A = a + \sum_i a_i \xi_i + \sum_{i,j} a_{ij} \xi_i \xi_j + \dots$
- Formally define "Integration" *via* $\int d\xi_N d\xi_{N-1} \dots d\xi_1 \xi_1 \xi_1 \dots \xi_N = 1$,
where integral becomes zero, if one of the ξ_i is missing.
 $\Rightarrow \int d\xi d\xi \exp(\xi a \bar{\xi}) = \int d\xi d\xi (1 + \xi a \bar{\xi}) = a$
 $\int d[\bar{\xi}] d[\xi] \exp(\sum_{ij} \xi_i A_{ij} \bar{\xi}_j) = \det(A)$
with $\int d[\bar{\xi}] d[\xi] := \int d\xi_N d\xi_{N-1} d\xi_{N-1} \dots d\xi_1 d\xi_1$
- Change of variables: Given a Grassmann integral $\int d[\xi] f[\xi]$
Linear substitution $\xi_i \rightarrow \theta_j = \sum_k J_{jk} \xi_k$
Then, one has (no proof): $\int d[\xi] f[\xi] = \int d[\theta] f[\xi[\theta]] \frac{1}{\det(J)}$
NB: For nonlinear substitution rules, the transformation rule may be more complicated, but we will not need that here!

(2) Strategy for solving the two dimensional Ising model (Samuel, 1980)

- ★ Starting point: High temperature expansion (Sec. 3.3.2)

$$\mathcal{Z}_N = 2^N (\cosh(\beta J))^{2N} \widehat{\mathcal{Z}}_N \text{ with } \widehat{\mathcal{Z}}_N = \sum_{\mathcal{C}_P} v^{l_P}, v = \tanh(\beta J)$$

with $\sum_{\mathcal{C}_P}$: Sum over all configurations of closed polygons

l_P : Total length of polygons

Idea: Generate sum over all polygon configurations
via Grassmann integral

- ★ Procedure

- Assign four Grassmann variables $\xi_{nm}^{(i)}$ ($i = 1 \dots 4$) to each lattice site (n, m)



- Define linker $\hat{l}$: Pairs of Grassmann variables

$$\text{Local: } \hat{e}_{nm}^{(ij)} = \xi_{nm}^{(i)} \xi_{nm}^{(j)} \text{ for } i < j \quad \cong \quad \begin{array}{c} \text{Diagram 1: A central red dot with four blue 'x' marks. Two blue arrows point from the central dot to the top and bottom 'x' marks, labeled '1' and '2'.} \\ \text{Diagram 2: A central red dot with four blue 'x' marks. Two blue arrows point from the central dot to the left and right 'x' marks, labeled '3' and '4'.} \end{array}$$

$$\text{Bond: } \begin{aligned} \hat{b}_{nm}^{(x)} &= \xi_{nm}^{(3)} \xi_{(n+1)m}^{(4)} & \begin{array}{c} \text{Diagram 1: A horizontal bond between two sites. The left site has a red dot and four blue 'x' marks. The right site has a red dot and four blue 'x' marks. A blue arrow points from the right 'x' of the left site to the left 'x' of the right site.} \\ \hat{b}_{nm}^{(y)} &= \xi_{nm}^{(1)} \xi_{n(m+1)}^{(2)} & \begin{array}{c} \text{Diagram 2: A vertical bond between two sites. The top site has a red dot and four blue 'x' marks. The bottom site has a red dot and four blue 'x' marks. A blue arrow points from the bottom 'x' of the top site to the top 'x' of the bottom site.} \end{array} \end{aligned}$$

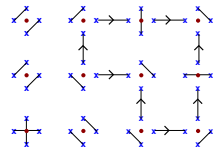
- Define "action" (quadratic in ξ)

$$S[\xi] = \sum_{nm} [v (a_x \hat{b}_{nm}^{(x)} + a_y \hat{b}_{nm}^{(y)}) + \sum_{i < j} a_{ij} \hat{e}_{nm}^{(ij)}] \equiv \sum_{\alpha} c_{\alpha} \hat{l}_{\alpha}$$

with $a_x, a_y, a_{ij} = \pm 1$ (sign to be determined below).

- Consider Grassmann integral $I = \int d[\xi] \exp(S[\xi])$
(Order: $\int d[\xi] = \int d\xi_{L_x, L_y}^{(4)} \dots d\xi_{L_x, L_y}^{(1)} \dots d\xi_{L_x-1, L_y}^{(4)} \dots d\xi_{1, L_y}^{(1)} \dots d\xi_{L_x, L_y-1}^{(4)} \dots d\xi_{L_x, 1}^{(1)}$)
 $\leadsto I$ has additive contributions from all configurations, in which $2L_x L_y$ linkers $\hat{l}_{\alpha}$ are distributed such that every position (n, m, i) is occupied by precisely one Grassmann variable.

Example:



Configurations contribute (additively)
with $\int d[\xi] \prod_{\alpha} c_{\alpha} \hat{l}_{\alpha} \propto \pm v^{l_P}$

Sign: Depends on the power of a_x, a_y, a_{ij} in I and the number of transpositions needed to sort $\prod_{\alpha} \hat{l}_{\alpha}$ by ascending $\xi_{nm}^{(i)}$

- $\Rightarrow$ - I sums automatically over all configurations with closed polygons. Free ends are not possible :-)
- Contribution of each polygon configuration is $\propto v^{l_P}$:-)
- But: Prefactor could be negative :-)

$\leadsto$ Goal: Choose $a_x, a_y, a_{ij} = \pm 1$ such that every polygon configuration has the weight v^{l_P} . Then we have $\widehat{\mathcal{Z}}_N = I$, and I can be calculated following the integration rules described in (1).

(3) Determination of coefficients a_x, a_y, a_{ij}

First consider configurations, in which polygons don't touch, i.e., don't share corners (For touching polygons see step (iii) below). Calculate their weight by rearranging, reorienting and reassigning linkers.

Notation: k_x, k_y : Number of bonds in x, y direction ($l_P = k_x + k_y$)

N_p : Number of polygons

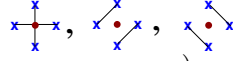
NB: Linkers commute, since they are pairs of Grassmann variables.

k_x and k_y are even, since polygons are closed.

Steps:

- (i) Calculate contribution of isolated lattice sites

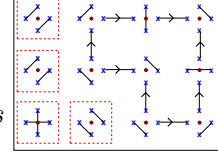
Three possibilities,



Factor: $(a_{12}a_{34} + a_{23}a_{14} - a_{13}a_{24})$ per site.

$\leadsto$ Postulate $(a_{12}a_{34} + a_{23}a_{14} - a_{13}a_{24}) \stackrel{!}{=} 1$

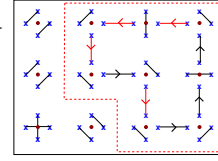
- (ii) Now consider polygons. Assemble all *bonds* belonging to same polygons together in chains.



- (iia) Reorient bonds in polygons such that they run counterclockwise.

Costs: Factor $(-1)^{(k_x+k_y)/2}$

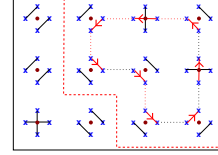
(half of all bonds must be reoriented)



- (iib) Shift linkers in polygon chains by one ξ
 $\leadsto$ New linkers are all local.

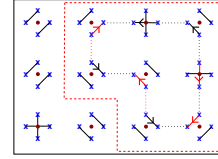
n_{ij} new linkers of the form $\hat{e}_{nm}^{(ij)}$.

Costs: $(-1)^{N_p}$ (one cyclic permutation of ξ variables per polygon)



- (iic) Reorient new linkers $\hat{e}^{(ij)}$ such that $i < j$

Costs: Factor $(-1)^{\sum_{i>j} n_{ij}}$.



- (iid) Determine weight of polygon elements:

- Bonds: $v^{l_P} a_x^{k_x} a_y^{k_y} = v^{l_P}$ (k_x, k_y even)

- Joints between bonds:

$$\begin{array}{ccccccc} \text{---} \times \text{---} & \text{---} \times \text{---} & \text{---} \times \text{---} & \text{---} \times \text{---} & \text{---} \times \text{---} & \text{---} \times \text{---} & \text{---} \times \text{---} \\ \bar{n}_{34} & \bar{n}_{12} & \bar{n}_{14} & \bar{n}_{23} & (-a_{13})\bar{n}_{24} & (-a_{24})\bar{n}_{13} & \end{array} \quad (\bar{n}_{ij} = n_{ij} + n_{ji})$$

(Sign: $\int d\xi^{(4)} d\xi^{(3)} d\xi^{(2)} d\xi^{(1)} \hat{e}^{(ij)} \hat{e}^{(kl)}$ for site with linkers $\hat{e}^{(ij)} \hat{e}^{(kl)}$)

- (ie) Summarize: Polygon configuration has weight $W v^{l_P}$ with

$$W = a_{12}^{\bar{n}_{34}} a_{34}^{\bar{n}_{12}} a_{23}^{\bar{n}_{14}} a_{14}^{\bar{n}_{23}} a_{13}^{\bar{n}_{24}} a_{24}^{\bar{n}_{13}} (-1)^{N_p + \frac{1}{2}(k_x+k_y) + \sum_{i>j} n_{ij} + \bar{n}_{24} + \bar{n}_{13}}$$

Exploit relations between $k_{x,y}$ and n_{ij} :

- Every straight polygon line has corners at both ends

$\Rightarrow$ Lines up: $k_y/2 - n_{21} = n_{24} + n_{23} = n_{41} + n_{31}$

Lines down: $k_y/2 - n_{12} = n_{42} + n_{32} = n_{14} + n_{13}$

Lines right: $k_x/2 - n_{43} = n_{41} + n_{42} = n_{13} + n_{23}$

Lines left: $k_x/2 - n_{34} = n_{14} + n_{24} = n_{31} + n_{32}$

- If one runs through a polygon in a counterclockwise way, one has four more left corners than right corners.

$\Rightarrow n_{24} + n_{32} + n_{13} + n_{41} = 4N_p + n_{42} + n_{14} + n_{31} + n_{23}$

- Collect all this:

$$n_{24} = N_p + n_{31}, n_{13} = N_p + n_{42}, n_{32} = N_p + n_{14}, n_{41} = N_p + n_{23}$$

$$\bar{n}_{14} = \bar{n}_{23}, \bar{n}_{13} = \bar{n}_{24}, k_y - \bar{n}_{12} = k_x - \bar{n}_{34} = \bar{n}_{13} + \bar{n}_{14}$$

$$\Rightarrow W = (a_{13}a_{24})^{\bar{n}_{13}} (-a_{14}a_{23})^{\bar{n}_{14}} (a_{12}a_{34})^{-\bar{n}_{13}-\bar{n}_{14}}$$

(iii) Possible choices for a_x, a_y, a_{ij} ★ Recall $|a_x| = |a_y| = |a_{ij}| = 1$

★ Further conditions from (i) and (ii)

(i) $a_{12}a_{34} + a_{23}a_{14} - a_{13}a_{24} \stackrel{!}{=} 1$

(ii) $W = (a_{13}a_{24})^{\bar{n}_{13}} (-a_{14}a_{23})^{\bar{n}_{14}} (a_{12}a_{34})^{-\bar{n}_{13}-\bar{n}_{14}} \stackrel{!}{=} 1 \quad \forall \bar{n}_{12}, \bar{n}_{14}$

$$\Rightarrow \boxed{a_{12}a_{34} = -1, \quad a_{13}a_{24} = -1, \quad a_{14}a_{23} = 1, \quad a_{x,y} = \pm 1}$$

Consistency check: What happens, if polygons touch each other?Corresponds to bond constellation  ("cross")Steps in (ii) turn this into  or  (equivalent) $\leadsto$ In W (iii), two "corners" are replaced by one "cross"

$$\begin{aligned} \begin{array}{c} \text{Two corners} \\ \text{Diagram 1} \end{array} &\cong (-a_{13})(-a_{24}) = -1 \rightarrow \begin{array}{c} \text{Cross} \\ \text{Diagram 2} \end{array} = -1 \quad \checkmark \\ \begin{array}{c} \text{Two corners} \\ \text{Diagram 3} \end{array} &\cong (a_{14})(a_{23}) = 1 \rightarrow \begin{array}{c} \text{Cross} \\ \text{Diagram 4} \end{array} = 1 \quad \checkmark \end{aligned}$$

Conclusion: Conditions (iii) make sure that I corresponds to a sum over all polygon configurations with weight v^{l_P} .

$$\Rightarrow I = \widehat{\mathcal{Z}} = \sum_{\mathcal{C}_P} v^{l_P}, \text{ hence } I \text{ can be used to calculate } \widehat{\mathcal{Z}}.$$

In practice, we still have some freedom and choose

$$\boxed{a_x = -1, \quad a_y = 1, \quad a_{12} = a_{24} = -1, \quad a_{13} = a_{14} = a_{23} = a_{34} = 1}$$

(4) Calculation of the partition function★ Remaining task: Calculate $\widehat{\mathcal{Z}}_N = \int d[\xi] \exp S[\xi]$

$$\text{with } S[\xi] = \sum_{nm} [v(a_x \hat{b}_{nm}^{(x)} + a_y \hat{b}_{nm}^{(y)}) + \sum_{i < j} a_{ij} \hat{e}_{nm}^{(ij)}] \quad (v = \tanh(\beta J))$$

and coefficients $a_{x,y}, a_{ij}$ from (3)

$$(\hat{e}_{nm}^{(ij)} = \xi_{nm}^{(i)} \xi_{nm}^{(j)}, \quad \hat{b}_{nm}^{(x)} = \xi_{nm}^{(3)} \xi_{(n+1)m}^{(4)}, \quad \hat{b}_{nm}^{(y)} = \xi_{nm}^{(1)} \xi_{n(m+1)}^{(2)})$$

★ Fourier transform: Assume periodic boundary conditions (as in 3.2.2).

Then, configurations exist where domain interfaces span the whole system, i.e., they do not form closed polygons. However, the statistical weight of such configurations decreases exponentially with increasing system size, and we will thus neglect them.

$$\text{Define } p_k = \frac{2\pi k}{L_x}, \quad q_l = \frac{2\pi l}{L_y} \text{ with } k \in [-\frac{L_x}{2}, \frac{L_x}{2}], \quad l \in [-\frac{L_y}{2}, \frac{L_y}{2}]$$

$$\text{and } \zeta_{kl}^{(i)} = \frac{1}{\sqrt{L_x L_y}} \sum_{mn} e^{-i(p_k n + q_l m)} \xi_{nm}^{(i)} \quad (\Rightarrow \xi_{-k, -l}^{(i)} = \xi_{kl}^{(i)*})$$

$$\begin{aligned} \Rightarrow \xi_{nm}^{(i)} &= \sqrt{L_x L_y}^{-1} \sum_{kl} e^{i(p_k n + q_l m)} \zeta_{kl}^{(i)} \\ \sum_{nm} \hat{e}_{nm}^{(ij)} &= \sum_{kl} \zeta_{kl}^{(i)} \zeta_{-k, -l}^{(j)} = \frac{1}{2} \sum_{kl} (\zeta_{kl}^{(i)} \zeta_{-k, -l}^{(j)} - \zeta_{kl}^{(j)} \zeta_{-k, -l}^{(i)}) \\ \sum_{nm} \hat{b}_{nm}^{(x)} &= \sum_{kl} \zeta_{kl}^{(1)} \zeta_{-k, -l}^{(3)} e^{-iq_l} = \frac{1}{2} \sum_{kl} (\zeta_{kl}^{(1)} \zeta_{-k, -l}^{(3)} e^{-iq_l} - \zeta_{kl}^{(3)} \zeta_{-k, -l}^{(1)} e^{iq_l}) \\ \sum_{nm} \hat{b}_{nm}^{(y)} &= \sum_{kl} \zeta_{kl}^{(2)} \zeta_{-k, -l}^{(4)} e^{-ip_k} = \frac{1}{2} \sum_{kl} (\zeta_{kl}^{(2)} \zeta_{-k, -l}^{(4)} e^{-ip_k} - \zeta_{kl}^{(4)} \zeta_{-k, -l}^{(2)} e^{ip_k}) \end{aligned}$$

$$\Rightarrow S = \frac{1}{2} \sum_{kl} \sum_{ij} \zeta_{kl}^{(i)} A_{ij}^{(kl)} \zeta_{-k, -l}^{(j)} = \sum'_{kl} \left(\sum_{ij} \zeta_{kl}^{(i)} A_{ij}^{(kl)} \zeta_{kl}^{(j)*} \right) =: S[\zeta, \zeta^*],$$

where $\sum'_{kl}$ sums only over half of the (kl) ,such that (kl) and $(-k, -l)$ are both fully covered

$$\text{and } A^{(kl)} = \begin{pmatrix} 0 & -1 - ve^{-iq_l} & 1 & 1 \\ 1 + ve^{iq_l} & 0 & 1 & -1 \\ -1 & -1 & 0 & 1 + ve^{-ip_k} \\ -1 & 1 & -1 - ve^{ip_k} & 0 \end{pmatrix}$$

(NB: $A_{ij}^{(kl)} = -A_{ji}^{(-k, -l)} = -A_{ji}^{(kl)*}$)

$\Rightarrow$ Partition function (using equations from (1))

$$\begin{aligned} \widehat{\mathcal{Z}}_N &= \int d[\xi] \exp S[\xi] \\ &\quad \left| \begin{array}{l} \text{(Jacobi determinant is one)} \end{array} \right. \\ &= \int d[\zeta^*] d[\zeta] \exp S[\zeta, \zeta^*] = \int d[\zeta^*] d[\zeta] \exp \left(\sum_{kl} \left(\sum_{ij} \zeta_{kl}^{(i)} A_{ij}^{(kl)} \zeta_{kl}^{(j)*} \right) \right) \\ &= \prod'_{kl} \det A^{(kl)} = \prod_{(kl)} \sqrt{\det A^{(kl)}} \\ &= \prod_{kl} \sqrt{(1 + v^2)^2 - 2v(1 - v^2)(\cos p_k + \cos q_k)} \end{aligned}$$

(5) Conclusion: Exact solution of the Ising model

Free energy: (From $\mathcal{Z}_N = 2^N (\cosh(\beta J))^{2N} \widehat{\mathcal{Z}}_N$)

$$\begin{aligned} F &= -k_B T \ln \mathcal{Z} \\ &= -N k_B T \left\{ \ln(2 \cosh^2 \beta J) + \frac{1}{2N} \sum_{kl} \ln \left[(1 + v^2)^2 - 2v(1 - v^2)(\cos p_k + \cos q_l) \right] \right\} \\ &\quad \left| \begin{array}{l} v = \tanh \beta J \end{array} \right. \\ &= -N k_B T \frac{1}{2N} \sum_{kl} \ln \left[4 \cosh^2(2\beta J) - 4 \sinh(2\beta J)(\cos p_k + \cos q_l) \right] \end{aligned}$$

Thermodynamic limit: $\sum_{kl} \rightarrow \frac{1}{(2\pi)^2} \iint_{-\pi}^{\pi} dp_x dp_y$

$$\Rightarrow \boxed{F = -N k_B T \frac{1}{8\pi^2} \iint_{-\pi}^{\pi} dp_x dp_y \ln \left[4 \cosh^2(2\beta J) - 4 \sinh(2\beta J)(\cos p_x + \cos p_y) \right]}$$

Corresponds to the result of Onsager!

Analysis:

A phase transition is expected, if the argument of $\ln[\dots]$ is zero.

$\leadsto \cosh^2(2\beta J) = \sinh(2\beta J)(\cos p_x + \cos p_y)$ for one (p_x, p_y)

$\leadsto$ Possible for $(\cos p_x + \cos p_y) = 2$, i.e., $(p_x, p_y) = (0, 0)$

Then, one has: $\cosh^2 2\beta_c J = 1 + \sinh^2 2\beta_c J \stackrel{!}{=} 2 \sinh 2\beta_c J$

$$\Rightarrow (1 - \sinh^2 2\beta_c J) = 0$$

$$\Rightarrow \beta_c J = \frac{1}{2} \operatorname{arsinh} 1 = \frac{1}{2} \ln(1 + \sqrt{2})$$

$\leadsto$ Same result as in Sec. 3.3.2!

But: from the exact solution, one can also calculate other quantities,

such as, e.g., the specific heat $\rightarrow$ Exercise

(One obtains $c \sim \ln(T - T_c)$: Logarithmic divergence)

3.4 Series Expansions: General Remarks

Last subsection (3.3.2): Introduction of the concept of series expansions – an important technique when studying phase transitions analytically

In particular, the high temperature expansion turns out to be a powerful and highly versatile tool in statistical physics.

Basic idea (in quantum mechanics notation)

- For arbitrary statistical averages (canonical ensemble), we have

$$\langle A \rangle_\beta = \frac{\text{Tr}(Ae^{-\beta H})}{\text{Tr}(e^{-\beta H})}$$
 (Classically, "Tr" refers to the suitable phase space integral or sum, e.g. in the Ising model, " $\sum_{\{S_i\}} \dots$ ", and $H \triangleq \mathcal{H}$ to the Hamiltonian.)
- Define $\mathcal{Z}_0 = \text{Tr}(1)$ and rewrite:

$$\begin{aligned} \text{Numerator of } \langle A \rangle_\beta: \quad \text{Tr}(Ae^{-\beta H}) &= \frac{1}{\mathcal{Z}_0} \langle Ae^{-\beta H} \rangle_0 \\ \text{Denominator of } \langle A \rangle_\beta: \quad \text{Tr}(e^{-\beta H}) &= \frac{1}{\mathcal{Z}_0} \langle e^{-\beta H} \rangle_0, \end{aligned}$$
 where $\langle \dots \rangle_0$: Statistical average at $\beta = 0$ ($T \rightarrow \infty$)
- Then expand $\langle A \rangle_\beta = \frac{\langle Ae^{-\beta H} \rangle_0}{\langle e^{-\beta H} \rangle_0}$ in powers of β

$$(e^{-\beta H} = 1 - \beta H + \frac{1}{2}\beta^2 H^2 + \dots)$$

Leading terms:

$$\begin{aligned} \langle A \rangle_\beta &= \frac{\langle A \rangle_0 - \beta \langle AH \rangle_0 + \frac{1}{2}\beta^2 \langle AH^2 \rangle_0 + \dots}{1 - \beta \langle H \rangle_0 + \frac{1}{2}\beta^2 \langle H^2 \rangle_0 + \dots} \\ &= \langle A \rangle_0 - \beta (\langle AH \rangle_0 - \langle A \rangle_0 \langle H \rangle_0) \\ &\quad + \frac{1}{2}\beta^2 (\langle AH^2 \rangle_0 - 2\langle AH \rangle_0 \langle H \rangle_0 - \langle A \rangle_0 \langle H^2 \rangle_0 + 2\langle A \rangle_0 \langle H \rangle_0^2) \\ &\quad + \mathcal{O}(\beta^3) \end{aligned}$$

Free energy ($\beta F = -\ln(\text{Tr}(e^{-\beta H}))$) can be expanded analogously.

Very general approach

Low temperature expansions are also possible (see, e.g., Sec. 3.3.2), but the design principles are less generic (Setting up such an expansion requires the knowledge of the elementary excitations in the system).

General remarks on series expansions

- In general, graphical methods are useful for the construction, see, e.g., the graphical expansions in Sec. 3.3.2 in polygon configurations (The "diagrams" of the expansion are the polygon configurations.)
- Simplifications can often be identified beforehand based on general considerations (e.g., symmetry considerations).
- Important example: **Linked Cluster Theorem**: Only connected diagrams (configurations with connected polygons) contribute to $F \propto \ln \mathcal{Z}$, diagrams with unconnected components cancel out.
 (Heuristic "proof": Every unconnected component comes with a combinatorial factor $\propto N$. However, F is extensive, therefore, they must all cancel each other!)

Analysis of series expansions

Starting point: Series $f(z) = \sum_n a_n z^n$

Only a finite number of coefficients are known.

Question: Assume that $f(z)$ has a singularity, $f(z) \sim (z - z_c)^{-\gamma}$

What can we learn from the series about the singularity?

Example: Consider simple function $f(z) = (1 - z/z_c)^{-\gamma}$ (with $\gamma > 1$)

$\Rightarrow$ Expansion $f(z) = \sum_n \binom{-\gamma}{n} \left(\frac{-1}{z_c}\right)^n z^n$

$$\Rightarrow a_n = \left(\frac{1}{z_c}\right)^n (-1)^n \binom{-\gamma}{n} = \left(\frac{1}{z_c}\right)^n \frac{\gamma(\gamma+1)\cdots(\gamma+n-1)}{n!}$$

$$\Rightarrow \frac{a_n}{a_{n-1}} = \frac{1}{z_c} \frac{\gamma+n-1}{n} = \frac{1}{z_c} \left(1 + \frac{\gamma-1}{n}\right)$$

$\Rightarrow$ Possible strategies for determining z_c :

- Simply plot $r_n = \frac{a_n}{a_{n-1}}$ versus $\frac{1}{n} \leadsto$ Axis intercept gives $1/z_c$!
(Generally, $\lim_{n \rightarrow \infty} \frac{a_{n-1}}{a_n}$ gives the radius of convergence of the series. Therefore, this method works, if the convergence radius is determined by the singularity at z_c)
- More efficient method: Eliminate term $\frac{\gamma-1}{n}$ in our example by choosing $r_n = n \frac{a_n}{a_{n-1}} - (n-1) \frac{a_{n-1}}{a_{n-2}}$
(Gives $r_n \equiv \frac{1}{z_c}$ in our example. In general, corrections apply.)
- There exist numerous other, much more sophisticated approaches, e.g., Padé approximants. Analyzing series expansions is an art in itself

If z_c is known, similar techniques can be applied to determine γ .

For example, a simple estimator is $S_n = 1 + n\left(\frac{a_n}{a_{n-1}} z_c - 1\right)$

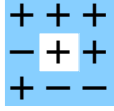
3.5 Mean-Field Approximation

Often less involved than series expansions, more general approach, not restricted to regions without singularities. "Sufficient" for many purposes.

But: Uncontrolled approximation

3.5.1 Simplest approach: Spins in mean fields

3.5.1.1 Approach *via* effective field (intuitive approach)



$$\mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j - H \sum_i S_i$$

nearest neighbors

$$\text{Interactions} \leftrightarrow \text{Effective field } H_{\text{eff}}^i = -\frac{\partial \mathcal{H}}{\partial S_i} = H + J \sum_j S_j$$

Mean-field approximation: Replace S_j by $\langle S \rangle = m$.

$$H_{\text{eff}} = H + Jqm, \text{ with } q: \text{coordination number (cubic lattice: } 2 \cdot D)$$

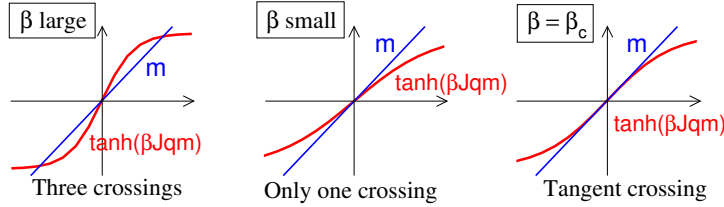
Consider single spin in the external field H_{eff} : $\mathcal{H}_{\text{eff}}^{(i)} = -H_{\text{eff}} S$

$$\leadsto \text{Partition function } \mathcal{Z} = e^{\beta H_{\text{eff}}} + e^{-\beta H_{\text{eff}}}$$

$$\text{Magnetization: } m = \frac{e^{\beta H_{\text{eff}}} - e^{-\beta H_{\text{eff}}}}{e^{\beta H_{\text{eff}}} + e^{-\beta H_{\text{eff}}}} = \tanh(\beta H_{\text{eff}})$$

$$\Rightarrow \text{Implicit, self consistent equation for } m: \boxed{m = \tanh(\beta(Jqm + H))}$$

At $H = 0$, the equation can be solved graphically:



At the critical point $\beta = \beta_c$

$\Rightarrow$ Only one crossing point, but slopes are equal

$$\Rightarrow \left. \frac{d}{dm} \tanh(\beta_c Jqm) \right|_{m=0} = \left. \frac{d}{dm} m \right|_{m=0} = 1$$

$$\Rightarrow \boxed{\beta_c Jq = 1}$$

Close to the critical point, $\tanh(\dots)$ can be expanded in powers of m .

$$\Rightarrow m = \tanh(\beta Jqm) \approx \beta Jqm - \frac{1}{3}(\beta Jq)^3 m^3 + \dots$$

$$\Rightarrow m(T) \approx \sqrt{3(\beta Jq - 1)/(\beta Jq)^3} = \sqrt{3 \frac{T}{T_c}} \sqrt{1 - \frac{T}{T_c}} \propto (T_c - T)^{1/2}$$

$$\Rightarrow \text{Critical exponent } \beta: \beta = 1/2$$

Within this approach, one can calculate the spontaneous magnetization and the susceptibility, but not the entropy or the free energy.

3.5.1.2 Approach *via* free energy (Bragg-Williams approximation)

Starting point: Free energy $F = U - T\mathcal{S}$

"Mean-field" approximation: Spins are not correlated:

$\leadsto$ Joint probability function factorizes: $P(S_1, S_2, \dots, S_N) \approx \prod_{j=1}^N p^{(1)}(S_j)$
with $p^{(1)}(S)$: probability distribution for single spin

$$\begin{aligned} \text{(a) Energy: } \frac{1}{N}U &= \frac{1}{N}\langle \mathcal{H} \rangle = \frac{1}{N}\left\langle -J \sum_{\langle ij \rangle} S_i S_j - H \sum_i S_i \right\rangle \\ &\approx \frac{1}{N}\left(-J \sum_{\langle ij \rangle} \langle S_i \rangle \langle S_j \rangle - H \sum_i \langle S_i \rangle \right) = -\frac{1}{2}Jq m^2 - H m \end{aligned}$$

$$\begin{aligned} \text{(b) Entropy: } \mathcal{S} &= -k_B \sum_{\{S_1, \dots, S_N\}} P(S_1, \dots, S_N) \ln(P(S_1, \dots, S_N)) \\ &\approx -k_B N \sum_S p^{(1)}(S) \ln p^{(1)}(S) \end{aligned}$$

Given magnetization m , uncorrelated spins S_j

$\leadsto$ Construct probability function $p^{(1)}(S)$ such that $\langle S \rangle = m$

Notation: $p_+^{(1)} := p^{(1)}(+1)$, $p_-^{(1)} := p^{(1)}(-1)$

$$\Rightarrow \langle S \rangle = p_+^{(1)} - p_-^{(1)} \text{ and } p_+^{(1)} + p_-^{(1)} = 1$$

$$\Rightarrow \langle S \rangle = 2p_+^{(1)} - 1$$

$$\Rightarrow p_+^{(1)} = (1+m)/2, \quad p_-^{(1)} = (1-m)/2$$

$$\begin{aligned} \Rightarrow \frac{1}{N}\mathcal{S} &= -k_B (p_+^{(1)} \ln p_+^{(1)} + p_-^{(1)} \ln p_-^{(1)}) \\ &= k_B \left[-\frac{1+m}{2} \ln \frac{1+m}{2} - \frac{1-m}{2} \ln \frac{1-m}{2} \right] \end{aligned}$$

$$\Rightarrow \text{Free energy: } \frac{F}{N} = -\frac{1}{2}Jqm^2 - Hm + k_B T \left[\frac{1+m}{2} \ln \frac{1+m}{2} + \frac{1-m}{2} \ln \frac{1-m}{2} \right]$$

$$\text{Minimization: } \frac{\partial F}{\partial m} = -qJm - H + k_B T \frac{1}{2} \ln \left(\frac{1+m}{1-m} \right) \stackrel{!}{=} 0$$

$$\Rightarrow \boxed{\ln \left(\frac{1+m}{1-m} \right) = 2\beta(qJm + H)} \Rightarrow \boxed{m = \tanh \beta(qJm + H)}$$

$\leadsto$ Approximation equivalent to the approximation of 3.5.1.1

3.5.1.3 Problems with this mean-field approximation

– Geometry enters only *via* coordination number q

$\leadsto$ no dependence on dimension, local structure etc.

– Predicts a phase transition also for one dimensional Ising model (clearly wrong)

– Wrong critical point T_c , wrong critical exponents

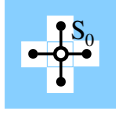
Example: Two dimensional Ising model on the square lattice:

$$\text{Mean-field} \rightarrow \beta_c J = \frac{1}{q}, \quad \text{Critical exponent } \beta = 1/2$$

$$\begin{aligned} \text{Exact} \quad \rightarrow \quad \beta_c J &= \frac{1}{q} 2 \ln(1 + \sqrt{2}) = \frac{1}{q} \cdot 1.76 \\ \text{Critical exponent } \beta &= 1/8 \end{aligned}$$

3.5.2 Improved theory: Clusters in mean fields

3.5.2.1 Approach *via* effective field (Bethe approximation)



Cluster with central particle "0"

$$\Rightarrow \mathcal{H}_{\text{Cluster}} = -J S_0 \sum_{j=1}^q S_j - H_{\text{eff}} \sum_{j=1}^q S_j$$

(Effective field H_{eff} acts on outer spins only
Central spin is treated exactly)

$$\Rightarrow \mathcal{Z}_{\text{Cluster}} = \left(e^{\beta(J+H_{\text{eff}})} + e^{-\beta(J+H_{\text{eff}})} \right)^q : \text{Contribution of } S_0 = +1$$

$$+ \left(e^{\beta(-J+H_{\text{eff}})} + e^{-\beta(-J+H_{\text{eff}})} \right)^q : \text{Contribution of } S_0 = -1$$

$$\langle S_0 \rangle = \frac{1}{\mathcal{Z}_{\text{Cluster}}} \left[\left(e^{\beta(J+H_{\text{eff}})} + e^{-\beta(J+H_{\text{eff}})} \right)^q - \left(e^{\beta(-J+H_{\text{eff}})} + e^{-\beta(-J+H_{\text{eff}})} \right)^q \right]$$

$$\langle S_j \rangle = \frac{1}{\mathcal{Z}_{\text{Cluster}}} \left[\left(e^{\beta(J+H_{\text{eff}})} + e^{-\beta(J+H_{\text{eff}})} \right)^{q-1} \cdot \left(e^{\beta(J+H_{\text{eff}})} - e^{-\beta(J+H_{\text{eff}})} \right) \right. \\ \left. + \left(e^{\beta(-J+H_{\text{eff}})} + e^{-\beta(-J+H_{\text{eff}})} \right)^{q-1} \cdot \left(e^{\beta(-J+H_{\text{eff}})} - e^{-\beta(-J+H_{\text{eff}})} \right) \right]$$

$$\leadsto \text{Condition for } H_{\text{eff}}: \quad \langle S_0 \rangle \stackrel{!}{=} \langle S_j \rangle (= m)$$

$$\Rightarrow \boxed{\frac{\cosh \beta(J + H_{\text{eff}})}{\cosh \beta(-J + H_{\text{eff}})} = e^{2\beta H_{\text{eff}}/(q-1)}}$$

Solutions:

- (i) $H_{\text{eff}} = 0$: Disordered state
- (ii) $H_{\text{eff}} \neq 0$ (if β is not too small): Ordered state

Transition point: Expand about small H_{eff}

$$\leadsto \left[\frac{\cosh \beta(J+H_{\text{eff}})}{\cosh \beta(-J+H_{\text{eff}})} \approx 1 + 2\beta H_{\text{eff}} \tanh \beta J \right] \stackrel{!}{=} \left[e^{2\beta H_{\text{eff}}/(q-1)} \approx 1 + 2\beta \frac{H_{\text{eff}}}{(q-1)} \right]$$

$$\Rightarrow \boxed{\coth(\beta_c J) = q - 1} \quad \Rightarrow \quad \boxed{2\beta_c J = \ln \left(\frac{q}{q-2} \right)}$$

Remarks:

- In one dimensions, one has $q = 2 \leadsto$ no phase transition ✓
- Two dimensional Ising model on the square lattice:
 - Exact: $\beta_c J = 0.44$
 - Bragg-Williams: $\beta_c J = 1/4 = 0.25$
 - Bethe: $\beta_c J = \ln(2) = 0.35$: Significant improvement!
- Higher coordination numbers:
 - Bragg-Williams: $2\beta_c J = 2/q$
 - Bethe: $2\beta_c J = \ln \frac{q}{q-2} = -\ln(1 - 2/q) = 2/q + \dots$
 - $\leadsto$ Bragg-Williams and Bethe approximation agree at lowest order of $1/q$. Results are never identical!
- Critical exponents in Bethe and Bragg-Williams approximation are the same: No improvement in this respect.

3.5.2.2 Approach *via* free energy (Guggenheim approximation)

Main approximation in Bragg-Williams theory: Independent spins

Guggenheim approximation: Independent clusters, neglect cluster correlations

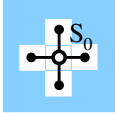
→ Improved treatment of pairs of neighbor spins

→ Improved treatment of pairs of neighbor spins

- Probability for one single cluster:

$$p_{\text{cluster}}(S_0; \{S_j\}) = p^{(1)}(S_0) \prod_{j=1}^q P(S_0 S_j | S_0)$$

conditional probability for $(S_0 S_j)$ given S_0

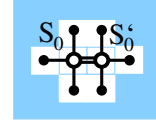


$P(S_0 S_j | S_0) = p^{(2)}(S_0 S_j) / p^{(1)}(S_0)$
 with $p^{(2)}(S_0 S_j)$: Pair probability

$$= p^{(1)}(S_0) \prod_{j=1}^q \frac{p^{(2)}(S_0 S_j)}{p^{(1)}(S_0)}$$

- Two neighbor clusters: Must correct for double counting of bonds

$$\begin{aligned} &\leadsto p_{\text{cluster}}(S_0; \{S_j\}) P_{\text{cluster}}(S'_0; \{S_j\} | (S_0 S'_0)) \\ &= p_{\text{cluster}}(S_0; \{S_j\}) p_{\text{cluster}}(S'_0; \{S_j\}) / p^{(2)}(S_0 S'_0) \end{aligned}$$



→ Whole system:

$$P(S_1, \dots, S_N) \approx \prod_{\langle ij \rangle} p^{(2)}(S_i S_j) / \prod_i p^{(1)}(S_i)^{q-1}$$

Construct probability functions such that $\langle S \rangle = m$

$$\begin{aligned} \text{Notation: } p_{\pm}^{(1)} &:= p^{(1)}(\pm 1), \quad p_{\pm\pm}^{(2)} := p^{(2)}(\pm 1, \pm 1), \quad p_{+-}^{(2)} = p_{-+}^{(2)} =: a \\ \Rightarrow p_{++}^{(1)} &= p_{++}^{(2)} + p_{+-}^{(2)} = \frac{1+m}{2}, \quad p_{--}^{(1)} = p_{--}^{(2)} + p_{+-}^{(2)} = \frac{1-m}{2} \\ \Rightarrow p_{++}^{(2)} &= \frac{1+m}{2} - a, \quad p_{--}^{(2)} = \frac{1-m}{2} - a \end{aligned}$$

$$\Rightarrow \text{Entropy: } \mathcal{S} = \sum_{\{S_1, \dots, S_N\}} P(S_1, \dots, S_N) \ln P(S_1, \dots, S_N)$$

$$\begin{aligned} \Rightarrow \frac{1}{N} \mathcal{S} &\approx -k_B \left(\frac{q}{2} \sum_{SS'} p^{(2)}(SS') \ln p^{(2)}(SS') - (q-1) \sum_S p^{(1)}(S) \ln p^{(1)}(S) \right) \\ &= -k_B \left\{ \frac{q}{2} \left[\left(\frac{1+m}{2} - a \right) \ln \left(\frac{1+m}{2} - a \right) + \left(\frac{1-m}{2} - a \right) \ln \left(\frac{1-m}{2} - a \right) \right. \right. \\ &\quad \left. \left. + 2a \ln a \right] - (q-1) \left[\left(\frac{1+m}{2} \right) \ln \left(\frac{1+m}{2} \right) + \left(\frac{1-m}{2} \right) \ln \left(\frac{1-m}{2} \right) \right] \right\} \end{aligned}$$

$$\text{Energy: } \frac{1}{N} U = \frac{1}{N} \langle \mathcal{H} \rangle = -J \frac{q}{2} [(p_{++}^{(2)} + p_{--}^{(2)}) - (p_{+-}^{(2)} + p_{-+}^{(2)})] = J \frac{q}{2} (4a - 1)$$

$$\text{Free energy: } F = U - \frac{1}{\beta} \mathcal{S}$$

$$\text{Minimize free energy: } \frac{\partial F}{\partial a} \stackrel{!}{=} 0, \quad \frac{\partial F}{\partial m} \stackrel{!}{=} 0$$

$$\begin{aligned} \bullet \quad \frac{1}{N} \frac{\partial F}{\partial a} &= 2qJ + \frac{1}{\beta} \frac{q}{2} \left[2 \ln(2a) - \ln((1+m-2a)(1-m-2a)) \right] \stackrel{!}{=} 0 \\ \Rightarrow \quad &\boxed{4\beta J = \ln \left(\frac{(1+m-2a)(1+m+2a)}{(2a)^2} \right)} \quad (i) \end{aligned}$$

$$\begin{aligned}
& \bullet \frac{1}{N} \frac{\partial F}{\partial m} = \frac{1}{\beta} \left[\frac{q}{4} \ln \frac{1+m-2a}{1-m-2a} - \frac{q-1}{2} \ln \frac{1+m}{1-m} \right] \stackrel{!}{=} 0 \\
& \Rightarrow \boxed{\frac{q}{2} \ln \left(\frac{1+m-2a}{1-m-2a} \right) = (q-1) \ln \left(\frac{1+m}{1-m} \right)} \quad (\text{ii})
\end{aligned}$$

Critical point: $m \rightarrow 0$

$$(\text{ii}) \Rightarrow \left[\frac{q}{2} \ln \left(1 + \frac{2m}{1-2a} \right) \approx \frac{q}{2} \frac{2m}{1-2a} \right] \stackrel{!}{=} \left[(q-1) \ln(1+2m) \approx (q-1)2m \right]$$

$$\Rightarrow 2a = \frac{q-2}{2(q-1)}, \quad 1-2a = \frac{q}{2(q-1)}$$

$$(\text{i}): \Rightarrow 4\beta_c J = 2 \ln \frac{1-2a}{2a} = 2 \ln \frac{q}{q-2} \quad \Rightarrow \quad \boxed{2\beta_c J = \ln \left(\frac{q}{q-2} \right)}$$

Remarks:

- Same result as in Bethe approximation ✓
- Systematic generalization to larger clusters is possible
 $\leadsto$ Cluster variation method
 Popular method in the context of order/disorder phase transitions
 For large clusters: Very good phase diagrams
 But still: wrong critical behavior (see next chapter)

3.5.3 Critical behavior in mean-field theory

As already mentioned earlier, one often observes critical behavior at continuous transitions: Many properties exhibit singularities when plotted against intensive variables such as temperature and magnetic field, which are often characterized by power laws.

At a qualitative level, the same behavior can already be seen in mean-field approximation. This will be shown in the present section.

Preview (defining $t = (T - T_c)/T_c$ and d : Spatial dimension)

<u>Quantity</u>	<u>Expo- nent</u>	<u>Power law</u>	<u>Value</u>		
			Mean-field	Ising exact 2D	3D
Magnetization m	β δ	$m \sim (-t)^\beta$ $m^\delta \sim H$ at $t = 0$	$\beta = 1/2$ $\delta = 3$	1/8 15	0.33 4.8
Susceptibility $\chi = \frac{\partial m}{\partial H}$	γ	$\chi \sim t ^{-\gamma}$	$\gamma = 1$	7/4	1.24
Specific heat $c_H = T \left(\frac{\partial S}{\partial T} \right)_H = \left(\frac{\partial E}{\partial T} \right)_H$	α	$c_H \sim t ^{-\alpha}$	$\alpha = 0$	0(log)	0.1
Correlations $G_{ij} = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle$ $=: G(\vec{r}_i - \vec{r}_j)$	η	$G(\vec{r}) \sim r^{2-d-\eta}$ at $t = 0$	$\eta = 0$	1/4 1/4	0.04 0.04
Correlation length $G(\vec{r}) \sim e^{-r/\xi}$	ν	$\xi \sim t ^{-\nu}$	$\nu = 1/2$	1	0.63

Calculation: In Bragg-Williams approximation

Bethe-Guggenheim calculation shall not be shown here, but the results are the same. In the next section we will see, why.

$$\text{Define } \boxed{h = \beta H} \quad \text{and} \quad \boxed{t = (T - T_c)/T_c = \beta_c/\beta - 1}$$

with $\beta_c = 1/qJ$ (q : Coordination number)

3.5.3.1 Magnetization

Starting point: (see Sec. 3.5.1.2): $m = \tanh \beta(qJm + H) = \tanh(\frac{\beta}{\beta_c}m + h)$

At $|t|, |h| \ll 1$, one has $|m| \ll 1$ and hence $m \approx \frac{\beta}{\beta_c}m + h - \frac{1}{3}(\frac{\beta}{\beta_c}m + h)^3$

Consider limit $t \rightarrow 0^-$, $h = 0$

$$\begin{aligned} \Rightarrow m &\approx \frac{\beta}{\beta_c}m - \frac{1}{3}(\frac{\beta}{\beta_c}m)^3 \\ \Rightarrow \frac{\beta}{\beta_c}m &= \sqrt{3}(-t)^{1/2} \quad \Rightarrow \quad m \sim (-t)^{1/2} \quad \Rightarrow \quad \boxed{\beta = 1/2} \end{aligned}$$

Consider limit $t = 0$, $h \rightarrow 0$ (i.e., $\beta/\beta_c = 1$)

$$\begin{aligned} \Rightarrow m &\approx m + h - \frac{1}{3}(m + h)^3 \\ \Rightarrow h &\approx \frac{1}{3}m^3 + \mathcal{O}(m^2h, mh^2) \quad \Rightarrow \quad h \sim m^3 \quad \Rightarrow \quad \boxed{\delta = 3} \end{aligned}$$

3.5.3.2 Susceptibility

Starting point: Same as before in Section 3.5.3.1

Consider limit $t \rightarrow 0$, $h \rightarrow 0$

$$\begin{aligned} \text{Define } g(m, h) &:= \tanh(\frac{\beta}{\beta_c}m + h) - m \approx m(\frac{\beta}{\beta_c} - 1) + h - \frac{1}{3}(\frac{\beta}{\beta_c}m)^3 \\ \Rightarrow g(m, h) &\equiv 0 \quad \Rightarrow \quad \frac{\partial m}{\partial h}\Big|_t = -\frac{\frac{\partial g}{\partial h}}{\frac{\partial g}{\partial m}} \\ \text{with } \frac{\partial g}{\partial h} &= 1, \quad \frac{\partial g}{\partial m} = (\frac{\beta}{\beta_c} - 1) - \frac{\beta}{\beta_c}(\frac{\beta}{\beta_c}m)^2 = -\frac{\beta}{\beta_c}(t + (\frac{\beta}{\beta_c}m)^2) \\ \Rightarrow \frac{\partial m}{\partial h}\Big|_t &= \frac{\frac{\beta_c}{\beta}}{t + (\frac{\beta}{\beta_c}m)^2} = \frac{\beta_c}{\beta} \begin{cases} t^{-1} & : t > 0 \ (m = 0) \\ (-2t)^{-1} & : t < 0 \ ((\frac{\beta}{\beta_c}m)^2 = -3t) \end{cases} \\ &\Rightarrow \quad \boxed{\gamma = 1} \end{aligned}$$

3.5.3.3 Specific heat

Starting point: $U = \langle \mathcal{H} \rangle = -J \sum_{\langle ij \rangle} \langle S_i \rangle \langle S_j \rangle = -NJ \frac{q}{2} m^2 = -N \frac{1}{2\beta_c} m^2$

$$\begin{aligned} \text{with } m^2 &= \begin{cases} 0 & : T > T_c \\ (-t)3\frac{\beta_c}{\beta} = \frac{(T-T_c)}{T_c} (\frac{T}{T_c})^2 & : T < T_c \end{cases} \\ \Rightarrow c_H &= \frac{\partial U}{\partial T}\Big|_H = \begin{cases} 0 & : T > T_c \\ -\frac{N}{2}k_B & : T \lesssim T_c \end{cases} \quad \text{with } (T \rightarrow T_c^-) \end{aligned}$$

Consider limit $t \rightarrow 0$: Finite jump $\Rightarrow \boxed{\alpha = 0}$

3.5.3.4 Correlation functions

Less straightforward, since correlations are ignored in mean-field theory.

Starting point: Consider Ising model at $H = 0$, regular lattice with simple unit cell and lattice vectors $\vec{r}_i$, d dimensions, periodic boundary conditions. The interaction range is characterized by a set of neighbor vectors $\{\vec{\tau}\}$, i.e., spins S_i, S_j interact if $\vec{r}_{ij} := (\vec{r}_j - \vec{r}_i) \in \{\vec{\tau}\}$. NB: If τ is a neighbor vector, then $(-\tau)$ is a neighbor vector as well.

Goal: Calculate $G(\vec{r}_{ij}) = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle$

Trick: Use general relation between fluctuations and susceptibilities

Consider generally an energy function of the form B : $\mathcal{H} = \mathcal{H}_0 - H_B B$

Then we have the general relation $\langle AB \rangle - \langle A \rangle \langle B \rangle = \frac{1}{\beta} \frac{\partial \langle A \rangle}{\partial H_B}$

$$\begin{aligned} (\text{Proof: } \langle A \rangle &= \frac{1}{\mathcal{Z}} \sum_{\text{Configurations}} e^{-\beta \mathcal{H}} A = \frac{\sum e^{-\beta \mathcal{H}_0 + \beta H_B B} A}{\sum e^{-\beta \mathcal{H}_0 + \beta H_B B}} \\ \Rightarrow \frac{\partial \langle A \rangle}{\partial H_B} &= \frac{\mathcal{Z} \sum e^{-\beta \mathcal{H}_0 + \beta H_B B} \beta B A - (\sum e^{-\beta \mathcal{H}_0 + \beta H_B B} \beta B) (\sum e^{-\beta \mathcal{H}_0 + \beta H_B B} A)}{\mathcal{Z}^2} \\ &= \beta \langle AB \rangle - \beta \langle A \rangle \langle B \rangle \quad \checkmark) \end{aligned}$$

Of course also valid in the case $H_B = 0$

Here: Consider $\mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j - \sum_i H_i S_i$

$\leadsto$ Inhomogeneous system with $\langle S_i \rangle = m_i$ different for all i

Solution as before: $m_i = \tanh(\beta(J \sum_{\text{neighbors } j \text{ of } i} m_j + H_i))$

Can be evaluated $\Rightarrow G_{\vec{r}_{ij}} = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle = \frac{1}{\beta} \frac{\partial m_i}{\partial H_j} \Big|_{h_k=0 \forall k}$

Solution for $T \geq T_c$:

$$G(\vec{r}) = \frac{1}{(2\pi)^d} \int_{\text{1st Brillouin zone}} d^d k \frac{1}{1 - \beta J \sum_{\vec{\tau}} \cos(\vec{k} \cdot \vec{\tau})} e^{i\vec{k} \cdot \vec{r}}$$

(Calculation:

First linearize: $m_i = \tanh(\beta(J \sum_{\text{neighbors}} m_j + H_i)) \approx \beta(J \sum_{\text{neighbors}} m_j + H_i)$

$$\Rightarrow \sum_j B_{ij} m_j = H_i \text{ with } B_{ij} = \frac{1}{\beta} \delta_{ij} - \begin{cases} J & : \vec{r}_{ij} \in \{\vec{\tau}\} \\ 0 & : \text{otherwise} \end{cases}$$

$$\Rightarrow m_i = \sum_j (B^{-1})_{ij} H_j \Rightarrow G(\vec{r}_{ij}) = \frac{1}{\beta} \frac{\partial m_i}{\partial H_j} = \frac{1}{\beta} (B^{-1})_{ij}$$

Then diagonalize and invert B by Fourier transform. Define $B_{ij} =: B(\vec{r}_{ij})$

$$\Rightarrow \tilde{B}(\vec{k}) = \sum_{\text{lattice vectors } \vec{r}} e^{-i\vec{k} \cdot \vec{r}} B(\vec{r}) = \frac{1}{\beta} - J \sum_{\vec{\tau}} \cos(\vec{k} \cdot \vec{\tau})$$

$$\Rightarrow \frac{1}{\beta} (B^{-1})_{ij} = \frac{1}{(2\pi)^d} \int d^d k (\beta \tilde{B}(\vec{k}))^{-1} e^{i(\vec{r}_i - \vec{r}_j) \cdot \vec{k}} \quad \checkmark)$$

Simplification for $t \rightarrow 0+$:

$$G(\vec{r}) = \frac{1}{(2\pi)^d} \int_{\infty} d^d k \frac{\beta_c / \beta}{t + k^2 v(\vec{e}_k)} e^{i\vec{k} \cdot \vec{r}}$$

$$\text{with } \vec{e}_k = \frac{\vec{k}}{k} \text{ and } v(\vec{e}) = \frac{1}{2q} \sum_{\vec{\tau}} (\vec{e} \cdot \vec{\tau})^2$$

(Calculation:

$$\text{Rewrite } B(\vec{k}) = \frac{1}{\beta_c} \left(t - \frac{1}{q} \sum_{\vec{\tau}} (1 + \cos(\vec{k} \cdot \vec{\tau})) \right)$$

$t \rightarrow 0$: Main contribution to integral stems from small $\vec{k}$!

$$\Rightarrow \text{Expand } \left[t + \frac{1}{q} \sum_{\vec{\tau}} (1 - \cos(\vec{k} \cdot \vec{\tau})) \right] \approx \left[t + k^2 v(\vec{e}_k) \right] \quad \checkmark)$$

Consider $t = 0$

$$\begin{aligned} \Rightarrow G(\vec{r}) &= \frac{1}{(2\pi)^d} \frac{\beta_c}{\beta} \int_{\infty} d^d k \frac{1}{k^2 v(\vec{e}_{\vec{k}})} e^{i\vec{k} \cdot \vec{r}} \stackrel{\vec{k}=\vec{k}r}{=} \underbrace{\frac{1}{(2\pi)^d} \frac{\beta_c}{\beta} \int_{\infty} d^d \tilde{k} \frac{1}{\tilde{k}^2 v(\vec{e}_{\tilde{k}})} e^{i\tilde{k} \cdot \vec{e}_{\vec{r}}} }_{\text{independent of } r} r^{2-d} \\ \Rightarrow \boxed{G(\vec{r}) \sim r^{2-d};} &\quad \Rightarrow \quad \boxed{\eta = 0} \end{aligned}$$

Now consider case $t \rightarrow 0$

$$\Rightarrow G(\vec{r}) = \frac{1}{(2\pi)^d} \frac{\beta_c}{\beta} \int_{\infty} d^d k \frac{1}{t + k^2 v(\vec{e}_{\vec{k}})} e^{i\vec{k} \cdot \vec{r}} \stackrel{\vec{k}=\vec{k}r}{=} \frac{1}{(2\pi)^d} \frac{\beta_c}{\beta} \int_{\infty} d^d \tilde{k} \frac{1}{r^2 t + \tilde{k}^2 v(\vec{e}_{\tilde{k}})} e^{i\tilde{k} \cdot \vec{e}_{\vec{r}}} r^{2-d}$$

- $r^2 t \ll 1 \Rightarrow r^2 t \approx 0 \Rightarrow G(\vec{r}) \sim r^{2-d}$ as before
- $r^2 t \gg 1$: Choose x direction in direction of $\vec{r}$. Other directions: $\vec{k}_{\perp}$
 $\Rightarrow G(\vec{r}) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk_x e^{ir k_x} \underbrace{\frac{\beta_c}{\beta} \frac{1}{(2\pi)^{d-1}} \int d^{d-1} k_{\parallel} \frac{1}{t + (k_x^2 + k_{\perp}^2) v(\vec{e}_{\vec{k}})}}_{=: g(k_x)}$

Use theorem of residues, search for poles p_j of $g(k_x)$ in the upper complex plane.

$$\Rightarrow \frac{1}{2\pi} \int_{-\pi}^{\pi} dk_x e^{ir k_x} g(k_x) = i \sum_j \lim_{z \rightarrow p_j} [(z - \bar{k}_j) f(z) e^{ir z}] \xrightarrow{r \rightarrow \infty} \text{const } e^{ir \bar{p}}$$

where $\bar{p}$ is the pole that is closest to the real axis.

Main contribution to the integral stems from $k_{\perp} \approx 0$

$$\Rightarrow \text{Pole at } t = -\bar{k}_x^2 v(\vec{e}_x) \Rightarrow \bar{k}_x = i\sqrt{t/v(\vec{e}_x)} =: i/\xi(\vec{e}_x)$$

$$\Rightarrow \boxed{G(\vec{r}) \sim e^{-r/\xi(\vec{e}_{\vec{r}})}} \quad \text{with} \quad \boxed{\xi \sim 1/\sqrt{t}} \quad \Rightarrow \quad \boxed{\nu = 1/2}$$

3.5.4 Validity of mean-field theory, Ginzburg criterion

3.5.4.1 Compare two methods for determining specific heat

Consider specifically the case $t > 0$, $t \rightarrow 0^+$

Recall Sec. 3.5.3.3: $c_H = \text{const} = 0$

Calculated from $U = -J \sum_{\langle ij \rangle} \langle S_i \rangle \langle S_j \rangle$

Now: Alternative calculation from $U = -J \sum_{\langle ij \rangle} \langle S_i S_j \rangle = -J \sum_{\langle ij \rangle} G_{ij}$
using the results from Sec. 3.5.3.4

$$\begin{aligned} U &= -N \frac{1}{(2\pi)^d} \int_{\text{1st Brillouin zone}} d^d k \frac{1}{1 - \beta J \sum_{\vec{\tau}} \cos(\vec{k} \cdot \vec{\tau})} \frac{J}{2} \sum_{\vec{\tau}} e^{i\vec{k} \cdot \vec{\tau}} \\ &\quad \left| \begin{array}{l} \text{Expansion about } k = 0 \\ \approx -\frac{N k_B T}{2} \frac{1}{(2\pi)^d} \int_{\infty} d^d k \frac{1 - k^2 v(\vec{e}_{\vec{k}})}{t + k^2 v(\vec{e}_{\vec{k}})} \\ \left| \begin{array}{l} \tilde{k} = \vec{k}/\sqrt{t}, \quad t \rightarrow 0^+ \\ \approx -\frac{N k_B T}{2} t^{d/2-1} \frac{1}{(2\pi)^d} \int_{\infty} d^d \tilde{k} \frac{1}{1 + v(\vec{e}_{\tilde{k}})} \propto T t^{d/2-1} \end{array} \right. \end{array} \right. \\ \Rightarrow c_H &= \frac{1}{N} \frac{\partial U}{\partial T} \propto t^{d/2-1} \quad (\text{at } t \rightarrow 0^+) \\ \Rightarrow c_H &\sim \begin{cases} \text{const} & \text{for } d > 4 : \text{consistent with Sec. 3.5.3.3} \\ \text{divergent} & \text{for } d > 4 : \underline{\text{not}} \text{ consistent with Sec. 3.5.3.3} \end{cases} \end{aligned}$$

$\Rightarrow$ Apparently, mean-field approximation breaks down for dimensions $d < 4$.

$\leadsto$ "Upper critical dimension"

3.5.4.2 Alternative argument: Ginzburg criterion

Mean-field theory neglects correlations.

$\leadsto$ should be oK, if the fluctuations within the correlation length ξ are small compared to the magnetization!

$$\begin{aligned}
 &\Rightarrow \underbrace{\sum_{V(\xi)} \sum_{V(\xi)} [\langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle]}_{\substack{|| \\ \xi^d \chi}} \ll \underbrace{\sum_{V(\xi)} \sum_{V(\xi)} \langle S_i \rangle \langle S_j \rangle}_{\substack{|| \\ (\xi^d)^2 m^2}} \\
 &\Rightarrow \frac{\chi}{\xi^d m^2} \ll 1 \qquad \text{with } \xi \sim |t|^{-\nu}, m \sim |t|^\beta, \gamma \sim |t|^{-\gamma} \\
 &\Rightarrow R |t|^{-\gamma + d\nu - 2\beta} \ll 1 \\
 &\quad R : \text{System dependent factor (range of interactions etc.)}
 \end{aligned}$$

At the critical point $t \rightarrow 0$

$$\begin{aligned}
 &\Rightarrow \text{Condition } d\nu - 2\beta - \gamma > 0 \text{ with } \gamma = 1, \beta = \nu = 1/2 \\
 &\Rightarrow \text{Fulfilled for } \frac{d}{2} - 2 > 0 \quad \Rightarrow \boxed{d > 4}
 \end{aligned}$$

$\leadsto$ Mean-field approximation captures correct critical behavior at $d > 4$.
However: Fails for $t \rightarrow 0^+$ at $d \leq 4$

3.6 The Monte Carlo method

Problem: Calculate partition functions, statistical expectation values, phase transitions in the Ising model or other "microscopic" models

Looking back: Approaches we have discussed so far

3.3: Exact techniques

→ Exact solutions for special cases (1D, 2D Ising)

3.4: Series expansions

→ Also exact, but limited applicability (convergence radius)

3.5: Mean-field approximation

→ More generally applicable, but uncontrolled approximation

Question: How can one obtain an "exact" solution in the general case?

Answer: Up to now - Only numerically

"Sledgehammer approach":

Calculate $\langle A \rangle = \frac{\sum e^{-\beta \mathcal{H}} A}{\sum e^{-\beta \mathcal{H}}}$ directly for finite systems

But: Use "smart" sledgehammer → Monte Carlo Simulations

Very general method

Broad applications in all areas of statistical physics and beyond. Also heavily used in Mainz. Shall therefore be briefly illustrated here at the example of the Ising model. (For more details see class "Computer simulations in statistical physics").

3.6.1 Main idea of Monte Carlo integration

Task: Calculate statistical expectation values $\langle A \rangle = \frac{\sum e^{-\beta \mathcal{H}} A}{\sum e^{-\beta \mathcal{H}}}$

Solution strategies

(a) **Exact enumeration** : Full Sum over all configurations

Pros: Exact

Cons: very time consuming, only possible for tiny systems

Inefficient at small temperatures, since most configurations don't contribute much to the sum

Way out: Monte Carlo Integration

Sum only over a random sample of configurations, not all!

(b) **Simple sampling** Entirely random sample (every configuration has equal probability)

(e.g.: Sample $j \leftrightarrow N$ random numbers $r_i^{(j)} \in [0 : 1]$,

$$S_i^{(j)} = \begin{cases} +1 & : r_i^{(j)} > 1/2 \\ -1 & : r_i^{(j)} < 1/2 \end{cases}$$

$$\text{Analysis: } \langle A \rangle = \lim_{n \rightarrow \infty} \frac{\sum_{j=1}^n A[\{S_i^{(j)}\}] e^{-\beta \mathcal{H}[\{S_i^{(j)}\}]}}{\sum_{j=1}^n e^{-\beta \mathcal{H}[\{S_i^{(j)}\}]}}$$

Pro: Results can already be obtained with small samples
 Can be improved systematically by increasing sample size
 $\leadsto$ One is less restricted with respect to system size

Cons: – No longer exact
 (however, accuracy can be controlled via sample size)
 – Still inefficient at low temperatures

(c) **Importance sampling** Draw sample according to the distribution
 $P\{S_i\} \propto e^{-\beta \mathcal{H}[\{S_i\}]}$

Analysis: $\langle A \rangle = \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{j=1}^n A[\{S_i^{(j)}\}]$

Pros: – First results can already be obtained with small samples
 Can be improved systematically by increasing sample size
 (as in (b))
 – Efficient: Configurations that contribute to the sum with
 higher weight are drawn more often
 (Cons: Not fully exact, but that's life!)

$\Rightarrow$ Importance sampling seems to be the method of choice, but ...

Question: How generate a sample with a prescribed probability distribution?

Solution: Generate a Markov Chain

★ Stochastic process without memory defined by

– State space (Here: Configuration space $\Gamma = \{S_i\}$)
 – Transition probability $W_{\Gamma \rightarrow \Gamma'}$

$\leadsto$ generates chain of states $\Gamma_0 \xrightarrow{W} \Gamma_1 \xrightarrow{W} \Gamma_2 \dots$
 or, respectively, chain of probabilities $P_n(\Gamma)$

Master equation: $P_{n+1}(\Gamma) = P_n(\Gamma) + \sum_{\Gamma'} \left\{ \underbrace{W_{\Gamma' \rightarrow \Gamma} P_n(\Gamma')}_{\text{flow in}} - \underbrace{W_{\Gamma \rightarrow \Gamma'} P_n(\Gamma)}_{\text{flow out}} \right\}$

★ For Markov chains with finite state space, one has a central limit theorem
 (stated without proof)

If the Markov chain is irreducible, i.e., every state can be reached
 from every other states (possibly by more than one step), then there
 exists a unique stationary limit distribution $\bar{P}(\Gamma)$ with $\lim_{n \rightarrow \infty} P_n(\Gamma) =$
 $\bar{P}(\Gamma)$, independent of the initial distribution $P_0(\Gamma)$

★ The stationary limit distribution fulfills $\sum_{\Gamma'} W_{\Gamma' \rightarrow \Gamma} \bar{P}(\Gamma') = \sum_{\Gamma'} W_{\Gamma \rightarrow \Gamma'} \bar{P}(\Gamma)$

★ $\Rightarrow$ Trick: (Metropolis, Rosenbluth, Teller)

Construct the transition function $W_{\Gamma \rightarrow \Gamma'}$ such that the limit distri-
 bution is just the target distribution function. This can be achieved
 with the following sufficient (but not necessary) conditions:

(i) irreducible (every state can be reached from every other state)

(ii) detailed balance $\frac{W_{\Gamma \rightarrow \Gamma'}}{W_{\Gamma' \rightarrow \Gamma}} = \frac{\bar{P}(\Gamma')}{\bar{P}(\Gamma)}$

One example of a popular implementation is the Metropolis algorithm

$$W_{\Gamma \rightarrow \Gamma'} = N_{\Gamma\Gamma'} \min(1, \frac{\bar{P}(\Gamma)}{\bar{P}(\Gamma')}) \quad \text{with } N_{\Gamma\Gamma'} = N_{\Gamma'\Gamma}$$

★ In particular, to obtain the Boltzmann distribution, one requires

$$\frac{W_{\Gamma \rightarrow \Gamma'}}{W_{\Gamma' \rightarrow \Gamma}} = e^{-\beta(\mathcal{H}(\Gamma) - \mathcal{H}(\Gamma'))} = e^{-\beta\Delta E}$$

which in the Metropolis algorithm results in

$$W_{\Gamma \rightarrow \Gamma'} = N_{\Gamma\Gamma'} \min(1, e^{-\beta\Delta E}) \quad \text{with } N_{\Gamma\Gamma'} = N_{\Gamma'\Gamma}$$

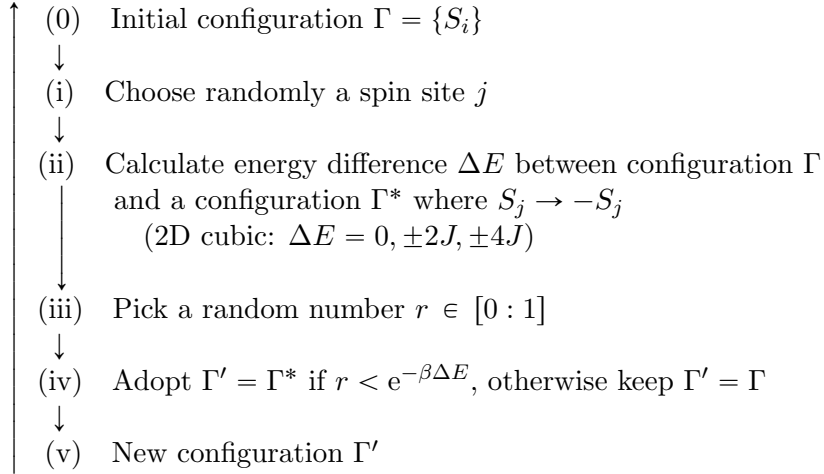
Remarks:

- The Metropolis algorithm is the most popular algorithm, but every other algorithm works too, as long as it fulfills the conditions (i) and (ii) or, instead of (ii), at least the condition of "global balance" $\sum_{\Gamma'} W_{\Gamma' \rightarrow \Gamma} \bar{P}(\Gamma') = \sum_{\Gamma} W_{\Gamma \rightarrow \Gamma'} \bar{P}(\Gamma)$
- It is not strictly necessary to target the Boltzmann distribution in the Markov chain (i.e., choose $\bar{P}(\Gamma) \sim e^{-\beta\mathcal{H}}$). In some cases, it may be more convenient to choose another target distributions and then "reweight" the data when calculating the expectation values.
($\leadsto$ "Reweight" methods such as "multicanonical" sampling, "Wang/Landau" sampling, "Metadynamics" etc.)

3.6.2 Examples of Monte Carlo algorithms

(a) Simple "Single Flip" Metropolis algorithm

Algorithm



Remarks:

- Similar algorithms can be designed easily also for other systems.
- Close to the critical point, spin clusters become very large
 $\leadsto$ Dynamics become very slow (critical slowing down)
 $\leadsto$ Sampling becomes inefficient!

(b) Ising model: Cluster algorithm (Wolff algorithm)

Algorithm

- (0) Initial configuration Γ
 $\downarrow$
 (i) Choose randomly a spin site j
 $\downarrow$
 (ii) Identify neighbors k of j with same spin direction $S_k = S_j$ and bonds (jk) that connect them
 $\downarrow$
 (iii) Assign bond variables u_{jk} to these bonds, choosing $u_{ij} = -1$ with probability $e^{-2\beta J}$. Spins connected by bonds with $u_{ij} = 1$ form a "cluster"
 $\downarrow$
 (iv) Identify neighbors of cluster with the same spin value. Assign bond variables to unoccupied connecting bonds. Extend cluster accordingly.
 $\downarrow$
 (v) Continue until cluster can no longer grow.
 $\downarrow$
 (vi) Change sign of all spins in the cluster ($S_k \rightarrow -S_k$)
 $\downarrow$
 (vi) New configuration Γ'

Proof that this algorithm fulfills detailed balance

Γ, Γ' : Configurations, in which light pink cluster contains spins $+1$ or -1 , respectively

Cluster is bounded by the contour $L = l^+ + l^-$ with l^+ : Boundary to spins $+1$ (dashed line)

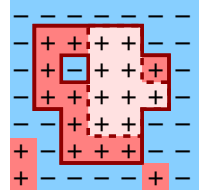
l^- : Boundary to spins -1 (solid line)

Transition $\Gamma \rightarrow \Gamma'$: Energy difference $\Delta E = 2J(l^+ - l^-)$

$$W_{\Gamma \rightarrow \Gamma'} = \underbrace{W_{\text{inside}}}_{\text{Probability of having selected pink cluster}} \cdot \underbrace{e^{-2\beta J l^+}}_{\text{Probability that cluster does not grow further}}$$

$$W_{\Gamma' \rightarrow \Gamma} = \underbrace{W_{\text{inside}}}_{\text{Probability of having selected pink cluster}} \cdot \underbrace{e^{-2\beta J l^-}}_{\text{Probability that cluster does not grow further}}$$

$$\Rightarrow W_{\Gamma \rightarrow \Gamma'} / W_{\Gamma' \rightarrow \Gamma} = e^{-2\beta J(l^+ - l^-)} = e^{-2\beta \Delta E} \quad \checkmark$$



Remark: Global dynamics, totally 'unrealistic',

but correlations break up much faster. $\leadsto$ more efficient sampling!

3.6.3 "Problems" with the Monte Carlo method

If one could invest an infinite amount of computing time, the Monte Carlo method would be exact, on principle. Nevertheless, one has to apply caution when analyzing the data.

- ★ In fact, the computing time is never infinite

$\leadsto$ Statistical error

- ★ The systems have finite size

$\leadsto$ Systematic error

 Causes problems in particular in the vicinity of critical points, where the correlation length diverges.

 Way out: Finite size scaling (Chapter 5)

- ★ When using importance sampling, the entropy and free energy cannot be calculated directly. (NB: Similar to experiments: Only observables can be calculated!)

$\leadsto$ Special methods must be developed, e.g., "thermodynamic integration", determination of free energy differences from histograms etc.

 (See textbooks on simulation methods)