Statistical mechanics, the Ising model and critical phenomena
— Lecture Notes —

September 26, 2017
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1 Scope of these notes

These notes accompany the lectures during approximately the first three weeks of the two-month course “Topics in Complex Systems” taught at Niels Bohr Institute, Copenhagen. The current notes should neither be considered complete nor to constitute an unbiased reference for the topics of critical phenomena and phase transitions. Rather, these notes make heavy use of well-established literature on the topic, e.g. the book by J. M. Yeomans [1], or the lecture notes by N. Goldenfeld [2]. Further recommended background reading are the statistical mechanics textbooks by S. K. Ma [3] and M. Plischke and B. Bergersen [4].

Primarily, the present notes are intended to serve as a brief introduction to the wide range of critical phenomena, roughly summarizing the lectures given during the course, and making heavy use of the Ising model as the canonical system. While simple and instructive, it should be kept in mind that this model is mostly a mathematical abstraction of reality, and — while initially intended as a crude approximation of magnetic systems — likely has more applications in other areas of physics and beyond. Using this model, several aspects of critical phenomena will be exemplified.

After briefly summarizing some crucial elements of statistical mechanics (Sec. 2), e.g. the partition function, entropy and free energy, we will start out with a definition of phase transitions and critical exponents (Sec. 3). We then define the Ising model (Sec. 4) and sketch a range of exact and approximate solutions. In Sec. 5 we discuss the transfer matrix method, which allows for an exact solution of the 1D Ising model, and is at the base of Onsager’s exact solution of the 2D version (which we leave out for brevity here). The mean field solution to the Ising model is shown in Sec. 6, which is supplemented by the phenomenological Landau theory (Sec. 7). As an important numerical method we describe the Monte Carlo method and the Metropolis algorithm (Sec. 8). A further approximate technique, which gives physical insight into basic excitations around either a low-temperature or high-temperature limit are series expansions (Sec. 9). We finally offer an outlook on the renormalization group, which — time permitting — will be discussed along practical implementation in selected 1D and 2D cases.

Homework exercises will be handed out as the course progresses. They will usually encompass a few exercises complementing the lecture notes, but generally covering closely related problems. Group work on homework problems is explicitly encouraged. You should work through all problems and if you get stuck, discuss with your classmates or visit me in my office.
2 Partition function and free energy

At the base of statistical mechanics lies the assumption that entropy, which is a measure of the "lack of information" about a given many-particle ensemble, must be maximized. Consider a large number of systems $N_S$, i.e. $N_S \to \infty$. Each of these systems can be in a certain state $i$, and $n_i$ counts the number of systems that are in the state $i$, one of a total of $q$ possible states (Fig. 2). If there were only one state, then we would have complete knowledge, since the state of all systems would be the same. If we had a number of possible states, we can measure the ignorance $I$ we have about the system. $I$ is the number of ways the $N_S$ systems can be re-arranged, i.e. the factorial $N_S!$ divided by the number of ways the systems of equal state can be re-arranged:

$$I \equiv \frac{N_S!}{n_1! \, n_2! \ldots \, n_q!}.$$  \hspace{1cm} (1)

$I$ simply measures the multiplicity of the outcome, where the states are populated according to the numbers $n_i$. The aim is to find the numbers $n_i$ such that ignorance is maximized while satisfying a constraint.

We are not forced to maximize $I$, instead, we could just as well maximize any monotonically increasing function of $I$. Instead of the ignorance $I$, for mathematical reasons it is convenient to use a different quantity $S$, the entropy, defined as

$$S \sim \frac{1}{N_S} \ln(I).$$  \hspace{1cm} (2)

When $I$ is maximized, so is $S$. We use the proportionality symbol in order to indicate, that one has the liberty to choose the proportionality constant as one pleases, the important aspect about $S$ is that it is an increasing function of the $I$. The use of $S$ is convenient, as for large numbers $N_S$ and $n_i$, Stirling’s approximation can be used to transition from the discrete factorial to continuous functions:

$$\lim_{N \to \infty} \ln N! = N \ln N - N + (1/2) \ln N + (1/2) \ln(2\pi) + 1/(12N) + \ldots,$$  \hspace{1cm} (3)

where for large $N$ retaining only the first two terms of the RHS is a very good

![Figure 1: Organizing $N_S$ systems into $q$ states.](image-url)
approximation. Using only these, for $N_S \to \infty$, which we sometimes call the thermodynamic limit, the entropy $S$ in Eq. 2 can be re-written as

$$S \sim \frac{1}{N_S} \left( N_S \ln N_S - \sum_i n_i \ln n_i - N_S + \sum_i n_i + \ldots \right)$$

(4)

$$\sim -\sum_i p_i \ln p_i .$$

(5)

The probabilities $p_i \equiv n_i / N_S$ thereby denote the likelihood that a given system is in state $i$. The proportionality allows free choice of a constant, and for physical systems

$$S = -k_B \sum_i p_i \ln p_i ,$$

(6)

with $k_B = 1.38 \times 10^{-23} \text{JK}^{-1}$ is conventional, hence entropy has units of energy divided by temperature. We note that it would be equally reasonable to absorb $k_B$ into the definition of temperature $T$, to be defined below. In that case, temperature would simply be measured in units of energy and entropy would remain dimensionless.

There are several aspects to point out about Eq. 5: Given that there is only one possible state $n_1$, then $n_1 = N_S$ and the entropy $S$ vanishes. For cases with more than one occupied state, $0 \leq p_i < 1 \forall i$, and entropy is always positive. As a measure of “disorder”, entropy $S$ is the fundamental quantity of statistical physics.

Langrange multipliers — maximization under constraints. As mentioned, statistical mechanics builds on the principle that entropy must be maximized. What we did not mention above is, that such a maximization takes place under a given a number of so-called constraints. The entropy (Eq. 5) is a multidimensional function of the values $p_i$. In 2D, i.e. $i \in \{1, 2\}$, its value can be visualized as a surface (Fig. 2) and the gradient $\nabla S$ is a vector pointing in the direction of steepest slope. Any constraint, $C(p_1, p_2, \ldots) = 0$, is also a function of the $p_i$, and we define such constraints to equal zero. In the 2D example (Fig. 2), a possible (but not at all physically inspired) constraint could be that $p_1^2 + p_2^2 - 1 = 0$, i.e. that the values of $p_i$ lie on a unit circle in the $p_1$-$p_2$-plane. The gradient of the constraint is $\nabla C(p_1, p_2, \ldots)$ and points in the direction, in which the constraint is most effectively modified. For the example of the circle, the gradient $\nabla C = 2(p_1, p_2)$, i.e. is the normal to the circle line.

Maximizing $S$ subject to $C$ means to find the values of $p_i$ where the gradients $\nabla S$ and $\nabla C$ align, i.e.

$$\nabla S = \lambda \nabla C ,$$

the gradients may thereby differ by a constant $\lambda$, which is termed Langrange multiplier. To ensure the constraint and express it analogously to the gradient,
one often employs the notation

$$\frac{\partial}{\partial \lambda}(S - \lambda C) = 0 .$$

Hence, the Langrange multiplier $\lambda$ can be seen as an extra dimension to the problem. By adding this dimension, one has the advantage of obtaining a maximization problem without constraint.

**Constraint of normalization of probability.** The previous example of a circle was entirely fabricated and physically not meaningful. In practice, one basic constraint is always present, namely that each system must be in one of the available states, i.e. total probability must equal unity, or

$$\sum_j p_j - 1 = 0 . \quad (7)$$

In this case, the problem to solve is:

$$\frac{\partial}{\partial p_i} k_B \left( \sum_j p_j \ln p_j - \lambda \left[ \sum_j p_j - 1 \right] \right) = 0 ,$$

$$\frac{\partial}{\partial \lambda} k_B \left( \sum_j p_j \ln p_j - \lambda \left[ \sum_j p_j - 1 \right] \right) = 0 .$$
These equations give
\[
\ln p_i = -\lambda - 1, \quad \text{hence } p_i = \exp(-\lambda - 1), \tag{8}
\]
as well as the imposed constraint \(\sum_j p_j = 1\). Eq. 8 hence expresses the uniform distribution of probabilities, that is, the fact that all states are equally likely — given that there are no additional constraints. The only constraint, that of normalized probabilities, is fulfilled by proper choice of \(\lambda = \ln q - 1\).

**Conserved quantities.** In the previous example we have already encountered a conserved quantity, namely total probability, stating that each system must be in one of the available states. However, in many physical contexts, such as a laboratory experiment, other quantities are also conserved — they might be controlled by the experimental setup, e.g. a closed container which constrains particle number or the total energy of the system.

**Constraint of total energy.** Consider total energy \(E\), and allow each possible state \(i\) to come with a specific energy \(\epsilon_i\). Then the constraint on total energy is
\[
\sum_j p_j \epsilon_j - E = 0. \tag{9}
\]
This additional constraint now requires one additional Lagrange multiplier and the complete equation for the gradients w.r.t. the \(p_i\) becomes
\[
\frac{\partial}{\partial p_i} k_B \left( -\sum_j p_j \ln p_j - \lambda \left[ \sum_j p_j - 1 \right] - \beta \left[ \sum_j p_j \epsilon_j - E \right] \right) = 0, \tag{10}
\]
where \(\beta\) is the Lagrange multiplier corresponding to the total energy constraint. Evaluating the derivatives yields the probabilities
\[
p_i = \exp(-1 - \lambda - \beta \epsilon_i) \sim \exp(-\beta \epsilon_i). \tag{11}
\]
Hence, the probability of occupying a given state is now dependent on the respective state energy and decays exponentially with that energy. Note that the exponentials in Eq. 11 are the usual Boltzmann probabilities. However, the new multiplier \(\beta\) must be fixed by ensuring that total energy equal \(E\). \(\beta\) is often referred to as “inverse temperature”, i.e. \(\beta = 1/k_B T\). We emphasize that the Boltzmann constant \(k_B\) generally appears together with \(T\), hence it is often easiest to absorb \(k_B\) into the definition of temperature — making the entropy dimensionless.

**Constraint of total particle number.** When total particle number is conserved, an additional Lagrange multiplier is required. In that case, the probabilities become
\[
p_i = \exp(-1 - \lambda - \beta \epsilon_i - \alpha N_i) \sim \exp(-\beta \epsilon_i - \alpha N_i), \tag{12}
\]
where \(N_i\) are the particle numbers for the different states \(i\) and \(\alpha\) is the Lagrange multiplier for particle number. For practical purposes, \(\alpha\) is often re-expressed as \(\alpha = -\mu/k_B T\), where \(\mu\) is the “chemical potential” and \(T\) temperature.
Critical Phenomena, by Jan O. Haerter

Statistical ensemble. Depending on which quantities are allowed to vary, statistical mechanics distinguishes several types of statistical ensembles. The micro-canonical ensemble considers both energy and particle number to be "fixed". By "fixed" it is hereby meant that the system has a specific value of total energy or particle number, no fluctuations regarding their values are allowed. This ensemble assumes that each state $i$ has the same energy and probability.

In practical terms, the microcanonical ensemble is less realistic, since an experimental system would generally allow for some uncertainty regarding the fluctuations of energy. The canonical ensemble relaxes the need for identical energy levels. It allows for the states $i$ to have distinct energy values but does require the total energy to be some average, or expectation value, $E$. The microstates are then occupied statistically, by the maximization of entropy under the total energy constraint, as discussed above. The grand canonical ensemble further relaxes the need for a fixed particle number in each state, but considers a total average $N$, which is again enforced as a constraint.

Partition function. With probabilities proportional to $\exp(-\beta \epsilon_i - \alpha N_i)$ and the normalization constraint on unit total probability, the normalization constant $Z$ can be defined as:

$$Z \equiv \sum_i \exp(-\beta \epsilon_i - \alpha N_i) , \quad (13)$$

through which the probabilities $p_i$ are

$$p_i = \frac{1}{Z} \exp(-\beta \epsilon_i - \alpha N_i) . \quad (14)$$

$Z$ is commonly referred to as the partition function, and can be useful in expressing observables, e.g. the average energy

$$\langle E \rangle = \frac{\sum_i \epsilon_i \exp(-\beta \epsilon_i - \alpha N_i)}{Z} = -\frac{\partial}{\partial \beta} \ln Z = T^2 \frac{\partial}{\partial T} \ln Z \quad (15)$$

or total particle number

$$\langle N \rangle = \frac{\sum_i N_i \exp(-\beta \epsilon_i - \alpha N_i)}{Z} = -\frac{\partial}{\partial \alpha} \ln Z = T \frac{\partial}{\partial \mu} \ln Z . \quad (16)$$

Note that, in the previous two equations, it is assumed that $\alpha$, respectively $\beta$, is held fixed when evaluating the derivatives.

Notably, the partition function is also related to the entropy:

$$S = -k_B \sum_i p_i \ln p_i = k_B \sum_i p_i (\ln Z + \beta \epsilon_i + \alpha N_i) \quad (17)$$

$$= k_B \ln Z + \langle E \rangle / T + \mu \langle N \rangle / T . \quad (18)$$

Thermodynamic potentials. Logarithms of partition functions are often referred to as thermodynamic potentials or free energies. When both particle
number and energy are allowed to vary, the corresponding potential is referred to as grand canonical potential,
\[ \Omega_{GC} \equiv k_B T \ln Z_{GC} = TS - \langle E \rangle + \mu \langle N \rangle , \]
which is a reformulation of Eq. 18.
In the canonical case, where only states of the same particle number are considered, the term \( \mu N \) is missing and the potential is referred to as the (Helmholtz) free energy,
\[ F \equiv -k_B T \ln Z_C = \langle E \rangle - TS , \]
where we note that the opposite sign is conventional as compared to Eq. 19.
In the microcanonical case, the potential is just the entropy.
Once the partition function is known, observables can be evaluated by taking appropriate derivatives, e.g. the internal energy
\[ \langle E \rangle = -\frac{\partial \ln Z}{\partial \beta} , \]
specific heat
\[ C_H \equiv \left( \frac{\partial \langle E \rangle}{\partial T} \right)_H = \frac{\partial \langle E \rangle}{\partial \beta} \frac{d\beta}{dT} = -\frac{\partial \langle E \rangle}{\partial \beta} = \frac{1}{k_B T^2} \frac{\partial^2 \ln Z}{\partial \beta^2} , \]
where \( H \) is some quantity that is held constant. Note that the derivative w.r.t. temperature could also be carried out explicitly in the partition function, as
\[ \frac{\partial \langle E \rangle}{\partial \beta} = -\frac{1}{k_B T^2} \frac{\partial}{\partial \beta} \sum \epsilon_n \exp(-\beta \epsilon_n) \sum \exp(-\beta \epsilon_n) \]
which leads to a relation between (microscopic) root-mean-square fluctuations \( \sigma_E \) and the (macroscopic) specific heat (see: exercises). One can hence measure the specific heat without perturbing the external temperature, it is sufficient to observe the fluctuations in equilibrium.
Once the free energy is known, various quantities can be obtained by taking derivatives w.r.t. the controllable variables:
\[ S = -\left( \frac{\partial F}{\partial T} \right)_H = \frac{\langle E \rangle - F}{T} , \]
magnetization
\[ M = -\left( \frac{\partial F}{\partial H} \right)_T , \]
or susceptibilities
\[ \chi_T = \left( \frac{\partial^2 F}{\partial H^2} \right)_T , \]
where the subscript \( T \) denotes that temperature is held constant while evaluating the derivative. We briefly remind of the origin of the derivative in Eq.
25: it is assumed that the energy has a term $-MH$ in addition to the internal degrees of freedom, where $M$ is the magnetization and $H$ an external magnetic field. $H$ can thereby be controlled within the experimental setting and acts as the “generalized force”, while $M$ acts as the “generalized displacement”. This should be compared to the usual term $-pV$, where the pressure $p$ is the generalized force and the volume $V$ the generalized displacement.

**Exercises**

1. **Two electrons.**

Consider two single-particle levels with energies $-\epsilon$ and $\epsilon$. In these levels place two electrons (no more than one electron of the same spin per level). As a function of $T$ find: (a) the partition function; (b) the average energy; (c) the entropy; (d) for microcanonical ensembles corresponding to each system energy level, compute the entropy; (e) for a–c, discuss the limits $T = 0$ and $T \to \infty$.

2. **Fluctuations.**

(i) Verify that

$$\langle (M - \langle M \rangle)^2 \rangle = \langle M^2 \rangle - \langle M \rangle^2 = k_B T^2 \frac{\partial^2}{\partial H^2} \ln Z = k_B T \chi_T .$$

(ii) Show in a similar way that the fluctuations in the energy are related to the specific heat at constant volume by

$$\langle (E - \langle E \rangle)^2 \rangle = k_B T C_V .$$

Use this equation to argue that $\Delta E \sim N^{1/2}$ where $N$ is the number of particles in the system.

---

2Yeomans: Problem 2.1
Figure 3: Cartoon of order parameters. For a zero-external-field ($H = 0$) magnetic system with symmetry regarding spin orientation (top) and a gas, where the order parameter can be defined as the difference in density for the liquid and gas phases.

### 3 Definition of phase transitions

Phase transitions are singularities in the free energy or one of its derivatives. Examples are the liquid-gas transition, the transition from a normal to a superconductor, or the transition from a paramagnet to a ferromagnet. A phase transition can be measured in terms of an order parameter, which changes with the phase transition. In the case of the liquid-gas transition, the order parameter is the difference in density of the liquid $\rho_{\text{liq}}(T)$ and that of the gas $\rho_{\text{gas}}(T)$. In magnetic systems, the order parameter is the magnetization $M(T)$ (Fig. 3).

In Sec. 4 we will analyze the Ising model \(^3\) as a crude description of magnetism. The Ising Hamiltonian is

$$\mathcal{H} = -J \sum_{(ij)} s_i s_j - h \sum_i s_i , \quad (27)$$

where $s_i$ is the “spin” at a lattice site $i$ and can take one of the values ±1. $h$ is the external magnetic field and $J$ is the coupling parameter. For a ferromagnet, which we qualitatively discuss here, $J > 0$, i.e. energy is minimized when spins have the same sign.

\(^3\)First studied by Lenz and Ising in 1925, see Brush [5] for a review on the model and its vast applications.
We qualitatively sketch some limits (Fig. 4): For very high temperature, spins are randomly oriented, all order disappears and there is no net magnetization. As temperature is lowered, the correlation length increases, i.e. the length at which spins are correlated and point in the same direction — "patchiness" increases. At the so-called critical temperature $T_c$, the correlation length "diverges", there are patches of correlated spins of all patch sizes. When an external field is absent ($h = 0$) there is however still no net magnetization. As temperature is lowered below $T_c$, nonzero magnetization emerges spontaneously, i.e. the system breaks the symmetry w.r.t. positive and negative spin, with one orientation dominating randomly. At $T = 0$, all spins are entirely aligned.

**First order vs. continuous phase transition.** A first order phase transition in a given quantity is present, when a derivative of the thermodynamic potential has a finite discontinuity. In the case of our magnetic system, the free energy is the appropriate thermodynamic potential. For $T < T_c$, there is a line of first order transitions at zero field $H$, where the free energy shows a kink and magnetization consequently is discontinuous. For $T > T_c$, the free energy is a smooth function of $H$ and magnetization varies continuously. When $T = T_c$, the magnetization varies continuously, hence the transition is not of first order. However, the slope at $H = 0$ is infinite, signaling a divergence in the derivative $\partial M/\partial H|_T$, i.e. the isothermal susceptibility. Hence, the transition here is of second order (continuous transition).

**Definition of correlation length.** While phase transitions are related to the macroscopic properties of a system, we will realize that many of such macroscopic properties are related to the microscopic configuration of the system. One crucial quantity that describes the microscopic state is the spin-spin correlation function. It is defined as

$$\Gamma(r_i, r_j) = \langle (s_i - \langle s_i \rangle)(s_j - \langle s_j \rangle) \rangle,$$

where $s_i$ is the value of spin at lattice position $r_i$, and $\langle ... \rangle$ denotes the ensemble average.
For translationally invariant systems, \( \langle s_i \rangle = \langle s_j \rangle \equiv \langle s \rangle \) and therefore the correlation function only depends on the distance vector between the two spins. It simplifies to

\[
\Gamma(r_i - r_j) \equiv \Gamma_{ij} = \langle s_i s_j \rangle - \langle s \rangle^2 .
\]

Away from the critical temperature \( T_c \), spins tend to be uncorrelated, i.e.

\[
\Gamma(r) \sim r^{-\tau} \exp(-r/\xi) ,
\]

where \( \tau \) is a number related to the critical exponent \( \eta \) (defined below) and \( \xi \) is the correlation length. Away from the critical temperature, the correlation length \( \xi \) is finite and the correlation between spins decays exponentially. However, as \( T_c \) is approached, the correlation length \( \xi \) diverges, i.e. \( \xi \to \infty \) and \( \exp(-r/\xi) \to 1 = const. \) Indeed, experiments as well as some exactly soluble models show that near criticality \( T \to T_c \), the value of the correlation function
decays as a power law with distance, i.e.

\[ \Gamma(r) \sim \frac{1}{r^{d-2+\eta}}. \]  

(31)

In this equation, \( \eta \) depends on some of the system properties and is an example of a so-called critical exponent.

One can relate the spin-spin correlation function to the susceptibility, i.e. the fluctuations in magnetization: The magnetic susceptibility at constant temperature is

\[ \chi_T = k_B T \frac{\partial^2}{\partial H^2} \ln Z \]  

(32)

\[ = \frac{1}{k_B T} ((\langle M^2 \rangle - \langle M \rangle^2)) \]  

(33)

\[ = \frac{1}{k_B T} ((\langle M - \langle M \rangle \rangle^2)) \]  

(34)

\[ = \frac{1}{k_B T} \left( \sum_i (s_i - \langle s_i \rangle) \sum_j (s_j - \langle s_j \rangle) \right) \]  

(35)

\[ = \frac{1}{k_B T} \sum_{ij} \Gamma_{ij} , \]  

(36)

where the total magnetization \( M \) was written as the sum over all spins. For the translationally invariant lattice, \( \sum_{ij} \Gamma_{ij} = N \sum_j \Gamma_{0j} \), which can be approximated by an integral near criticality, where the lattice structure is unimportant:

\[ N \sum_j \Gamma_{0j} \sim N \int dr \Gamma(r) r^{d-1} \sim \chi_T . \]  

(37)

Hence, for correlations to remain, one needs to require \( \eta < 2 \). Overall, divergent susceptibility (a macroscopic quantity) implies divergence also in the fluctuations of magnetization (a microscopic property).

**Definitions of critical exponents.** To measure the deviation from the critical temperature, it is convenient to define the dimensionless quantity

\[ t \equiv \frac{T - T_c}{T_c} . \]  

(38)

In terms of \( t \), a critical exponent is generally defined as the limit

\[ \lambda = \lim_{t \to 0} \frac{\ln |F(t)|}{\ln |t|} , \]  

(39)

or equivalently \( F(t) \sim |t|^\lambda \).
Table 1: **Critical exponents for several models.**

<table>
<thead>
<tr>
<th>Universality class</th>
<th>symmetry</th>
<th>$\alpha$</th>
<th>$\beta$</th>
<th>$\gamma$</th>
<th>$\delta$</th>
<th>$\nu$</th>
<th>$\eta$</th>
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<tbody>
<tr>
<td>2D Ising</td>
<td>2-component scalar</td>
<td>0</td>
<td>1/8</td>
<td>7/4</td>
<td>15</td>
<td>1</td>
<td>1/4</td>
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<td>4.8</td>
<td>0.63</td>
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<td>4.8</td>
<td>0.66</td>
<td>0.04</td>
</tr>
<tr>
<td>3D Heisenberg</td>
<td>3-dimensional vector</td>
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<td>1.39</td>
<td>4.8</td>
<td>0.71</td>
<td>0.04</td>
</tr>
<tr>
<td>mean field</td>
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<td>1/2</td>
<td>1</td>
<td>3</td>
<td>1/2</td>
<td>0</td>
</tr>
<tr>
<td>2D Potts, $q = 3$</td>
<td>$q$-component scalar</td>
<td>1/3</td>
<td>1/9</td>
<td>13/9</td>
<td>14</td>
<td>5/6</td>
<td>4/15</td>
</tr>
</tbody>
</table>

Commonly used critical exponents are

\[
C_H \sim |t|^{-\alpha} \text{ zero-field specific heat} \quad (40)
\]

\[
M \sim (-t)^{\beta} \text{ zero-field magnetization} \quad (41)
\]

\[
\chi_T \sim |t|^{-\gamma} \text{ zero-field isothermal susceptibility} \quad (42)
\]

\[
H \sim |M|^\delta \operatorname{sgn}(M) \text{ critical isotherm } (t = 0) \quad (43)
\]

\[
\psi \sim |t|^{-\nu} \text{ correlation length} \quad (44)
\]

\[
G(r) \sim \frac{1}{r^{d-2+\eta}} \text{ pair-correlation function at } T_c. \quad (45)
\]

The critical exponents are largely universal, meaning that they depend only on a few fundamental parameters, e.g. the dimensionality of space and the symmetry of the order parameter. For a brief overview, we list several common models along with their critical exponents (Tab. 1). Note that the critical exponents for the mean field system can be thought of as corresponding to four dimensional space, i.e. when the exponents for lower dimensions are known, the mean field exponents in some sense are an “extrapolation” to the next dimension. In fact, in 4D the mean field critical exponents are exact, $d = 4$ is therefore sometimes called the *upper critical dimension*. The mean field approach does not consider the dimensionality of the problem, only the *coordination number* of the lattice, i.e. the number of nearest neighbors, enters into the calculation. The mean field assumption implies that neighboring spins are uncorrelated. This assumption becomes more and more reasonable, when the number of nearest neighbors increases with the dimensionality of the problem. Therefore it seems intuitive that most critical exponents in the 3D Ising model (numerical solution) agree better with the mean field exponents than those of the 2D Ising model.

**Exercises**

1. **Paramagnet**

   A paramagnetic solid contains a large number $N$ of non-interacting, spin-1/2 particles, each of magnetic moment $\mu$ on fixed lattice sites. This substance is placed in a uniform magnetic field $H$.

   \(^4\)Yeomans: Problem 2.2
(i) Write down an expression for the partition function of the solid, neglecting lattice vibrations, in terms of \( x = \mu H/k_B T \).

(ii) Find the magnetization \( M \), the susceptibility \( \chi \), and the entropy \( S \), of the paramagnet in the field \( H \).

(iii) Check that your expressions have sensible limiting forms for \( x \gg 1 \) and \( x \ll 1 \). Describe the microscopic spin configuration in each of these limits.

(iv) Sketch \( M, \chi, \) and \( S \) as a function of \( x \).

(Answers: (i) \( Z = (2 \cosh x)^N \), (ii) \( M = N \mu \tanh x, \chi = N \mu^2 / (k_B T \cosh^2 x), S = N k (\ln 2 + \ln(\cosh x) - x \tanh x) \)).

2. Critical Exponents

Determine the critical exponents \( \lambda \) for the following functions as \( t \to 0 \):

- \( f(t) = A t^{1/2} + B t^{1/4} + C t \)
- \( f(t) = A t^{-2/3} (t + B)^{2/3} \)
- \( f(t) = A t^2 e^{-t} \)
- \( f(t) = A t^2 e^{1/t} \)
- \( f(t) = A \ln(\exp(1/t^4) - 1) \)

Consider a model equation of state that can be written

\[ H \sim aM(t + bM^2)^\theta \]  \hspace{1cm} (46)

where \( 1 < \theta < 2, a, b > 0 \) near the critical point. Find the exponents \( \beta, \gamma, \) and \( \delta \) and check if they obey the inequality \( \gamma \geq \beta(\delta - 1) \) as an equality.

3. Rushbrooke inequality. As the different observables are not independent, also the corresponding critical exponents are related to one another. Consider the specific heats at constant field \( H \) and constant magnetization \( M \), respectively:

\[ C_H \equiv T \left( \frac{dS}{dT} \right)_H, \] \hspace{1cm} (47)
\[ C_M \equiv T \left( \frac{dS}{dT} \right)_M, \] \hspace{1cm} (48)

as well as the magnetic susceptibility

\[ \chi_T \equiv \left( \frac{\partial M}{\partial H} \right)_T. \] \hspace{1cm} (49)

Consider now the entropy \( S = S(T, H) \) and the total derivative \( dS \). Use the Maxwell relation \( \left( \frac{\partial S}{\partial H} \right)_T \equiv \left( \frac{\partial M}{\partial T} \right)_H \) and the chain rule \( \left( \frac{\partial^2}{\partial x \partial y} \right)_z \equiv -1 \) to obtain a relation between the above observables:

\[ \chi_T(C_H - C_M) = T \left( \frac{\partial M}{\partial T} \right)_H^2. \] \hspace{1cm} (50)

\(^5\)Yeomans: Problems 2.3 and 2.5
Using the definitions of the critical exponents for these observables, verify the Rushbrooke inequality $\alpha + 2\beta + \gamma \geq 2$. 
4 Definition of the Ising Model

The Ising model represents one example of a lattice model, where one variable is located at each site of a regular grid. The state of the variables is determined by a Hamiltonian. Such models have been successful in the description of critical phenomena, (quantum) magnetism and models for high-temperature superconductivity and phase diagrams, disordered and non-equilibrium systems. With its simplicity, the Ising model is the most heavily studied lattice model in physics. We will use the Ising model in the following aspects: Phase transitions and critical exponents, mean field theory, series expansion techniques, as well as phenomenological models, such as Landau theory. We will also address the Monte Carlo technique, a numerical method to approximate the dynamics of a many particle system.

The Ising model encompasses a lattice of $N$ sites $i$, each of which contains an object $s_i$ (originally representing the magnetic dipole moment of an atomic spin or simply spin), which can be in one of two states that take values $\pm 1$. The Hamiltonian of the Ising model is

$$H \equiv -\sum_{\langle ij \rangle} J s_i s_j - h \sum_i s_i,$$

(51)

where $\langle ij \rangle$ denotes that a sum is to be carried out over all nearest-neighbor pairs of sites $i$ and $j$, and $J$ is the coupling between these neighboring sites. The quantity $h$ represents an external magnetic field which interacts with the magnetic moment $s_i$. The magnetization is then defined as the system's macroscopic magnetic moment $M = \sum_i s_i$.

It is important to note that the sign of $J$ plays an important role in determining the ordering of the system. For $J > 0$, energy is minimized if all spins align, i.e. neighboring $s_i$ and $s_j$ have the same sign. Such interaction is commonly referred to as ferromagnetic, and at low temperatures magnetic order is expected. If $J < 0$, neighboring spins tend to anti-align, in order to minimize energy. Depending on the lattice geometry, at low temperatures, a checkerboard pattern may result, which is referred to as anti-ferromagnetism. Notably, when the lattice is not bipartite, i.e. in cases where two sites can have a common nearest neighbor, an anti-ferromagnetic coupling ($J < 0$) can cause disordering effects, known as frustration (Fig. 4).

This is most easily exemplified by a triangle with only three spins. For $J > 0$, all spins align and $E = -3J$ for the ground state. There will be two configurations for the ground state, all spins either pointing “up” or “down”. For $J < 0$, the situation is more complicated. Out of the three bonds in the triangle, always one will be forced to have spins aligned, i.e. boost the energy along that bond to $+J$, yielding a ground state energy of $-J$. It is easy to verify that the ground state of such systems is far from unique and the number of states in the ground state increases with system size. In other words, the ground state entropy per site $(F/N)$ is finite for an anti-ferromagnetic triangular lattice, while it is zero for the ferromagnetic case. This is an example of ground state entropy (see Exercises).
At high temperatures, spins fluctuate thermally and order is generally destroyed. The macroscopic magnetic moment will vanish. This phase is referred to as paramagnetic phase. Note that the situation becomes already more complicated, when the lattice is not square, i.e. a simple anti-ferromagnetic order of the checkerboard-type is not possible. Consider a triangular lattice, where two neighboring sites may have a common neighbor. In this case, anti-alignment is not consistently possible, a case referred to as a frustrated spin system. We will however focus primarily on the square lattice geometry or one-dimensional systems.

To give an overview, whether an analytical solution exists for the Ising model depends on the dimension of the lattice. In 1D, an analytical solution exists, which we will discuss in Sec. 5. In 2D, Lars Onsager in 1944 obtained an analytical solution, which is however very technical. In 3D, no analytical solution exists to date. In 4D, it has been shown that the exact solution is identical to the mean-field solution, which we will discuss in Sec. 6.

4.1 Applications of the Ising model

Originally, Ising received the model from his Ph.D. supervisor as an exercise, and it was intended as a simple model for magnetism. While this is indeed one (qualitative) application of the model, many others exist.

Lattice gas. One intriguing variant is that of the lattice gas, where particles (they might be atoms or molecules) are considered to be located on the sites of a lattice, but the sites can also be empty (Fig. ??). Further, only nearest neighbors are taken to interact, an interaction which can be thought of as a lowering (or raising) of potential energy, depending on the sign. In short, we have

- states: occupied or empty,
- energy of interaction: $-\epsilon$ of neighboring sites are occupied.
The goal of the lattice gas model is that, as particle number can vary, so can density (since the total number of sites in the lattice is fixed). This means that, as temperature is lowered, one might find that the system spontaneously chooses a particular configuration of density, such that the respective thermodynamic potential is minimized. Since particle number is now not fixed, one must consider the Gibbs free energy and the grand canonical partition function (see Sec. 2). This brings in another Lagrange multiplier, namely the chemical potential \( \mu \), which is conjugate to the total particle number. We will later see that \( \mu \) can be associated with the external magnetic field of the Ising model, and that the grand canonical partition function is associated with the canonical one in the case of the Ising model. This means that, below \( T_c \), small changes in chemical potential can bring about a first order transition in density, moving between the “liquid” (i.e. density \( \rho_{\text{liq}} \)) and the “gas” (i.e. density \( \rho_{\text{gas}} \)) state abruptly. At temperatures close to \( T_c \) but below this value the system will spontaneously collapse to either \( \rho_{\text{liq}} \) or \( \rho_{\text{gas}} \).

The fortunate feature of the lattice gas model is that it maps exactly onto the Ising model, hence, finding a solution for one means having the solution for the other — there is no further approximation. How does this mapping work? For each site (“cell”), we define the spin as \( s_i = +1 \) (occupied) respectively \( s_i = -1 \) (empty). To be able to count particles, we make the unique transformation \( n_i = \frac{(s_i + 1)}{2} \),

where \( n_i \) now measures the number of particles at the site, i.e. either 0 or 1. For a lattice of \( N \) sites, the total number of particles is

\[
N_p = \frac{1}{2} \sum_i (s_i + 1) = \frac{1}{2} \sum_i s_i + \frac{N}{2}.
\]
The interaction between neighboring sites \( i \) and \( j \) is

\[
\epsilon_{ij} = -\epsilon \text{ if } s_i = s_j = 1 , \\
\epsilon_{ij} = 0 \text{ otherwise}.
\]

This can equivalently be written as

\[
\epsilon_{ij} = -\frac{1}{4}\epsilon(s_i + 1)(s_j + 1)
\]

and the total energy is

\[
E_p = -\frac{\epsilon}{8}\sum_{\langle ij \rangle}(s_i + 1)(s_j + 1) = -\frac{\epsilon}{8}\sum_{\langle ij \rangle}s_is_j - \frac{z\epsilon}{4}\sum_i s_i - \frac{zN\epsilon}{8}.
\]

In its original form the lattice gas model requires a grand canonical ensemble, since the total number of particles \( N_p \) may be varied (Sec. 2). The grand partition function then reads

\[
Z_G = \sum_{\{s\}} \exp(\beta\mu N_p - \beta E_p).
\] (52)

Notably, the probability weights in \( Z_G \) increase for large values of \( \mu \) (promoting larger numbers of particles, hence larger density), or by smaller values of the total energy. Re-writing \( Z_G \) in the “language” of the Ising model, we obtain an equivalent canonical partition function

\[
Z_C = \sum_{\{s\}} \exp(-\beta E_{\text{eff}}),
\] (53)

where

\[
E_{\text{eff}} = -\frac{\epsilon}{8}\sum_{\langle ij \rangle} - \left(\frac{\mu}{2} + \frac{z\epsilon}{4}\right)\sum_i s_i - \frac{zN\epsilon}{8} + \frac{\mu N}{2}.
\] (54)

This effective energy now highlights the correspondence between the two models:

- \( J \) corresponds to \( \frac{\epsilon}{8} \)
- \( h \) corresponds to \( \frac{\mu}{2} + \frac{z\epsilon}{4} \)
- \( M \) corresponds to density \( \rho \equiv N_p/N \)
- susceptibility \( \chi \) corresponds to compressibility \( \alpha \).

Note that the symmetry of the Ising model regarding \( \pm h \) is not preserved regarding occupied/unoccupied sites in the lattice gas model, i.e. there is no symmetry \( \rho \leftrightarrow (1 - \rho) \).

**Lattice binary mixture.** This is a model for an incompressible mixture of chemical species A and B (Fig. 4.1). In this case, the total number of particles
is fixed, but the difference of particles of types A and B may vary, i.e. \( N_A - N_B \). One option for defining the energy is that nearest-neighbor contacts of similar species, i.e. AA or BB contribute zero energy while those of different species, i.e. AB, give a contribution \( \epsilon \). Species would then attempt to avoid mixing, something that might be observed when oil and water are brought into the same volume. Similar to the lattice gas, we could define a cell \( i \) occupied by A to have \( s_i = +1 \) and those with B as \( s_i = -1 \). The energy of interaction between nearest neighbors \( i \) and \( j \) is then

\[
\epsilon_{ij} = \frac{1}{2} \epsilon (1 - s_is_j),
\]

and the total energy becomes

\[
E_p = \frac{\epsilon}{4} \sum_{(ij)} (1 - s_is_j) = \frac{zN\epsilon}{4} - \frac{\epsilon}{4} \sum_{(ij)} s_is_j.
\]

For a fixed mixing ratio of A and B, i.e. \( \langle N_A - N_B \rangle \) is constrained, the “grand” partition function is

\[
Z_G = \sum_{\{s\}} (\exp \beta \Delta \mu (N_A - N_B) - \beta E_p) = \sum_{\{s\}} \exp -\beta E_{\text{eff}}.
\]

Note that this is not actually a grand partition function, since total particle number is conserved, only the difference of particle numbers may be varied (hence the quotation marks). The effective energy this time is

\[
E_{\text{eff}} = -\frac{\epsilon}{4} \sum_{(ij)} s_is_j - \Delta \mu \sum_i s_i + \frac{zN\epsilon}{4},
\]

which again allows us to identify the mapping of parameters, i.e. \( J \to \frac{\epsilon}{4} \) and \( h \to \Delta \mu \).

**Models related to the Ising model.** A number of models are related to the Ising model, but are usually more complicated. It is useful to know about these models, to be able to compare them with the Ising model solution, which is often known or more easily available (e.g. by a simple computation). One simple extension of the Ising model are so-called Potts models, where \( s_i \) can take more than two values, but only when neighboring sites have the same value, is the energy value changed, i.e.

\[
\epsilon(i, j) = \delta(s_i - s_j),
\]

where \( \delta_x \) specifies the delta function which is unity when \( x = 0 \) and zero otherwise. Such Potts models can describe e.g. opinion dynamics in a population, where “agreement” of opinion could cause a negative value of energy.

The spins \( s_i \) could also take vectorial values, such that \( s_i \cdot s_j \) would become the inner product of two vectors. This model is called the Heisenberg model.
and describes isotropic magnetic moments in a lattice, i.e. moments that are not confined to one of the crystal axes. The Heisenberg model can also be applied to quantum spins, such that the vectors are interpreted as quantum spin operators $\hat{s}_i$.

Often, more complex lattices are introduced with non-trivial unit cells, e.g. fcc, bcc, or hexagonal lattices. These introduce further complications, which are often necessary when describing metals more quantitatively. Realistic descriptions generally also demand inclusion of further-neighbor interactions, beyond the range of nearest neighbors.

When the coupling parameter $J$ is made entirely random, then so-called “glassy” materials can be described, e.g. spin-glasses. Also time-dependent models are possible, leading altogether away from equilibrium statistical physics.

**Exercises**

1. **Ground state for simple models.** The ground state of a system (stable state at $T = 0$) often serves as the starting point for finite temperature investigations, e.g. the low-temperature expansion technique (later in the course). This is because it can dominate the partition function, even at $T > 0$. It is therefore important to develop some intuition for the ground state of simple models. Find the ground state for the following systems:
   
   (i) The 1d Ising model with first and second neighbor interactions
   
   $$\mathcal{H} = -J_1 \sum_i s_i s_{i+1} - J_2 \sum_i s_i s_{i+2},$$
   
   where both positive and negative values of the exchange parameters should be considered.

   (ii) The 1d $p$-state chiral clock model
   
   $$\mathcal{H} = -J \sum_i \cos(2\pi(n_i - n_j + \Delta)/p)$$
   
   for $J > 0$ and all values of $\Delta$.

   (iii) For the antiferromagnetic, zero-field spin-$1/2$ Ising model on a triangular lattice
   
   $$\mathcal{H} = J \sum_{(ij)} s_i s_j$$
   
   with $J > 0$, find the ground state energy and a possible representation of it.
5 1D Ising model

Ising was able to solve the model in 1D exactly during his thesis. Ising found that the 1D version of the model did not exhibit any phase transitions (except, strictly speaking, at $T = 0$).

In one dimension, the Ising model can be solved exactly by the so-called transfer matrix method. For simplicity, consider a periodic 1D lattice consisting of $N$ sites (a ring, see Fig. 5). The corresponding 1D Hamiltonian is

$$\mathcal{H}_N = -J \sum_{i=0}^{N-1} s_i s_{i+1} - h \sum_{i=0}^{N-1} s_i ,$$

(58)

where periodic boundary conditions mean that $s_N = s_0$.

The partition function for the $N$ sites is

$$Z_N = \sum_{\{s\}} \exp(\beta J (s_0 s_1 + s_1 s_2 + \cdots + s_{N-1} s_0) + \beta h (s_0 + s_1 + \cdots + s_{N-1})) ,$$

(59)

where the notation $\{s\}$ means that all configurations of the different $s_i$ are summed over in Eq. 59, $J$ is again the nearest neighbors coupling and $H$ the external magnetic field. The idea is now to break down the partition function into pairs of each two neighboring spins, yielding

$$Z_N = \sum_{\{s\}} \exp(\beta J (s_0 s_1 + s_1 s_2 + \cdots + s_{N-1} s_0) + \beta h (s_0 + s_1 + \cdots + s_{N-1})) \exp(\beta J s_1 s_2 + \beta h \frac{s_1 + s_2}{2}) \cdots \exp(\beta J s_{N-1} s_0 + \beta h \frac{s_{N-1} + s_0}{2}) .$$

(60)

Noticeable, each of the factors in the argument of exp in Eq. 61 can take one of four values, depending on the configuration of the two spins involved. It is more convenient to collect these four terms as the coefficients of a $2 \times 2$-matrix,

$$T_{i,i+1} = \exp(\beta s_i s_{i+1} + \beta h (s_i + s_{i+1})/2) ,$$

Figure 8: **1D Ising model.** Each of the $N$ sites $i$ has two nearest neighbors. Note the periodic boundary conditions, which are enforced by demanding $S_0 = S_N$, i.e. the 1D system becomes a closed loop of $N$ sites.
or more explicitly
\[
\begin{bmatrix}
  e^{\beta(J+h)} & e^{-\beta(J)} \\
  e^{-\beta(J)} & e^{\beta(J-h)}
\end{bmatrix}
\]

(62)

where the rows correspond to the two values of \(s_i = \pm 1\) and columns correspond to the two values of \(s_{i+1} = \pm 1\). It is more intuitive here to think of summing over configurations of bonds, rather than configurations of spins. In more mathematical language, what one is doing here is to switch to the dual lattice, the lattice of bonds. Note that in the one dimensional nearest-neighbor Ising model, the dual lattice is still a one-dimensional chain. For a 2D square lattice, the dual lattice is also a square lattice, while for a 2D triangular lattice, the dual becomes the hexagonal lattice, since each site there has six nearest neighbors.

We return to the one-dimensional problem: The partition function thus turns into a product of \(N\) identical \(2 \times 2\) matrices, where matrix multiplication beautifully ensures the constraint that the choice of spin orientation at site \(i\) has to be consistent from one matrix to the next (the configuration of columns for one matrix matches the configuration of rows for the neighboring). The partition function hence simplifies to

\[
Z_N = \sum_{s_0 = \pm 1} (T^N)_{0,0} = \text{Tr}(T^N) = \sum_i \lambda_i^N ,
\]

where \(\lambda_i\) are the eigenvalues of \(T\).

The problem hence boils down to finding the eigenvalues of \(T\), i.e. solving \(\det(T - \lambda I) = 0\).

This gives

\[
\left( e^{\beta(J+h)} - \lambda \right) \left( e^{\beta(J-h)} - \lambda \right) - e^{-2\beta J} = 0 ,
\]

yielding

\[
\lambda_{1/2} = e^{\beta J} \cosh \beta h \pm \sqrt{e^{2\beta J} \sinh^2 \beta h + e^{-2\beta J}}.
\]

**Free energy.** In the thermodynamic limit, i.e. \(N \to \infty\), the free energy per site is easy to compute. Assuming that the eigenvalues are listed in decreasing magnitude, i.e. \(\lambda_1 > \lambda_2\),

\[
f = -k_B T \lim_{N \to \infty} \frac{1}{N} \ln \left( \lambda_1 + \lambda_2 \right)
\]

In the thermodynamic limit, the ratio \(\left( \frac{\lambda_2}{\lambda_1} \right)^N \to 0\) and the free energy per site is just

\[
f = -k_B T \ln \lambda_1
\]

\[
= -k_B T \ln \left[ e^{\beta J} \cosh \beta h + \sqrt{e^{2\beta J} \sinh^2 \beta h + e^{-2\beta J}} \right].
\]
Critical Phenomena, by Jan O. Haerter

Figure 9: Spin-spin correlation function. Spin chain with two spins separated by $R$ sites, $\tanh x$, with $x = \beta J$, is the correlation function between two neighboring spins.

In the zero temperature limit, $\beta \to \infty$, 

$$f \to -k_B T \ln \left[ e^{\beta J} (\cosh \beta h + \sinh \beta h) \right] = -J - H ,$$

which is the ground state energy of a single spin.

**Correlation function.** To compute the correlation function (Fig. 5), in principle, the transfer matrix method could be exploited, both for $h = 0$ and $h \neq 0$. However, for $h = 0$, i.e. absence of an external magnetic field, there is a simpler way to compute the correlation between two spins that are separated by $R$ lattice sites. Consider first the correlation of any two neighboring spins, i.e. sites with a separation of unity:

$$\Gamma(1) = \langle s_i s_{i+1} \rangle = \frac{\sinh \beta J}{\cosh \beta J} = \tanh \beta J ,$$

a result that is simply obtained by summing over the two different values of the bond energy between sites $i$ and $i + 1$, namely $\pm J$. Now consider two spins that are separated by a distance of $R$ lattice sites instead:

$$\Gamma(R) = \langle s_i s_{i+R} \rangle , \quad (63)$$

and realize that the expectation value in Eq. 63 will not change by inserting products $s_j s_j = 1$, hence

$$\Gamma(R) = \langle s_i s_{i+1} s_{i+1} s_{i+2} s_{i+2} \ldots s_{i+R} \rangle .$$

Note that the expectation value now factorizes into a product of bond expectation values, when one simply considers the energy of each bond, not the sites themselves, i.e.

$$\Gamma(R) = \tanh^R \beta J .$$

Note that as $R$ increases, the correlation falls off exponentially with distance. There is hence no long-ranged order in the 1D Ising model, which would require a power-law dependence on distance.
Exercises

1. **Pair correlation function in 1D.** (repetition of notes above)
   The 1D Ising model has the advantage of showing an exact solution, but has the disadvantage, that it has no finite critical temperature, i.e. $T_c = 0$.

   To see a manifestation of this, consider now the spin-spin correlation function
   \[ \Gamma(1) = \langle s_i s_{i+1} \rangle \]
   for two neighboring spins in the absence of an external magnetic field ($h = 0$). Can you compute the correlation function of two spins separated by a distance $R$, i.e.
   \[ \Gamma(R) = \langle s_i s_{i+R} \rangle \]
   by making use of $\Gamma(1)$?

   Discuss that the dependence $\Gamma(R) \sim p(T)^R$ with $p(T) < 1$, i.e. that correlations decay exponentially at finite $T > 0$. What about $T = 0$?
   *(Hint: Make use of multiple insertions of unity and think more of summations over bonds than sites.)*

2. **No finite temperature phase transition in 1D Ising model.**
   The free energy of the $h = 0$ ferromagnetic Ising model for a state of fixed energy $E_\Omega$ can be calculated from
   \[ F_\Omega = E_\Omega - TS_\Omega = -J \sum_{\langle ij \rangle} s_i s_j - T k_B \log(\#\text{states}) . \]
   Here, $\Omega$ indicates possible multiplicity of states of the same internal energy.

   (i) Consider first a simple spin-$\frac{1}{2}$ Ising chain and compute the ground state internal energy and entropy to obtain $F_\Omega$. Consider then an excited state with a single domain wall along the chain. Compute the corresponding internal energy and entropy. Use the free energy difference to argue for a breakdown of the ordered state for any $T > 0$.

   (ii) Consider now a square lattice (2D) and again the formation of a domain wall, described by a region of $\uparrow$-spin enclosed by a region of $\downarrow$-spin. Take the region of $\uparrow$-spins to be bounded by a path of length $n$ lattice spacings. Estimate the number of such paths by approximating the upper bound for the number of paths. Then again compute the free energy difference and argue for a finite transition temperature.
6 Mean field solution

Various approximate approaches to the solution of the Ising model are termed “mean field”. In essence, mean field theory builds on the assumption, that the surroundings of each spin, or more generally each particle, act as a joint “field” on this particle, thereby, the individual correlations to each surrounding site are ignored (Fig. 6).

In the following, we give two approaches.

6.1 Using a trial Hamiltonian

We here want to approximate the solution to the zero-external-field Ising Hamiltonian. In mean field theory, it is assumed that each spin of the system interacts with its surroundings, but the surroundings represent a “mean field”, i.e. there is no explicit interaction with each nearest-neighbor site, but it is assumed that all nearest-neighbor sites produce a joint field, which is the same for each site of the system. The Hamiltonian we want to solve is

$$\mathcal{H} = -J \sum_{ij} s_i s_j,$$

where a ferromagnetic coupling $J > 0$ is taken.

We use the Bogoliubov inequality, which states that

$$F \leq \Phi = F_0 + \langle \mathcal{H} - \mathcal{H}_0 \rangle_0,$$

where $\mathcal{H}_0$ is the zero-field Hamiltonian.

Figure 10: Cartoon of the mean field assumption. The surroundings of a given site act as an effective “mean field” $h$, thereby any correlations between individual sites are ignored. The equation is closed by assuming that the site itself contributes to the mean field seen by its neighbors. By this assumption, a self-consistent equation is obtained for the field $h$, which is proportional to the magnetization of each spin $m$. 

![Cartoon of the mean field assumption](image-url)
where \( F \) is the true free energy, \( F_0 \) is the free energy obtained from a trial Hamiltonian \( \mathcal{H}_0 \) and \( \langle ... \rangle_0 \) denotes the expectation value computed in the ensemble defined by \( \mathcal{H}_0 \). The trial Hamiltonian \( \mathcal{H}_0 \) thereby depends on a parameter \( h_0 \), which is then used to minimize \( \Phi \). A common choice is the take \( \mathcal{H}_0 \) as the free Hamiltonian, i.e.

\[
\mathcal{H}_0 = -h_0 \sum_i s_i .
\]

The trial free energy is (see exercises)

\[
F_0 = -N k_B T \ln(2 \cosh \beta h_0) ,
\]

and the expectation value of spin is

\[
\langle s \rangle_0 = \tanh \beta h_0 .
\]

We now evaluate the expectation value in Eq. 65, yielding

\[
\langle \mathcal{H} - \mathcal{H}_0 \rangle_0 = \sum_{\{s\}} \frac{(-J \sum_{\langle ij \rangle} s_is_j + h_0 \sum_i s_i) \exp(\beta h_0 \sum_i s_i)}{\sum_{\{s\}} \exp(\beta h_0 \sum_i s_i)}
\]

\[
= -J \sum_{\langle ij \rangle} \langle s_i \rangle_0 \langle s_j \rangle_0 + h_0 \sum_i \langle s_i \rangle_0 ,
\]

note the difference between the symbols \( \mathcal{H}_0 \) and \( h_0 \). Using translational invariance of the lattice (all sites are equivalent),

\[
\langle s \rangle_0 \equiv \langle s_i \rangle_0 = \langle s_j \rangle_0 ,
\]

we have

\[
\langle \mathcal{H} - \mathcal{H}_0 \rangle_0 = -JzN\langle s \rangle_0^2/2 + Nh_0\langle s \rangle_0 .
\]

The approximate free energy then is

\[
\Phi = -N k_B T \ln(2 \cosh \beta h_0) - JzN\langle s \rangle_0^2/2 + Nh_0\langle s \rangle_0
\]

\[
= -N k_B T \ln(2 \cosh \beta h_0) - JzN \tanh^2 \beta h_0 + Nh_0 \tanh \beta h_0 .
\]

Minimizing w.r.t. \( h_0 \) we obtain

\[
\frac{d\Phi}{dh_0} = N k_B T \tanh \beta h_0 - JzN \tanh \beta h_0 k_B T \cosh^2 \beta h_0 + \frac{N}{k_B T} h_0 \frac{1}{\cosh^2 \beta h_0} + N \tanh \beta h_0
\]

\[
= \frac{N}{k_B T \cosh^2 \beta h_0} (h_0 - Jz \tanh \beta h_0) .
\]

Minimization requires the last factor to vanish, i.e. \( h_0 = Jz \langle s \rangle_0 \). This gives a condition for the mean field magnetization (compare Fig. 6.1):

\[
\langle s \rangle_0 = \tanh(\beta Jz \langle s \rangle_0) .
\]

(66)
Inserting this into the approximate free energy $\Phi$ yields the mean field free energy:

$$\Phi_{mf} = -Nk_B T \ln(2 \cosh \beta J z \langle s \rangle_0) + \frac{JzN}{2} \langle s \rangle_0^2.\quad (67)$$

**Finding the critical temperature $T_c$.** Recall that the critical temperature is defined as the temperature, where a transition from a ferromagnetic to a paramagnetic phase is observed. The expression for the mean field magnetization (Eq. 66) implicitly defines $\langle s \rangle_0$, even though an analytical solution does not exist. However, one does not need an explicit expression for $\langle s \rangle_0$, if one only is interested in the transition temperature $T_c$, i.e. where magnetization just barely becomes finite.

A practical way to obtain this transition is to just plot both sides of Eq. 66 as a function of $\langle s \rangle_0$. The LHS just gives a straight line of slope unity, while the RHS gives a monotonically increasing concave function, however, the slope depends on temperature. The concavity guarantees that, if the slope is less than unity at $\langle s \rangle_0 = 0$, there will be no further intersections for positive (or negative, by symmetry) magnetization.

All we need to do is hence to look for an argument of the tanh that gives

$$\lim_{\langle s \rangle_0 \to 0} \frac{\partial \tanh(\beta J z \langle s \rangle_0)}{\partial \langle s \rangle_0} \approx \beta J z = 1,$$

i.e. the critical temperature $T_c$ becomes

$$T_c = \frac{J z}{k_B},$$

a quantity that notably only depends on the coordination number $z$, that is, the number of nearest neighbors of each site, but not on the dimensionality of the lattice.
Now that $T_c$ is known, we can define the dimensionless temperature

$$t \equiv \frac{T - T_c}{T_c},$$

i.e. $T = T_c(t + 1) = \frac{Jz}{k_B}(t + 1)$.

How does magnetization scale as we approach the critical point, i.e. what is the exponent $\beta$ in $M \sim (−t)^\beta$? Since this still only requires small deviations from $T_c$ and small values of $\langle s \rangle_0$, it is sufficient to expand the $\tanh$ in a Taylor series:

$$\langle s \rangle_0 = \tanh(\beta Jz \langle s \rangle_0) = \tanh\left(\frac{1}{t + 1} \langle s \rangle_0\right),$$

yielding

$$\langle s \rangle_0 = \frac{\langle s \rangle_0}{1 + t} - \frac{(\langle s \rangle_0)^3}{3(1 + t)^3} + \mathcal{O}\left(\frac{(\langle s \rangle_0)^5}{(1 + t)^5}\right)$$

$$= \langle s \rangle_0(1 - t) - \frac{(\langle s \rangle_0)^3}{3} + \mathcal{O}\left(\langle s \rangle_0^2, \langle s \rangle_0^4, \langle s \rangle_0^5\right).$$

Hence, $-t = (\langle s \rangle_0^2)/3$, or

$$\langle s \rangle_0 = 3(-t)^{1/2},$$

i.e. $\beta_{mf} = 1/2$, that is, when temperature is lowered from $T_c$, the magnitude of total magnetization increases as a square root dependency with the temperature difference $T_c - T$.

Similarly, we can now evaluate the specific heat critical exponent $\alpha$: $C_H \sim |t|^{-\alpha}$:

$$C_H = T \left(\frac{\partial S}{\partial T}\right)_h,$$

where the external field $h$ is held fixed and the entropy $S = -\left(\frac{\partial F}{\partial T}\right)$ (exercise).

As result, it is found that

$$T < T_c: C_H = \frac{3}{2}Nk + \mathcal{O}(t)$$

$$T > T_c: C_H = 0,$$

hence, the specific heat has a jump discontinuity at $T_c$, but is otherwise constant. Therefore, $\alpha_{mf} = 0$.

It is also possible to compute the critical isotherm exponent $\delta$, which is defined at $t = 0$, as $h \sim |M|^\delta \text{sgn}(M)$. This requires the addition of a small magnetic field $h$ to the Ising Hamiltonian:

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j - h \sum_i s_i,$$

hence,

$$\langle s \rangle_0 = \tanh(\beta (Jz \langle s \rangle_0 + h)).$$
With $T = T_c$, $\beta Jz = 1$, hence $\langle s \rangle_0 = \tanh(\langle s \rangle_0 + h/Jz)$, which can now be expanded for small $\langle s \rangle_0$ and $h$, yielding

$$\langle s \rangle_0 = \langle s \rangle_0 + \frac{h}{Jz} - \frac{\langle s \rangle_0^3}{3} + \mathcal{O} \left( \langle s \rangle_0^2 h, \langle s \rangle_0 h^2, h^3, \langle s \rangle_0^5 \right).$$

Therefore, $h \sim \langle s \rangle_0^3$ and $\delta_{mf} = 3$.

In analogous ways, the susceptibility exponent $\gamma$ in $\chi_T \sim |t|^{-\gamma}$ can be computed, yielding $\gamma_{mf} = 1$ (left as exercise).

### 6.2 Mean field solution (alternative approach)

While more elegant and general, the use of a trial Hamiltonian (Sec. 6.1) comes with a more technical nature of the derivation. A simpler, yet more “hands on” approach is the following: Take again the Ising Hamiltonian

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j - h \sum_i s_i. \quad (69)$$

The average magnetization per site is

$$m = \frac{1}{N} \sum_{j=1}^N \langle s_j \rangle.$$

We can re-write the spin of each particle relative to this average as

$$s_i = m + (s_i - m)$$

and obtain for the product of spins in Eq. 69

$$s_i s_j = (m + (s_i - m))(m + (s_j - m)) = m^2 + m(s_i - m) + m(s_j - m) + (s_i - m)(s_j - m). \quad (70)$$

Assuming that fluctuations are small (generally a poor assumptions), we neglect the second-order fluctuation term (4th term in Eq. 70). This is the basis of the mean field assumption, i.e. that products of spins with spins can be ignored and only products of spins and a “mean field” need to be taken into account. This assumption then yields the mean field energy

$$E_{MF} = -J \sum_{\langle ij \rangle} (-m^2 + m(s_i + s_j)) - h \sum_i s_i. \quad (71)$$

We have hence replaced the (microscopic) interaction between each spin and each neighbor by an average magnetic field, produced jointly by all the neighbors. Eq. 71 can be simplified by noting that $-J \sum_{\langle ij \rangle} (-m^2) = \frac{JNz}{2} m^2$, where $z$ is the coordination number, i.e. number of nearest neighbors, of the lattice;
further, $\sum_{\langle ij \rangle} (s_i + s_j) = z \sum_j s_j$, since all spins are equivalent. The mean field energy then is

$$E_{MF} = \frac{JNz}{2} m^2 - (Jzm + h) \sum_{j=1}^{N} s_j.$$ 

We can now write the mean field partition function as

$$Z_{MF} = \sum_{\{s_j\}} \exp \left( -\beta E_{MF} \right)$$

$$= \exp \left( -\beta \frac{NJzm^2}{2} \right) \sum_{s_1} \cdots \sum_{s_N} \prod_{j=1}^{N} \exp \beta (Jzm + h) s_j$$

$$= \exp \left( -\beta \frac{NJzm^2}{2} \right) \left[ \sum_{s_1} \exp \beta (Jzm + h) s_1 \right] \cdots \left[ \sum_{s_N} \exp \beta (Jzm + h) s_N \right]$$

$$= \exp \left( -\beta \frac{NJzm^2}{2} \right) [\cosh(Jzm\beta + h\beta)]^N. \quad (73)$$

It is now straightforward to compute the magnetization per site:

$$m = \frac{1}{N} \sum_{j=1}^{N} \langle s_j \rangle = \langle s \rangle,$$

where translational invariance was assumed. Hence

$$m = \frac{1}{Z_{MF}} \exp \left( -\beta \frac{NJzm^2}{2} \right) [2 \cosh( Jzm\beta + h\beta )]^{N-1} [2 \sinh( Jzm\beta + h\beta )]$$

$$= \tanh( Jzm\beta + h\beta ),$$

which is, for $h = 0$, again the self-consistent equation for $m$ (compare Fig. 6.1).

The mean field free energy can be computed from Eq. 73 as usual, yielding

$$f_{MF} = -\frac{k_B T}{N} \ln Z_{MF} = \frac{Jzm^2}{2} - k_B T \ln [2 \cosh( Jzm\beta + h\beta )]. \quad (75)$$

For the following, it is useful to work in dimensionless units by dividing Eq. 75 through by $zJ$ and introducing the rescaled quantities $h' = \frac{h}{zJ}$ as well as $\theta = \frac{k_B T}{zJ}$. We then have

$$\frac{f_{MF}}{zJ} = m^2 + \theta \ln 2 - \theta \ln \cosh \left( \frac{m + h'}{\theta} \right). \quad (76)$$

**Mean field specific heat.** In the following, we will compute the specific heat $c_H$ (in the absence of a magnetic field). We will find that $c_H$ has a jump discontinuity (first order transition) as $T_c$ is crossed. Consider what we have: the free energy is presently a function of temperature $\theta$ and magnetization $m$. The latter, in turn, depends on temperature. Keeping this in mind, we nonetheless want to find a condition for when the free energy is minimized through finite
values of \( m \), i.e. when the system “decides” to break the symmetry w.r.t. the two spin configurations.

As will be discussed further (Sec. 7), a fourth order polynomial in \( m \) is a reasonable starting point for observing such a transition. Even without knowing this, one might be tempted to expand \( \cosh (m/\theta) \) in Eq. 76 in a Taylor series, yielding

\[
\frac{f_{MF}}{zJ} = \frac{m^2}{2} - \theta \ln 2 - \theta \ln \left[ 1 + \frac{1}{2} \frac{m^2}{\theta^2} + \frac{1}{24} \frac{m^4}{\theta^4} + \mathcal{O} \left( \frac{m^6}{\theta^6} \right) \right]. \tag{77}
\]

Using the additional expansion \( \ln(1 + x) = x - \frac{x^2}{2} + \ldots \) the final logarithm in Eq. 77 simplifies to yield

\[
\frac{f_{MF}}{zJ} = \frac{m^2}{2} - \theta \ln 2 - \theta \ln \left( 1 + \frac{1}{2} \frac{m^2}{\theta^2} - \frac{1}{12} \frac{m^4}{\theta^4} + \mathcal{O} \left( \frac{m^6}{\theta^6} \right) \right)
= \frac{m^2}{2} \left( 1 - \frac{1}{\theta} \right) - \theta \ln 2 + \frac{m^4}{12\theta^3} + \mathcal{O} \left( \frac{m^6}{\theta^6} \right).
\]

We are now in a position to ask for extrema of \( f_{MF} \) regarding \( m \), which require that we set the derivative \( \partial f_{MF}/\partial m = 0 \), hence

\[
\frac{1}{zJ} \frac{\partial f_{MF}}{\partial m} = m \left( 1 - \frac{1}{\theta} \right) + \frac{1}{3} \frac{m^3}{\theta^3} = 0.
\]

This leads to

\[
m^2 = 3(1 - \theta)\theta^2 = 3(-t)\theta^2, \tag{78}
\]

where we have re-introduced the previous reduced temperature \( t \). Note that \( \theta^2 \) in the vicinity of \( T_c \) acts as a constant, since the relevant variations occur in the variable \( t \) (not \( \theta \), is the small quantity). Note that Eq. 78 again delivers the mean field critical exponent \( \beta = 1/2 \), and further allows us to substitute \( m^2 \) back into the free energy \( f_{MF} \). This yields

\[
\frac{f_{MF}}{zJ} = -\frac{3}{2}(1 - \theta)^2 - \theta \ln 2 + \frac{3}{4} \theta(1 - \theta)^2 + \text{higher order terms}
\]

Substituting “solitary” appearances of \( \theta \) by unity (we are very close to \( T_c \)), we have

\[
\frac{f_{MF}}{zJ} = -\frac{3}{4}(1 - \theta)^2 - \theta \ln 2 + \text{higher order terms},
\]

and can check that, with \( t < 0 \) the free energy is actually reduced as compared to the symmetric choice of \( m = 0 \) — hence, free energy is minimized, not maximized for our choice of \( m^2 \).

We are now in a position to proceed with entropy \( S \) and specific heat \( c_H \) as derivatives of the free energy, i.e.

\[
S = -\frac{\partial f_{MF}}{\partial T} = -\frac{\partial f_{MF}}{\partial \theta} \frac{\partial \theta}{\partial T} = -k_B \left( \frac{3}{2} (1 - \theta) + \ln 2 \right).
\]
The specific heat becomes
\[ c_H = T \frac{\partial S}{\partial T} = \theta \frac{\partial S}{\partial \theta} = \frac{3}{2} k_B \theta. \]

Taking the limit \( T \to T_c \) is now simply the statement \( \theta = 1 \), hence \( c_H = \frac{3}{2} k_B \).

Since \( c_H = \text{const} \), the specific heat critical exponent \( \alpha_{MF} = 0 \).

For \( T > T_c \), \( m = 0 \) and the paramagnetic free energy only depends linearly on temperature \( (f_{MF} = -k_B T \ln 2) \), yielding constant entropy \( S_{\text{para}} = k_B \ln 2 \).

Hence, also for \( T > T_c \) the specific heat critical exponent \( \alpha_{MF} = 0 \).

Mean field magnetic susceptibility. We return to the self-consistency condition

\[
m = \tanh \beta (J_z m + h) = \tanh \left( \frac{J_z}{k_B T} m + \frac{h}{k_B T} \right) = \tanh \left( \frac{1}{1 + t} m + \frac{1}{J_z} \frac{h}{1 + t} \right),
\]

using the usual replacements \( \frac{J_z}{k_B T} = \frac{1}{1 + t} \) and \( \frac{1}{k_B T} = \frac{1}{1 + t} \).

Note that, as an implicit equation in \( m \), Eq. 79 cannot directly be solved for \( m \) to evaluate \( \partial m / \partial h \). However, one could apply \( \partial / \partial h \) to both sides of the equation, hoping that this will make it possible to proceed.

Before doing so, we remember that we are looking for solutions near the critical temperature, where we expect \( m \) to be very small. For this reason, we expand \( \tanh x = x - x^3 + \ldots \) to low order in a power series, where we introduced \( x \equiv \frac{1}{1 + t} m + \frac{1}{J_z} \frac{h}{1 + t} \).

We find that
\[
\frac{\partial m}{\partial h} = (1 - x^2) \frac{\partial x}{\partial h},
\]
where
\[
\frac{\partial x}{\partial h} = \frac{1}{1 + t} \left( \frac{\partial m}{\partial h} + \frac{1}{J_z} \right).
\]

Taking now the limit of \( h \to 0 \), we have
\[
\lim_{h \to 0} (1 - x^2) = \frac{(1 + t)^2 - m^2}{(1 + t)^2}
\]
and the susceptibility becomes
\[
\chi = \frac{\partial m}{\partial h} \bigg|_{h \to 0} = \frac{1}{(1 + t)^3} \left( \chi + \frac{1}{J_z} \right) ((1 + t)^2 - m^2).
\]

After some further transformations we have
\[
\chi = \frac{1}{J_z} \frac{(1 + t)^2 - m^2}{t + m^2}.
\]
Considering that \( t \) and \( m^2 \) are both small and of similar order while \( 1 \gg t \), we can safely ignore the term \(+t\) in the numerator and obtain

\[
\chi = \frac{1 - m^2}{Jz t + m^2}.
\]

Given that near \( T_c \) for \( T < T_c \) \( m \) and \( t \) are related by Eq. 68 and similarly 78, in the ferromagnetic case we have that

\[
\chi = \frac{1}{Jz} \frac{1 + 3t}{-2t} \sim \frac{1}{-2Jzt},
\]

while in the paramagnetic case \((t > 0, m = 0)\)

\[
\chi = \frac{1}{Jzt}.
\]

However, in both limits the critical exponent \( \gamma = 1 \) (in \( \chi \sim |t|^{-\gamma} \)).

**Exercises**

1. **Specific heat and susceptibility in the mean field approximation.**
   (reproducing results above)
   Starting from the mean field free energy with \( h = 0 \), expand to fourth order in \( m \) and find the minimum in free energy to obtain the mean field magnetization as function of temperature (it is useful to introduce the dimensionless temperature \( \theta \equiv \frac{k_B T}{Jz} \), where \( J \) is the coupling and \( z \) the coordination number of the lattice (number of neighbors of a site.) The free energy is now only a function of temperature. By taking the derivative w.r.t. temperature, obtain entropy \( S \). Differentiating again w.r.t. temperature, obtain \( c_v \). Discuss the difference of \( c_v \) for \( t > 0 \) and \( t < 0 \) near \( t = 0 \). What is the critical exponent \( \alpha \) (in \( C_H \sim |t|^\alpha \))?
   By using the self-consistency expression

\[
m = \tanh(\beta(Jzm + h))
\]

and inserting the reduced temperature \( t = (T - T_c)/T_c \), obtain the magnetic susceptibility \( \chi_T \equiv \partial m/\partial h \) (i.e. the limit \( h \to 0 \) is taken before the limit \( t \to 0 \)). Can you obtain the critical exponent \( \gamma \) (in \( \chi_T \sim |t|^{-\gamma} \))? (Hint: Start by expanding out \( \tanh x \approx x - x^3/3 \) and ignore higher order contributions.)

2. **Landau free energy from mean field free energy.**
   By expanding out the mean field free energy (Eq. 75) to fourth order in \( m \), show that the resulting expression in symmetric regarding the transformation \( m \to (-m) \) and that the coefficient \( a_2 \) of the quadratic term is temperature dependent (i.e. \( a_2(T)m^2 \)).
7 Landau theory

Landau proposed a phenomenological approach that does not consider the details of the interaction, but simply writes an expression for the free energy as a power series of the order parameter, the magnetization $m$, i.e. $F(m) = \sum a_q m^q$. The only constraint imposed was that the functional form should respect the symmetry of the problem, i.e. in the absence of an external magnetic field both orientations of spin should be equivalent. Hence, only even powers of $m$ should be allowed, yielding

$$F(m) = F_0 + a_2 m^2 + a_4 m^4 + \text{higher order terms} \tag{80}$$

for the first few terms.

Dropping all terms beyond the quartic contribution, one additionally has to consider that free energy should be a minimum at equilibrium. However, a minimum can only be obtained, if the coefficient $a_4 > 0$, otherwise there would be no lower bound to $F$. The coefficient $a_2$ may however vary and it was Landau’s contribution to consider that it might depend on temperature. Let us distinguish several cases:

- $a_2 > 0$: $F(m)$ has only one minimum, namely at $m = 0$,
- $a_2 < 0$: $F(m)$ has two additional minima,
- $a_2 = 0$: This is the transition between the case of a single minimum and three minima.

If we now choose $a_2$ to have an explicit temperature dependence, $a_2 = \tilde{a}_2 t$, then a continuous transition occurs at $t = 0$.

**Figure 12:** Landau free energy for different values of temperature. Zero external field ($h = 0$). For $T > T_c$ and $T = T_c$ the minimum of the free energy is located at $m = 0$. For $T < T_c$, there are two minima which are symmetrically located at finite magnetization.
The reader is encouraged to check that our previous expansion of the mean field free energy (Eq. 77), obtained from the microscopic partition function, yields a similar temperature dependence as Eq. 80.

**Critical exponents.** It is even possible to compute critical exponents from Landau’s theory. Consider again $\beta$, in $m \sim (-t)^\beta$ near $t = 0$. First, we obtain the value of magnetization when $t < 0$ by searching for extrema in $F$:

$$\frac{dF(m)}{dm} = 0 = 2\tilde{a}_2tm + 4a_4m^3 = m(2\tilde{a}_2t + 4a_4m^2),$$

yielding $m = 0$ and

$$|m| = \sqrt{t\tilde{a}_2/2a_4}, \quad (81)$$

hence $\beta = 1/2$. Notably, this is the same critical exponent which we previously obtained within the explicit mean field derivation.

The specific heat critical exponent is obtained by differentiating $F$ twice w.r.t. $t$. Using Eq. 81 in the free energy (Eq. 80), we have for $t < 0$

$$F = F_0 - \frac{\tilde{a}_2t^2}{4a_4} + \mathcal{O}(t^3), \quad (82)$$

hence, the specific heat tends to a constant as $t \to 0^-$. For $t > 0$, $m = 0$ and the specific heat vanishes, we hence recover the jump discontinuity found in the mean field solution, and $\alpha = 0$.

To obtain $\gamma$ and $\delta$ one needs to add a magnetic field term to the free energy, hence breaking the previous symmetry regarding overall spin flip. The free energy then reads

$$F = F_0 - hm + \tilde{a}_2tm^2 + a_4m^4, \quad (83)$$

Minimizing w.r.t. $m$ gives

$$\frac{dF}{dm} = -h + 2\tilde{a}_2tm + 4a_4m^3 = 0,$$

which yields the critical isotherm (setting $t = 0$) as $h \sim m^3$, i.e. $\delta = 3$.

My similar means one can also compute the isothermal susceptibility $\chi_T \sim |t|^{-\gamma}$ (exercises).

Overall, the Landau critical exponents are the same as those obtained from the mean-field theory of the Ising model. To see that this is not a surprise, we return to the Ising mean field free energy (Eq. 67):

$$\Phi_{mf} = -Nk_B T \ln(2 \cosh \beta Jz\langle s \rangle_0) + \frac{Jz N}{2} \langle s \rangle_0^2, \quad (84)$$

and expand this in a Taylor series for small $\langle s \rangle_0$. Using

$$\cosh x = 1 + \frac{1}{2}x^2 + \mathcal{O}(x^4), \text{ where } x \equiv \beta Jz\langle s \rangle_0 \text{ and}$$

$$\ln(1 + y) = y - \frac{1}{2}y^2 + \mathcal{O}(y^3), \text{ where } y \equiv \frac{1}{2}x^2,$$
we have
\[ F_{mf} = F_0 + \frac{NJ_z}{2} (s)_0^2 (1 - \beta J_z) + O((s)_0^4) . \]
The factor \( \frac{NJ_z}{2} (1 - \beta J_z) \) can be identified with \( a_2 \), vanishes at \( T = T_c \), becomes negative as \( T > T_c \) and negative as \( T < T_c \).
8 Monte Carlo method

It is important to thoroughly understand so-called *Monte Carlo* methods due to their wide range of applicability. Monte Carlo methods are generally computer simulations which help to compute the ensemble average when analytical approaches fail or are too cumbersome — a situation that is often encountered in statistical physics and condensed matter physics. Monte Carlo methods are widely used in science and technology, also in areas far away from lattice models as we study them here, e.g. traffic flow. Plainly speaking, the aim generally is to obtain an approximation to the expectation value of an observable $A$, i.e.

$$
\langle A \rangle = \frac{\sum_{\{s\}} A \exp(-\beta H)}{\sum_{\{s\}} \exp(-\beta H)}.
$$

Using again the Ising model as our “canonical” example,

$$
H = -J \sum_{\langle ij \rangle} s_i s_j - h \sum_i s_i,
$$

common expectation values are

$$
\langle s_i \rangle = \langle s \rangle = \frac{\sum_{\{s\}} s_i \exp(-\beta H)}{\sum_{\{s\}} \exp(-\beta H)},
$$

$$
\langle s_i s_j \rangle = \frac{\sum_{\{s\}} s_i s_j \exp(-\beta H)}{\sum_{\{s\}} \exp(-\beta H)},
$$

$$
\langle H \rangle = \frac{\sum_{\{s\}} H \exp(-\beta H)}{\sum_{\{s\}} \exp(-\beta H)}.
$$

One could hence imagine to simply sum over all configuration and obtain an exact number for the expectation value of interest. However, even on modern-day computers, summing over $2^N$ configuration for an $N$-site lattice of more than a few dozen sites is prohibitively costly.

But do we really need to sample the entire space of configurations to get a reasonable estimate of the expectation values? The idea of Monte Carlo techniques is, to sample mainly those configurations that are likely to occur. Take intermediate temperatures, where $J/k_B T \sim 1$. Further, take the external field to be absent, i.e. $h = 0$. When all $N$ spins are aligned, the contribution to the partition function is $\exp Nz/2$, where $z$ is the coordination number. Conversely, a state where all spins are anti-aligned gives a contribution of $\exp -Nz/2$. Notably, the former configuration is $\exp Nz$ times more likely that the latter, an enormous number even for modest $N$.

Now the idea is to sample phase space by importance. This can be thought of a *Markov chain*, where, in principle, each state of the system can be visited in finite time. However, the probability of entering states of low likelihood will be reduced — to finally yield the proper Boltzmann distribution of weights as
Figure 13: Cartoon of possible Monte Carlo timeseries. Points show system averages of magnetization \( m \) after various system updates for a Monte Carlo simulation with fixed \( T \) and parameters \( J \) and \( H \), \( n_0 \) and \( n_{max} \) indicate system updates between which the asymptotic behavior is estimated. A “system update” corresponds to \( N \) attempted spin flips, where \( N \) is the system size. Far from \( T_c \) one expects relatively fast convergence, close to \( T_c \) an aspect known as “critical slowing down” causes the convergence time to diverge.

it appears in the partition function. The goal is, to achieve the equilibrium distribution

\[
P^\text{eq}_l = \frac{e^{-\beta E_l}}{\sum_m e^{-\beta E_m}},
\]

when continuing the Markov chain infinitely long. \( l \) labels a given spin configuration and \( P^\text{eq}_l \) is the equilibrium probability of this configuration. This requirement puts constraints on the transition probability between states.

The probability to reside in state \( l \) at time \( t+1 \) is

\[
P_l(t+1) = P_l(t) \left( 1 - \sum_{m \neq l} w_{l \rightarrow m} \right) + \sum_{m \neq l} P_m(t) w_{m \rightarrow l}, \tag{85}
\]

where \( w_{i \rightarrow j} \) labels the transition probability from configuration \( i \) to \( j \) and the summations are carried out to include all possible configurations \( m \). It is further useful to define \( w_{l \rightarrow l} = 1 - \sum_{m \neq l} w_{l \rightarrow m} \), i.e. the probability to remain in configuration \( l \). Note also that \( \sum_m w_{l \rightarrow m} = 1 \), hence compactly

\[
P_l(t+1) = \sum_m P_m(t) w_{m \rightarrow l}.
\]

We check that probabilities are normalized correctly:

\[
\sum_l P_l(t+1) = \sum_{m,l} P_m(t) w_{m \rightarrow l} = \sum_{m,l} P_l(t) w_{l \rightarrow m} = \sum_l P_l(t) = 1.
\]
For the stationary solution we therefore have
\[ P_l(t + 1) = P_l(t) , \]
hence
\[ \sum_m [P^e_{l \rightarrow m} w_{l \rightarrow m} - P^e_{m \rightarrow l} w_{m \rightarrow l}] = 0 . \] (86)

A simple way to achieve the condition in Eq. 86 is to ensure that every term vanishes, i.e.
\[ P^e_{l \rightarrow m} w_{l \rightarrow m} = P^e_{m \rightarrow l} w_{m \rightarrow l} , \]
i.e.
\[ \frac{w_{l \rightarrow m}}{w_{m \rightarrow l}} = \frac{P^e_{m}}{P^e_{l}} = e^{-\beta(E_m - E_l)} \equiv e^{-\beta \Delta E} . \] (87)

Notably, Eq. 87 ensures that probabilities are assigned by the standard Boltzmann weights in the canonical partition function. This condition is referred to as **detailed balance**, which stresses that a balance of probabilities exists between any two states individually. In principle, detailed balance is not required in the Monte Carlo procedure, what *is* strictly required is that equilibrium probabilities are consistent with the Boltzmann distribution. There can be other ways than detailed balance to achieve this, but they are generally much more difficult to prove. A further requirement is **ergodicity**, which in this context means that each state can be visited within infinite time during a Monte Carlo simulation. In practice it is often hard to prove that ergodicity is fulfilled and there are situations where a Monte Carlo simulation can become “trapped” in a local minimum of the free energy.

There are several ways to accomplish this. We therefore label a particular choice of transition probabilities as \( a_{l \rightarrow m} \), to distinguish from the general \( w_{l \rightarrow m} \). We make the ansatz that \( a_{l \rightarrow m} \) should be a function of \( e^{-\beta \Delta E} \), i.e.
\[ a_{l \rightarrow m} = F(e^{-\beta \Delta E}) , \]

by symmetry hence
\[ a_{m \rightarrow l} = F\left(\frac{1}{e^{-\beta \Delta E}}\right) = F\left(\frac{1}{x}\right) , \]
with \( x \equiv e^{-\beta \Delta E} \).

It results that
\[ \frac{a_{l \rightarrow m}}{a_{m \rightarrow l}} = \frac{F(x)}{F(1/x)} = x , \]
whence it must be ensured that \( 0 \leq F(x) \leq 1 \) for meaningful transition probabilities. The choice of \( F(x) \) is not unique. Popular choices are

1. \( F(x) = \min(x, 1) \), Metropolis algorithm,
2. \( F(x) = \frac{x}{1 + x} \), heat bath algorithm,
3. $F(x) = \frac{1}{2} (1 - \tanh(\beta \Delta E/2))$, Glauber dynamics.

**Practical implementation on a computer.**

The basic set-up of a Monte Carlo simulation is rather straightforward:

- set up lattice sites $i$ and spins $s_i$, define Hamiltonian $H$, define total number of steps $n_{\text{max}}$ and $n_0 < n_{\text{max}}$,
- set the system to an initial configuration of spins (either a random configuration or one that is meaningful for the problem of interest),
- flip a spin (note the example in Fig. 8), compute $r = e^{-\Delta E/k_B T}$, generate random number $q$ between $[0, 1]$, if $r > q$ perform the Monte Carlo move (e.g. flip the spin), otherwise do not,
- compute $A_n$, i.e. the expectation value of $A$ at time step $n$, if $n > n_0$, if $n \leq n_0$, we are still in the period considered transient,
- repeat until $n_{\text{max}}$ is reached,
- calculate $\langle A \rangle = \frac{1}{n_{\text{max}} - n_0} \sum_{n>n_0} A_n$.

Difficulties usually lie in the proper choice of system size $N$, the choice of the transient period $n_0$, and the duration of the sampling period $n_{\text{max}}$. Generally, fluctuations increase in the vicinity of $T_c$ and achieving robust results may require increasing both system size and sampling time.

**Critical slowing down.**

One well-known issue with Monte Carlo simulations is that near the critical temperature $T_c$ the correlation length of the lattice diverges (i.e. $\xi \sim t^{-\nu}$, see also the discussion following Eq. 30), hence clusters of arbitrary size form.
Figure 15: Performing the Monte Carlo step. Example of a spin flip by which the change of energy is negative for $J > 0$ and $h > 0$. In the Metropolis algorithm this step would always be accepted. Imagine going the opposite direction: The energy difference would be $\Delta E = +4J + 2h$. The probability of accepting this move would then become $\exp(-\beta(4J + 2h))$. Note also that $\Delta E$ can be computed entirely locally, since the remainder of the lattice maintains its energy. Considering this speeds up the computation enormously.

Within these clusters, any Monte Carlo update is unlikely to lead to any long-lasting changes and the overall correlation time $\tau$, which for an observable $A$ can be defined as

$$\tau = \frac{\int_0^\infty dt \langle [A(t) - \langle A \rangle] \rangle}{\int_0^\infty dt \langle [A(t) - \langle A \rangle] \rangle},$$

(88)

can be shown to diverge, i.e. $\tau \sim \xi^z \sim t^{-z\nu}$. The number $z$ is thereby a dynamical critical exponent associated with the observable $A$, and $\langle A \rangle$ is the equilibrium average of $A$, i.e. the average of $A$ after the system has reached an equilibrium configuration. Since the autocorrelation time diverges, it becomes more and more time consuming to achieve statistically independent samples of the system, as $T_c$ is approached. There are sophisticated methods to (partially) alleviate the problem of statistical slowing down, e.g. cluster update algorithms, which however come with their own set of complications [6]. A useful precaution to at least quantify the required sampling time is to measure the autocorrelation $C_A(k)$ as the simulation is running:

$$C_A(t) = \frac{\langle A_n A_{n+k} \rangle - \langle A_n \rangle \langle A_{n+k} \rangle}{\langle A_n^2 \rangle - \langle A_n \rangle^2}.$$ 

$n$ and $k$ are “times” measured in units of Monte Carlo updates, where one Monte Carlo update represents the attempted update of $N$ sites ($N$ is system size). In general, $C_A(t) \sim \exp(-t/\tau_{auto})$, hence $\tau_{auto}$ can be estimated and one can decide how many steps are required for a large enough, independent, sample. More more details on Monte Carlo methods the reader is referred to the literature [6].
Exercises

Monte Carlo Simulation.
Consider a 2D spin-$\frac{1}{2}$ Ising model on a square lattice. Write a computer program (choose your favorite programming language) where you define the sites $i$ and their spins $s_i$. Make sure to store your program, so that we can build on it later on. Start with a small number of sites, perhaps $20 \times 20$. Consider periodic boundary conditions, i.e. each site has four nearest neighbors that are cyclically defined at the boundaries.

1. Define variables for the constants $J$, $h$ and $k_BT$ as well as the maximum number of spin configurations $n_{\text{max}}$, i.e. the number of configurations the program will sample before terminating. Define also a number $n_0 < n_{\text{max}}$ beyond which expectation values should be computed. Define also a function that computes the energy corresponding to a given spin configuration, i.e. $E = -J \sum_{(ij)} s_is_j + h \sum_i s_i$. Further, define a function that flips a (random or deterministic) spin, as well as the exponential $x \equiv \exp \left( -\Delta E / k_BT \right)$ with $\Delta E$ the energy difference between two states $l$ and $m$ and define the acceptance procedure for a transition $a_{l \rightarrow m}$.

2. Make a loop that iterates over the procedure. Starting from a random configuration, carry out the Monte Carlo simulations.

3. For $h = 0$, compute the internal energy $\langle E \rangle$ and the magnetization per site $\langle s \rangle$ as function of $k_BT$, by evaluating the expectation value for all $n > n_0$. Plot a timeseries of $\langle E \rangle$ and $|\langle s \rangle|$ as function of $n_0$. Determine a minimal $n_0$ so that the expectation values are not affected by the transient behavior. (Note that you may need to make adequate adjustments to $n_{\text{max}}$ in this process.)

4. Obtain the expectation values for various temperatures and plot them as function of $k_BT/J$.

5. Repeat the simulation several times for each observable and temperature to obtain a distribution of results for that data point. Use the distribution to quantify the sampling error and plot the error bars.

6. Try to determine $k_BT_c/J$ and $\beta$ numerically and compare your results to the exact results $\langle s \rangle^8 = 1 - (\sinh 2J/kT)^{-4}$ and $\beta = 1/8$ (Onsager’s solution).

7. Plot also the corresponding temperature dependence using a finite magnetic field $h$.

8. Repeat for a larger system size and make notes of your findings for $n_0$ and $n_{\text{max}}$ and discuss (qualitatively) how these values and the error bars depend on the reduced temperature $t$. 
9. Change your lattice geometry to the 4d spin-$\frac{1}{2}$ nearest-neighbor Ising model, find $T_c$ and plot $\langle s \rangle$ as well as $\langle E \rangle$ vs. $k_B T/J$. Compare to the mean field solution with the corresponding value of coordination number $z$. 
9 Series expansion techniques

While brute force computation allows numerical approximations to the state of a certain, finite, system at a given temperature, external field and system parameters, it is generally advisable to seek results for the infinite system — at the very least to check for consistency of the solutions using numerical computations.

9.1 High temperature expansion

We again use the zero field Ising model on a 2D square lattice as a simple example. Consider the term

\[ e^{\beta J s_i s_j} = \cosh \beta J + s_i s_j \sinh \beta J \equiv \cosh \beta J (1 + s_i s_j v) \]

where \( v \equiv \tanh \beta J \). This choice is made in order to have a small parameter, which approaches zero at high temperatures, i.e. \( v \to 0 \) as \( \beta \to 0 \). In other words, \( s_i s_j = 1 \) becomes equally likely as \( s_i s_j = -1 \) in the limit of high temperature.

The partition function is

\[
Z = \sum_{\{s\}} \prod_{\langle ij \rangle} e^{\beta J s_i s_j} = (cosh \beta J)^B \sum_{\{s\}} \prod_{\langle ij \rangle} (1 + s_i s_j v) \]

\[
= (cosh \beta J)^B \sum_{\{s\}} \left( 1 + \sum_{\langle ij \rangle} s_i s_j v + v^2 \sum_{\langle ij \rangle;\langle kl \rangle} s_i s_j s_k s_l + \ldots \right),
\]

where \( B \) denotes the total number of bonds on the lattice, i.e. for a 2D square lattice of \( N \) sites \( B = 2N \). Since \( v \) is the small parameter in inverse temperature, including more orders of \( v \) means approaching lower and lower temperatures.

Consider now terms of the form

\[
\sum_{\{s\}} \left( s_i^{n_i} s_j^{n_j} s_k^{n_k} \ldots \right) = 2^N \text{ all } n_i \text{ even},
\]

\[
= 0 \text{ otherwise.} \quad (89)
\]

Here, \( N \) denotes the total number of spins on the lattice, as before. The result in Eq. 89 means that only closed loops contribute to the sum.

We finally end up with the partition function

\[
Z = (cosh \beta J)^B 2^N (1 + N v^4 + 2N v^6 + \frac{1}{2} N(N+9) v^8 + 2N(N+6) v^{10} + \ldots) \quad (90)
\]
Figure 16: Examples of motifs in high temperature expansion. Note that motifs with “loose ends” do not contribute, while closed loops do.

For simplicity, we introduce $K \equiv \beta J$ in the following. Several transforma-
tions are required to get a handy expression for the free energy.\textsuperscript{6}

In this process, it turns out that terms involving powers greater than linear in \(N\) drop out, which they should, since the free energy should be extensive (i.e. \(\sim N\)). The high-temperature free energy finally is

\[
\mathcal{F} = -NkT \left( \ln 2 + v^2 + \frac{3}{2}v^4 + \frac{7}{3}v^6 + \frac{19}{4}v^8 + \frac{61}{5}v^{10} + \mathcal{O}(v^{12}) \right).
\]

Some applications. Note a few simple lessons from the high-temperature expansion. Returning to our 1D Ising model (Sec. 5), we have a chain of \(N\) spins, which we can apply our formalism to. Consider first the case of open boundary conditions, i.e. sites 0 and \(N - 1\) only have one neighbor each. In that case, no closed loops are possible, and

\[
Z_{1D}^{\text{open}} = 2^N \cosh^B \beta J,
\]

where \(B = N - 1\), i.e. the number of bonds in the open 1D chain. For the periodic chain \((B = N)\), one closed loop of length \(N\) is possible, i.e. a single contribution arises from \(v^N\), and

\[
Z_{1D}^{\text{closed}} = 2^N \cosh^B \beta J(1 + v^N),
\]

\textsuperscript{6}To compute the free energy, one needs to take the logarithm of the partition function, as usual. However, note that this requires to expand in small powers of \(v\); For this purpose, note that, with \(B = 2N\), \(\ln(\cosh K)^B = N \ln(\cosh^2 K)\). Further, the square of \(\cosh K\) can be expanded as a power series in \(v = \tanh K\), i.e.

\[
\cosh^2 K = \frac{1}{1 - v^2} = 1 + v^2 + v^4 + v^6 + v^8 + v^{10} + \mathcal{O}(v^{12}),
\]

which makes it compatible with the final term in Eq. 90. Remembering that \(\ln x = x - x^2/2 + x^3/3 - \ldots\), we get the power series

\[
\ln(\cosh^2 K) = \ln(1 + v^2 + v^4 + \ldots) = v^2 + \frac{v^4}{2} + \frac{v^6}{3} + \frac{v^8}{4} + \frac{v^{10}}{5} + \mathcal{O}(v^{12}).
\]

We also need to “process” the final factor in Eq. 90, i.e.

\[
\ln(1 + X)
\]

with

\[
X \equiv (Nv^4 + 2Nv^6 + \frac{1}{2}N(N + 9)v^8 + 2N(N + 6)v^{10} + \ldots),
\]

and making use of the the power series \(\ln(X) = X - X^2/2 + \mathcal{O}(X^3)\) to second order, we have

\[
\ln(1 + X) = X - \frac{N^2v^8}{2} + 2N^2v^{10} + \mathcal{O}(v^{12})
\]

\[
= Nv^4 + 2Nv^6 + \frac{9}{2}Nv^8 + 12Nv^{10},
\]

where we note that the two terms quadratic in \(N\) have dropped out, hence all remaining terms are linear in system size (\(\sim N\)), as we expect it for physical reasons for the free energy. Putting it all together, we can proceed and write down the free energy.
Figure 17: **Internal energy for the zero-field triangular lattice.** Comparison of a Monte Carlo simulation (red solid curve) and a high-temperature expansion to 6th order in \( v = \tanh \beta J \) (green dashed curve).

where the contribution from \( v^N \) scales to zero at any finite \( T \) in the thermodynamic limit, meaning that the boundary condition does not later the result.

Note also, that it is straightforward to compute spin-spin correlation functions \( \langle s_m s_n \rangle \) using the same formalism, when considering that the product \( s_m s_n \) just acts as an additional factor in any of the products of bonds in the series expansion. this means, that

\[
\langle s_m s_n \rangle = \frac{\sum_{\{s\}} \left( \prod_{\langle ij \rangle} e^{\beta J s_i s_j} \right) s_m s_n}{Z} = \frac{2^N \cosh^B \beta J \sum_{\text{graphs w. even powers except at } m \text{ and } n} v^{\# \text{ bonds}}}{2^N \cosh^B \beta J \sum_{\text{all graphs}} v^{\# \text{ bonds}}}.
\]

In other words, \( m \) and \( n \) should be the endpoints of lines on the lattice. In the 1D lattice this is just the path connecting the points \( m \) and \( n \) and

\[
\langle s_m s_n \rangle = v^{|m-n|} = \exp \left( -\frac{|m-n|}{\xi} \right),
\]

with the correlation length \( \xi \equiv -1/(\ln \tanh \beta J) \). Hence, we recover the result from Sec. 5, that correlations decay exponentially in one dimension.
Figure 18: **Computation of the correlation function in 2D.** Red points show two point between which the correlation function is to be computed. Black and green path indicate possible graphs contributing to the correlation function, both of order \( v^5 \).

### 9.2 Low temperature expansion

At low temperature, it is convenient to order the partition function starting from the ground state energy (given that it is known) and consecutively add excitations of increasing energy. Consider the partition function

\[
Z = e^{-E_0/k_BT} \left( 1 + \sum_{n=1}^{\infty} \Delta Z^{(n)}_N \right) .
\]

\( E_0 \) thereby denotes the ground state energy and \( \Delta Z^{(n)}_N \) are all Boltzmann factors corresponding to excitations relative to the ground state. The label \( (n) \) indicates that \( n \) spins were flipped relative to the ground state.

For example, if one bond is anti-aligned, this leads to an energy “cost” of \( 2J \), yielding a Boltzmann factor \( x = e^{-2J/k_BT} = e^{-2K} \). A single spin flip in a 2D square lattice hence requires a factor \( x^4 \).

When two spins are flipped, one needs to distinguish two cases: either, these particular spins are neighbors, in that case, six bonds become anti-aligned and the energy cost is \( 12J \); or the spins are not neighbors, in which case 8 bonds are anti-aligned and the cost is \( 16J \). Again, one needs to keep track of multiplicities: in the first case, there are \( 2N \) ways to choose neighboring spins, in the latter, there are \( N \) ways to choose the first spin, and \( N - 5 \) to choose the second, so that the two are *not* neighbors. To avoid double counting, an additional factor of \( 1/2 \) needs to be applied, yielding \( N(N - 5)/2 \) configurations.
Continuing systematically in the fashion for increasing numbers of flipped spins, one obtains an increasingly close approximation of the partition function

\[
Z = e^{-E_0/k_BT} \left( 1 + Nx^4 + 2Nx^6 + \frac{1}{2}N(N+9)x^8 + 2N(N+6)x^{10} + O(x^{12}) \right).
\]  

(91)

### 9.3 Duality of the 2D square lattice Ising model

Comparing the terms in Eq. 90 and Eq. 91, it is clear that, in the present example of the 2D square lattice, there is a complete correspondence between \(x = \exp(-2K)\) and \(v = \tanh K\) for the low and high temperature series. Referring to the final factors in Eqs 90 and 91 as \(g(v)\) and \(g(x)\), respectively, one can equate the free energies of the two cases as

\[
\frac{-F}{Nk_BT} = \ln Z/N = \frac{E_0}{Nk_BT} + g(x) = \ln(2 \cosh^2 K) + g(v),
\]

(92)

where \(g(x)\) and \(g(v)\) are infinite power series in their respective arguments. From other arguments (e.g. a Monte Carlo simulation or the mean field approximation) we might suspect a (single) critical temperature somewhere between the lowest and highest temperatures, i.e. \(T = 0\) and \(T \to \infty\). If this is so, then the singular contribution, i.e. that which leads to divergences at \(T_c\), should match for the two expansions at hand. Since \(\frac{E_0}{Nk_BT}\) and \(\ln(2 \cosh^2 K)\) are both perfectly “well-behaved” functions for \(T > 0\), we are not concerned with these and focus only on the correspondence between \(g(x)\) and \(g(v)\). Even without know all the terms in these functions, it is possible to exploit the topological fact that they both contain the same type of terms. If we can ensure that \(g(x) = g(v)\) at some “transition temperature”, located in between the low and high temperature expansion, we have a path to finding \(T_c\). However,

\[
v = x, \text{ i.e. } \tanh K = \exp(-2\tilde{K})
\]

(93)
does not bring out any symmetry regarding the temperature $T = J/k_B K$. Here we have used different symbols $K$ and $\tilde{K}$ to make clear that we are referring to (presently distinct) temperatures below and above $T_c$.

We can re-write Eq. 93 in a symmetric form by using that

$$\sinh 2\tilde{K} = \frac{1}{2} (\exp(2\tilde{K}) - \exp(-2\tilde{K}))$$

$$= \frac{1}{2} \left( \frac{1}{\tanh K} - \tanh K \right)$$

$$= \frac{1}{\sinh 2K},$$

which finally gives the symmetric form

$$\sinh 2\tilde{K} \cdot \sinh 2K = 1.$$

Due to the complete symmetry of $g(x)$ and $g(v)$ the only solution for $K = \tilde{K}$, i.e. in the limit of $T \to T_c$, is that

$$\sinh 2K = 1 = \frac{1}{2} (\exp 2K - \exp(-2K)).$$

Introducing $q \equiv \exp(2K)$ gives a quadratic in $q$, yielding

$$q_{1/2} = 1 \pm \sqrt{2}.$$

Discarding the negative solution for physical reasons, we obtain the critical temperature

$$\frac{k_B T_c}{J} = \frac{2}{\ln(1 + \sqrt{2})} \approx 2.27.$$

**Exercises**

1. For a 2D Ising model on a triangular lattice, construct the high temperature expansion for the partition function. Continue the expansion to at least sixth order in the expansion parameter $v$. Compute the free energy $F$ and show that term of higher power than linear in $N$ cancel out — by which it is ensured that $F$ is extensive (scales with system size).

2. Compute also the low temperature expansion for the triangular lattice partition function.

3. Compute the internal energy for the high temperature expansion, either by a derivative of the partition function w.r.t. $\beta$ or by subtracting $TS$ from the free energy.

4. Use a Monte Carlo simulation to compute the internal energy per site for the 2D triangular lattice. Plot your results for the high and low temperature expansions together with the Monte Carlo result, as a function of temperature.
10 Basic concepts of renormalization

In a renormalization group transformation the original Hamiltonian, usually defined in dimensionless form $\hat{H} \equiv \mathcal{H}/k_B T$, is transformed by an operation $\mathcal{R}$ to obtain the modified Hamiltonian $\hat{H}'$, i.e.

$$\hat{H}' = \mathcal{R}\hat{H}.$$ 

In this operation, some of degrees of freedom of $\hat{H}$ are removed, i.e.

$$N' = b^{-d}N,$$

where $b$ is the linear rescaling, $d$ is the dimensionality of the lattice and $N$ ($N'$) is the original (transformed) number of lattice sites.

The general idea is, that a partial trace, i.e. a summation over a subset of spins (more generally: degrees of freedom) is performed, to obtain a new partition function that has fewer remaining summations to be carried out. In the case of the example in Fig. 10, it might be that the even-numbered sites each have a spin-half particle. One then rewrites the partition function to allow these sites to actually take on the available spin values. This will be practically carried out in the subsequent section (Sec. 10). The art of renormalization is to relate back the resulting Hamiltonian $\hat{H}'$ to take on the same functional form as the original $\hat{H}$, albeit with “rescaled” coefficients.

In general, the partition function should remain unchanged, i.e.

$$Z_{N'}(\hat{H}') = Z_N(\hat{H}).$$

Since this also leaves the free energy unchanged, the free energy per site in the new Hamiltonian will increase by the rescaling $b^d$. Similarly, linear lengths are rescaled as $b^{-1}$, respectively momenta as $b$.

![Figure 20: Basic concept behind an RG transformation. In a first step, a partial trace is carried out, removing a fraction of the original degrees of freedom (gray sites). In a second step, the Hamiltonian is “coarse grained”.](image)

The aim is to find the fixed points of the renormalization procedure, i.e. the parameter values where

$$\hat{H}' = \hat{H} \equiv \hat{H}^*.$$  \hspace{1cm} (94)
RG for 1D Ising model

Consider the partition function for the 1D Ising model of $N$ sites. Define $K \equiv \beta J$ and $h = \beta H$, where $J$ and $H$ are the coupling constant and the external magnetic field. The Hamiltonian hence reads

$$\mathcal{H} = -K \sum_i s_i s_{i+1} - h \sum_i s_i .$$

When we consider only sites of even index $2i$, then each of these sites is only connected to odd-index neighbors. The goal is to evaluate the possible configurations for the even sites and perform a partial sum. Doing this, in terms of these three constants, the partition function is

$$Z(N, K, h) = \sum_{\{s\}} \left[ e^{(K + h/2) (s_1 + s_3) + h} + e^{(-K + h/2) (s_1 + s_3) - h} \right] \times \ldots . \quad (95)$$

The goal is now to put the resulting partition function in a form that resembles that of the original partition function, but where the even sites are left out. To achieve this, the constants $N$, $K$, and $h$ are allowed to be rescaled.

$$Z(N, K, h) = e^{Ng(K,h)} Z\left(\frac{N}{2}, K', h'\right) = e^{Ng} \sum_{\{s\}} e^{-H'}, \quad (96)$$

where $\mathcal{H}' = -K' \sum_{i \text{ odd}} s_i s_{i+2} - h' \sum_{i \text{ odd}} s_i$. The rescaled Hamiltonian hence indeed represents a “coarse grained” version of the original Hamiltonian, where the lattice spacing has decreased by a factor two by removing half the sites. To accomplish this, the constants have to be rescaled. Matching each of the factors in Eq. 95 with the corresponding factors in Eq. 96, means that for each value of $s_i$, $s_{i+2} = \pm 1$

$$e^{(K + h/2) (s_i + s_{i+2}) + h} + e^{(-K + h/2) (s_i + s_{i+2}) - h} = e^{K' s_i s_{i+2} + h' (s_i + s_{i+2}) + 2g} .$$

Inserting the different combinations of $s_i$ and $s_{i+2}$ gives the three conditions

$$e^{2K+2h} + e^{-2K} = e^{K'+h'+2g}$$
$$e^h + e^{-h} = e^{-K'+2g}$$
$$e^{-2K} + e^{2K-2h} = e^{K'-h'+2g} .$$

These equations can be solved for $K'$, $h'$ and $g$, yielding

$$K' = \frac{1}{4} \frac{\cosh(2K + h) \cosh(2K - h)}{\cosh^2 h}$$
$$h' = h + \frac{1}{2} \ln \frac{\cosh(2K + h)}{\cosh(2K - h)}$$
$$g = \frac{1}{8} \ln \left[ 16 \cosh(2K + h) \cosh(2K - h) \cosh^2 h \right] . \quad (97)$$
The equations in Eq. 97 are recursive relations and specify the fixed points and flow diagram of the system. The action of an iteration is to remove half the degrees of freedom, by which the number of sites \( N' = N/b \) with \( b = 2 \). The lattice spacing is increased to \( a' = b \, a \). Other quantities depend on the lattice spacing and are correspondingly rescaled, e.g. the correlation length \( \xi' = \xi/b \). The spins remaining in the new Hamiltonian interact through the rescaled coupling \( K' \) and act under the rescaled field \( h' \). Noticeable, the renormalization for the 1D Ising model is exact, the resulting coarse-grained Hamiltonian looks exactly like the original, in the sense that no new terms are generated, e.g. interactions between three particles. The only thing that is necessary, is to define how the parameters of the system “scale” as the transformation is performed. This exactness is the crucial difference between a 1D and a 2D Ising model. In the latter, such exact mapping is not possible, the transformation always produces additional terms that are not present in the original Hamiltonian. The additional challenge in 2D hence becomes, to discard some of those additional terms, to be able to derive a self-consistent renormalization (Sec. 10).

Defining for simplicity, \( x \equiv e^{-4K} \), \( y \equiv e^{-2h} \), and \( z \equiv e^{-8g} \), the recursion relations are

\[
\begin{align*}
x' &= x \frac{(1 + y)^2}{(x + y)(1 + xy)} , \\
y' &= y \frac{x + y}{1 + xy} , \\
z' &= z^2 xy^2 \frac{1}{(x + y)(1 + xy)(1 + y)^2} .
\end{align*}
\]

(98)

The first two equations do not depend on \( z \), which means that the singular behavior of the free energy does not depend on a shift in energy scale. Investigating the fixed points in the \( x-y \) plane it is first seen that \( x = 1 \) is always a fixed point, irrespective of \( y \), i.e. for any \( 0 \leq y \leq 1 \). These fixed points are infinite temperature sinks.

Notably, the equations in Eq. 98 constitute a dynamical system in 3D parameter space. The linear stability in the vicinity of any fixed point \( X^* \) can be assessed by the Jacobian

\[
J \equiv \frac{\partial q'}{\partial q} \bigg|_{X^*} ,
\]

where \( q \) is any of the three variables and \( q' \) represents the primed variables, i.e. the LHS of Eq. 98. At the ferromagnetic fixed point \( X^* = \{ x^*, y^* \} = \{ 0, 1 \} \) (where the continuous phase transition occurs, and we are therefore interested in), the Jacobian (Eq. 99) turns out to already be diagonal, and gives

\[
\begin{align*}
\frac{\partial x'(x, y)}{\partial x} \bigg|_{X^*} &= 4 , \\
\frac{\partial y'(x, y)}{\partial y} \bigg|_{X^*} &= 2 .
\end{align*}
\]

(100)
hence \( x' \sim 4x \) and \( \epsilon' \sim 2\epsilon \) near the fixed point \( X^* \), where \( \epsilon = y^* - 1 \), i.e. a small parameter proportional to the magnetic field near \( y = 1 \). As the Jacobian \( J \) is diagonal, the coefficients in the Eq. 100 represent the eigenvalues of the Jacobian. Notably, if we are working in the range where a linearized description of the transformation in Eq. 98 is appropriate, i.e. sufficiently close to a fixed point, then a repeated application of the transformation will just lead to an additional scaling of the type in Eq. 100. This means, that the eigenvalues of a duplicate application will become

\[
\lambda_i(b)\lambda_i(b) = \lambda_i(b^2),
\]

where \( b \) refers to the rescaling of spatial scales accomplished by the renormalization procedure. I.e. the repeated application just gives powers of the eigenvalues, which then represent the eigenvalue corresponding to \( J^2 \) (you can check this by just multiplying \( J \) with itself and finding the corresponding eigenvalues). But if Eq. 101 holds, then \( \lambda_i \) must have the form

\[
\lambda_i(b) = b^{y_i},
\]

where \( y_i \) is a coefficient.

Notably, for \( x \) and \( \epsilon \) these coefficients are different: the coupling \( x \) scales with \( y_1 = 2 \) while the field has \( y_2 = 1 \). Hence, as one zooms out of the lattice, “temperature” increases quadratically with the rescaling, while the “field” goes only linearly.

These consideration have broader implications: Given that, under suitable rescaling of the parameters, the renormalization should keep the total partition function unchanged, the free energy per spin, \( f \) should increase by a factor of \( b^2 \) in each step, where \( b \) is the rescaling of space. If we write the singular part \( f^{(s)} \) of the free energy, i.e. the part that can produce divergences in one of the derivatives, before and after renormalization as a function of the different variables, e.g. temperature \( t \) and field \( h \), we have (with Eq. 102)

\[
f^{(s)}(t, h, \ldots) \sim b^{-d} f^{(s)}(b^{y_1} t, b^{y_2} h, \ldots)
\]

in the limit where \( t \) and \( h \) approach zero, i.e. near \( T_c \).

Even though the exact form of the free energy might not be known at \( T_c \), knowing the scaling of \( f^{(s)} \) and its parameters we should be in a position to analyze its scaling and that of its derivatives, e.g. the specific heat coefficient at zero magnetic field,

\[
C \sim \left( \frac{\partial^2 f^{(s)}}{\partial t^2} \right)_{h=0} \equiv f_{tt}^{(s)}(h = 0) \sim |t|^{-\alpha}.
\]

In fact, it is straightforward to write down \( f_{tt} \) at zero magnetic field:

\[
f_{tt}^{(s)}(t, 0) \sim b^{-d+2y_1} f_{tt}^{(s)}(b^{y_1} t, 0). (103)
\]
How can we obtain the temperature dependence of the RHS of the equation 103? One needs to notice that the rescaling by a factor of $b$ is arbitrary, any number could be chosen for $b$. So why not choose

$$b = |t|^{-1/y_1},$$

i.e. make the first argument in $f_{tt}^{(s)}$ become a constant? With this choice, the prefactor in Eq. 103 becomes a function of $t$:

$$f_{tt}(t, 0) \sim |t|^{(d - 2y)/y_1} f_{tt}(\pm 1, 0),$$

which allows us to read off the critical exponent of specific heat,

$$\alpha = 2 - d/y_1.$$

Similarly, the exponent $\beta$ is obtained to be

$$\beta = (d - y_2)/y_1.$$

The exponents corresponding to the magnetic susceptibility $\chi \sim |t|^{-\gamma}$ and that of the critical isotherm $H \sim |M|^\delta sgn(M)$ can be computed analogously.

Notably, by this procedure four critical exponents have been expressed in terms of only two variables $y_1$ and $y_2$. As a consequence, there must be two relations between these critical exponents. It can be checked that these area

$$\alpha + 2\beta + \gamma = 2,$$

i.e. the one we obtained from the Rushbrooke inequality in Sec. 3, as well as

$$\gamma = \beta(\delta - 1).$$

Another consequence is that the scaling above and below the critical temperature should be the same, which is easily seen by inspecting Eq. 104.

When re-considering the pair-correlation function (Eq. 28), one obtains

$$\Gamma(r, t, h, \ldots) \sim c^2(b) \Gamma(b^{-1}r, b^{y_1}t, b^{y_2}h, \ldots),$$

(105)

where it was used that all spatial scales are diminished by the factor $b^{-1}$ at each renormalization step and $c(b)$ is some function of the spatial rescaling only, which however remains to be specified. At zero field ($h = 0$), one can employ a similar “trick” as before, setting $b \sim |t|^{-1/y_1}$ and obtains

$$\Gamma(r, t) \sim c^2(|t|^{-1/y_1}) \Gamma(|t|^{1/y_1}r, \pm 1),$$

therefore the critical exponent $\nu = 1/y_1$.

To obtain $c(b)$ one can now set both $t$ and $h$ to zero in Eq. 105 and remember the Eq. ??, where

$$\Gamma(r) \sim r^{-(d + 2 + \eta)}.$$

(106)
Using our previous equation
\[ \chi_T \sim N \int \Gamma(r)r^{d-1}dr \] (107)
together with Eq. 106, we have that
\[ \chi_T \sim \xi^{2-\eta} . \] (108)

Writing both \( \chi_T \) and \( \Gamma \) in terms of \( t \) we have
\[ t^{-\gamma} \sim t^{-(2-\eta)\nu} , \] (109)
which then yields the additional exponent relation
\[ \gamma = (2 - \eta)\nu . \] (110)

In summary, it can be seen that all exponent relation result from the RH scaling. What is — of course — left to do is to obtain the values of \( y_i \), which define the scaling w.r.t. the different variables \( t, h, \) etc. Once these \( y_i \) are known, all critical exponents can be computed. Note that the dimensionality of space \( (d) \) enters naturally in the previous equations, as \( d \) relates the different critical exponents to the (linear) rescaling of space \( b \).

**RG for 2D Ising model**

As mentioned in Sec. 10, the two-dimensional case presents further complications, not present in 1D. An exact mapping from a given Hamiltonian to one where only parameters are rescaled, is now generally not possible. We here discuss only the simplest 2D case, where the lattice is first broken down into larger clusters of so-called “block spins”, which are taken as the “unperturbed” Hamiltonian. The interaction between the block spins is then incorporated perturbatively.

To this end, consider a triangular lattice spin-\( \frac{1}{2} \) Ising model with a ferromagnetic coupling \( J > 0 \). The energy hence is
\[ \mathcal{H} = K \sum_{<ij>} s_is_j + h \sum_i s_i , \] (111)
where \( K \equiv -\beta J \) and \( h \equiv -\beta H \) and \( <ij> \) denotes nearest neighbor sites \( i \) and \( j \). The lattice is now broken down in triangular blocks of three sites each (Fig. 10), and we define the block spin of each triangle \( I \) by a “majority rule”
\[ S_I \equiv \text{sign}\{S_I^1 + S_I^2 + S_I^3\} . \] (112)

By this definition of block spins the lattice constant has been enlarged by a factor \( l = \sqrt{3} \).
As a first step, we want to express the original Hamiltonian by a formally exact Hamiltonian using however the block spins. For this purpose we first define the collection of spins which constitute one triangle $I$ as

$$\sigma_I \equiv \{S^I_1, S^I_2, S^I_3\},$$ (113)

yielding $2^3 = 8$ possible combinations of spins. Under the majority rule (Eq. 112) there are four combinations of spins with $S_I = 1$ and four with $S_I = -1$. In this sense, the total number of degrees of freedom has been preserved.

The coarse grained Hamiltonian is

$$e^{\mathcal{H}(S_I)} = \sum_{\sigma_I} e^{\mathcal{H}(S_I, \sigma_I)}.$$ 

The goal is to approximate $\mathcal{H}'$. To this end, we break $\mathcal{H}$ down into the interaction within block spins $\mathcal{H}_0$ and those between block spins $V$,

$$\mathcal{H} = \mathcal{H}_0 + V.$$
The Hamiltonian $H_0$ is

$$H_0 = K \sum_I \sum_{i,j \in I} S_i S_j,$$

while the “perturbation”, i.e. the interaction between the blocks, is

$$V = K \sum_{I \neq J} \sum_{i \in I, j \in J} S_i S_j.$$

We can now write the average of any quantity $A$ with respect to $H_0$ as

$$\langle A(S_I) \rangle_0 \equiv \frac{\sum_{\sigma_I} e^{H_0(S_I, \sigma_I)} A(S_I, \sigma_I)}{\sum_{\sigma_I} e^{H_0(S_I, \sigma_I)}}.$$

The equation for the coarse grained Hamiltonian thus becomes

$$e^{\mathcal{H}'(S_I)} = \langle e^V \rangle_0 \sum_{\{ \sigma_I \}} e^{H_0(S_I, \sigma_I)}.$$

Notably, since for the second factor on the RHS all blocks are independent, this factor can be evaluated to give

$$\sum_{\sigma_I} e^{H_0(S_I, \sigma_I)} = Z_0(K)^M,$$

where $Z_0(K)$ is the partition function for one block

$$Z_0(K) = \sum_{S_1 S_2 S_3} e^{K(S_1 S_2^T + S_2 S_3^T + S_3 S_1^T)}.$$

Notably, the value of $Z_0(K)$ does only depends on bond configurations, i.e. the relative orientation of neighboring spins. Hence, the overall orientation $S_I$ is irrelevant. There is only one way to obtain a sum of $3K$, but three configuration where two bonds are frustrated, i.e. two spins are anti-aligned, each with energy $-K$, hence

$$Z_0(K) = 3e^{-K} + e^3 K.$$

The problem left to solve is hence

$$e^{\mathcal{H}'(S_I)} = \langle e^V \rangle_0 Z_0(K)^M,$$

with $M$ the total number of blocks in the system.

A cumulant expansion of $\langle e^V \rangle_0$ gives

$$\langle e^V \rangle_0 = \langle 1 + V + \frac{V^2}{2} + \ldots \rangle_0$$

$$= 1 + \langle V \rangle_0 + \frac{\langle V^2 \rangle_0}{2} + \ldots .$$
Figure 22: Definition of block spins in 2D triangular lattice. Block spins (yellow triangles) each consist of three spins and form a “coarse grained” triangular lattice of lattice constant enlarged by a factor $\sqrt{3}$. Schematic (right) shows the numbering of sites for two sub-lattice $J$ and $I$ and possible interactions between $I$ and $J$.

Notably, we consider the “perturbation” $V$ to be small, and in doing so we will neglect higher order terms in $V$. Using

$$\log(1 + x) = x - \frac{x^2}{2} + \mathcal{O}(x^3),$$

we have

$$\log \langle e^V \rangle_0 = \langle V \rangle_0 + \frac{1}{2} \langle V^2 \rangle_0 - \frac{\langle V \rangle_0^2}{2} + \mathcal{O}(V^3).$$

Re-exponentiating, we have

$$\langle e^V \rangle_0 = \exp \left( \langle V \rangle_0 + \frac{1}{2} [\langle V^2 \rangle_0 - \langle V \rangle_0^2] + \mathcal{O}(V^3) \right).$$

The Hamiltonian $\mathcal{H}'$ can now be expressed approximately as

$$\mathcal{H}' = M \log Z_0(K) + \langle V \rangle_0 + \frac{1}{2} [\langle V^2 \rangle_0 - \langle V \rangle_0^2] + \mathcal{O}(V^3).$$

$\langle V \rangle_0$ couples nearest neighbor blocks. Explicitly it is with

$$V = \sum_{I \neq J} V_{IJ},$$

where

$$V_{IJ} = k(S^I_3)(S^J_1 + S^J_2),$$

thus $\langle V \rangle_0 = 2K \langle S^I_3 S^J_1 \rangle_0$ (compare schematic Fig. 10). Since $\mathcal{H}_0$ does not couple different blocks, i.e. cannot induce any correlations between spins on different blocks, The expectation value factorizes, giving

$$\langle V_{IJ} \rangle_0 = 2K \langle S^J_3 \rangle_0 \langle S^I_1 \rangle_0.$$
But
\[ \langle S_J^3 \rangle_0 = \frac{1}{Z_0} \sum_{\sigma_J} S_J^3 e^{K[S_I^I S_J^J + S_I^J S_J^J + S_J^J S_I^J]}. \]

For \( S_J = 1 \) we have
\[ \langle S_J^3 \rangle_0 = \frac{e^{3K} + e^{-K}}{e^{3K} + 3e^{-K}}, \]
while for \( S_J = -1 \) we have
\[ \langle S_J^3 \rangle_0 = -\frac{e^{3K} + e^{-K}}{e^{3K} + 3e^{-K}}, \]

hence the expectation value of \( V \) within the unperturbed Hamiltonian becomes
\[ \langle V \rangle_0 = 2K\Phi(K)^2 \sum_{IJ} S_I S_J \]
with \( \Phi(K) \equiv \frac{e^{3K} + e^{-K}}{e^{3K} + 3e^{-K}} \). In total, the effective Hamiltonian, to first order in \( V \) is
\[ \mathcal{H}'\{S_I\} = M \log Z_0(K) + K' \sum_{IJ} S_I S_J + \mathcal{O}(V^2), \]
where \( K' = 2K\Psi(K)^2 \). We have hence achieved the goal of deriving an RG transformation that allows a rough approximation to the recursion relation for the coupling constant \( K \).

**Fixed points and critical exponents.** What are the fixed points of the recursion relation we just obtained? Fixed points satisfy
\[ K^* = 2K^*\Phi(K^*)^2, \]
which has three solutions
\[ K^* = 0 \quad K^* = \infty \quad \Phi(K^*) = 1/\sqrt{2}. \]

Using \( x \equiv \exp(4K) \), the latter relation can be inverted, giving a non-trivial fixed point
\[ K_c = \frac{1}{4} \log(1 + 2\sqrt{2}) \approx 0.34, \]
whereas the exact result (Onsager) is \( K_c = (\log 3)/4 \approx 0.27 \).

**Exercises**

1. **Exponent relations.**
Starting from the scaling for the singular part of the free energy
\[ f^{(s)}(t, h) \sim b^{-d} f^{(s)}(b^{\mu_1} t, b^{\mu_2} h) \tag{114} \]

\[ ^7 \text{Yeomans, problem 8.2} \]
where \( t \equiv (T - T_c)/T_c \) and \( h = h_0/k_B T \) show that \( \alpha = 2 - d/y_1 \), \( \beta = (d - y_2)/y_1 \), \( \gamma = (2y_2 - d)/y_1 \) and \( \delta = y_2/(d - y_2) \) and hence confirm that \( \alpha + 2\beta + \gamma = 2 \), and \( \gamma = \beta(\delta - 1) \).

Set \( T = T_c \) in your 2D square lattice zero-field Monte Carlo simulation and make lattice size \( N \) sufficiently large (say, \( N \sim 100 \times 100 \)). For a snapshot of your simulation near equilibrium, perform a ”numerical renormalization“,
where you apply the following majority rule: For any square consisting of \( 2 \times 2 \) sites, color this square by the majority of spins, i.e. if more are pointing up than down, the ”block spin“ will point up. For a ”tie“, choose randomly between up and down for the block spin. The resulting lattice will then only have \( N^2/4 \) sites and represent a zoomed-out version of the original. Repeat this procedure several times and observe the patterns obtained for the various iterations. If you are close to \( T_c \) you should observe that patches at different scales remain, even when you rescale several times.

Now repeat this exercise for a temperature slightly below \( T_c \), e.g. \( T = .99T_c \). Now you should find that the resulting patterns ”flow“ towards one of the polarized extremes, either all spins pointing up or down.

Repeat again for \( T \) slightly larger than \( T_c \), say \( T = 1.01T_c \). Now the result should be that pattern become random, you will end up with a featureless mix of up and down spins.
References


