Seminar on Statistical Physics
at the University of Heidelberg

The Ising Model in One and Two Dimensions

Johannes Obermeyer

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Lecturer: Prof. Dr. G. Wolschin

Abstract

The Ising model is a theoretical model in statistical physics to describe ferromagnetism. It simplifies the complex properties of solids by assuming only nearest neighbor interaction between lattice sites and allowing only two opposite pointing orientations of each lattice site's magnetic moment. It is analytically exactly solvable in one and two dimensions by means of different mathematical approaches. The Ising model shows the expected phase transition for a ferromagnet only in two and higher dimensions.

29 may 2020

Contents

1. Basic idea and motivation

The Ising model is a theoretical model in statistical physics that was developed to describe ferromagnetism. The ferromagnet in one or two dimensions can be modeled as a linear chain or rather a rectangular lattice with one molecule or atom at each lattice site i. To each molecule or atom a magnetic moment is assigned that is represented in the model by a discrete variable σ_i. The possible values of σ_i are +1 and -1 which correspond to alignments of the magnetic moments parallel or anti-parallel to some preferred axis. For a lattice with N_{tot} lattice sites the two possible σ_i-values lead to $2^{N_{\text{tot}}}$ possible configurations σ of the arrangement of molecules. The original Ising model further considers only nearest neighbor interaction since we assume that the molecules exert only short-range forces. A system of two (neighboring) lattice sites is considered to be in a lower energetic state if the two magnetic moments are aligned, i.e. the σ_i-values are both either +1 or -1, and to be in a higher energetic state if the magnetic moments point in opposite directions, i.e. the σ_i-values are different. Due to this interaction the system tends to align all magnetic moments in one direction in order to reach the lowest energetic state. If nearly all magnetic moments point in the same direction the arrangement of molecules behaves like a macroscopic magnet.

The attention of this seminar talk in Statistical Physics is focused on phase transitions, i.e. a transition between an ordered and a disordered state. A ferromagnet above a critical temperature T_{C}, also known as the *Curie Temperature*, is in a disordered state that in the Ising model corresponds to a uniform but random distribution of the σ_i-values. Below the critical temperature T_{C} (nearly) all magnetic moments are aligned even in the absence of an external applied magnetic field $\vec{B}$. In the regime below the critical temperature the magnetization M of a ferromagnet at zero applied magnetic field is called the spontaneous magnetization M_0. Heating up a strongly cooled ferromagnet, the spontaneous magnetization vanishes at the Curie point T_{C} and the ferromagnet switches from an ordered to a disordered state which is the phase transition of second order that shall be investigated by the Ising model [Gal72].

2. History of the Ising model

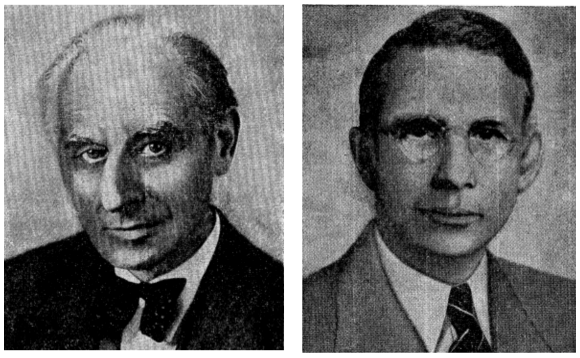

Figure 2.1: Photograph of Wilhelm Lenz (left) and Ernst Ising (right). Source: [Bru67].

In 1920, Wilhelm Lenz (figure 2.1, left) proposed the model nowadays known as the Ising model to his PhD-student Ernst Ising (figure 2.1, right) [Bru67]. Ising then worked on the problem of the one-dimensional model and found a combinatorial, exact solution in 1924 that he published in 1925. In Ising's solution of the one-dimensional ferromagnet there is no phase transition at any temperature. Ising therefore assumed that the model can not describe ferromagnetic behavior and even tried to extend the non-existence of spontaneous magnetization in his solution to two dimensions [Isi25]. Due to Ising's results for the one-dimensional problem, the model was no longer of great interest for most physicists and only in 1928 Heisenberg cited Ising's original paper from 1925 once in order to justify the need for his more complex *Heisenberg model* [Isi17]. Nonetheless, the model was studied in the following years in the context of order-disorder transitions in alloys for example. In 1936, R. Peierls published a paper in which he showed that although there is no phase transition in one dimension, there is a phase transition in two dimensions [Pei36]. Shortly after that, in 1941, H. A. Kramers and G. H. Wannier had developed an algebraic method to calculate the exact solution of the two-dimensional Ising model. L. Onsager used parts of this method to calculate the exact solution of the Ising model in two dimensions and published his results in 1942 [Ons44]. Since then there have been successfully found various approaches for exactly solving the two-dimensional Ising model and these results are nowadays used in different scientific fields.

3. Ising model

In this chapter, solutions for the Ising model in one and two dimensions are discussed. For the one-dimensional model, E. Ising's original solution as well as the transfer matrix formalism are derived in detail. For the two-dimensional model, the transfer matrix formalism is expanded to higher dimensions and the exact solution from L. Onsager is given without further derivation.

As mentioned in the introduction (see chap. 1), the Ising model was invented to describe the physical system of a ferromagnet and especially its behavior at the critical point T_C. In order to describe the system, its thermodynamic quantities are derived from the partition function

$$Z = \sum_s \exp(-\beta E(s))\,. \tag{3.1}$$

Here, the sum is over all possible micro-states s, $E(s)$ is the energy of the corresponding micro-state s and $\beta = 1/(k_\mathrm{B}T)$. The energy of a micro-state $E(s)$ is given in the model by the energy of a certain configuration σ of the magnetic moments [Bax89]:

$$\begin{aligned} E(\sigma) &= E_0(J,\sigma) + E_1(B,\sigma) \\ &= E_0(J,\sigma) - B\sum_{i=1}^{N}\sigma_\mathrm{i}\,. \end{aligned} \tag{3.2}$$

Here, the first term represents the energy due to the molecular interaction with bond strength J. The second term corresponds to the energy of the system in an external applied magnetic field $\vec{B}$ parallel to the preferred axis whereas here and in the following the Bohr magneton is equal to unity. The free energy per site f in the thermodynamic limit can be calculated by

$$f(B,T) = -k_\mathrm{B}T \lim_{N\to\infty}\frac{1}{N}\ln(Z(B))\,. \tag{3.3}$$

The magnetization M of the system is given by the average of the magnetic moments σ_i per site:

$$\begin{aligned} M(B,T) &= \frac{1}{N}\langle\sigma_1 + ... + \sigma_N\rangle \\ &= \frac{1}{N}\frac{1}{Z}\sum_\sigma(\sigma_1 + ... + \sigma_N)\exp[-\beta(E_0(J,\sigma) - B\sum_{i=1}^{N}\sigma_\mathrm{i})]\,. \end{aligned} \tag{3.4}$$

Using equation (3.3), the magnetization can be calculated as the derivative of the free energy f per site with respect to the magnetic field strength B:

$$M = -\frac{\partial}{\partial B} f(B,T)\,. \tag{3.5}$$

3.1 One-dimensional Ising model

3.1.1 Ernst Ising's origianl solution

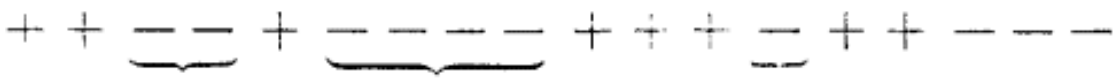

Figure 3.1: Configuration of a linear chain with $N = 18$ lattice sites i, each assigned with a σ_i-value of +1 or -1. The number of groups of negative lattice sites embedded by positive lattice sites (see brackets) is $s = 3$. Source: [Isi25].

E. Ising's original solution [Isi25] for the linear chain (see figure 3.1) assumes a configuration of N elements with ν_1 positive and ν_2 negative σ_i-values such that

$$N = \nu_1 + \nu_2\,. \tag{3.6}$$

Further, the groups of connected lattice sites with $\sigma_i = -1$ that are embedded by lattice sites with $\sigma_i = +1$ are counted by the variable s and shown in figure 3.1 by the curved brackets. The variable δ is either 0 or 1, depending on whether the chain ends on the right with $\sigma_i = +1$ or $\sigma_i = -1$. All possibilities to arrange a fixed number of ν_1 positive and ν_2 negative lattice sites such that the chain always starts with a positive lattice site on the left are given by

$$\binom{\nu_1 - 1}{s} \cdot \binom{\nu_2 - 1}{s + \delta - 1}\,. \tag{3.7}$$

Here, the first binomial coefficient counts the possibilities to choose the s gaps between the ν_1 positive lattice sites. The second binomial coefficient in equation (3.7) counts the possibilities to distribute the ν_2 negative lattice sites on $s + \delta$ positions in the chain. If the linear chain starts with a negative lattice site instead of a positive one on the left side, the number of possible configurations can be obtained from equation (3.7) by replacing ν_1 with ν_2 and vice versa:

$$\binom{\nu_2 - 1}{s} \cdot \binom{\nu_1 - 1}{s + \delta - 1}\,. \tag{3.8}$$

The energy E_0 for a system of two neighboring magnetic moments in this approach is considered to be zero if the moments are aligned. If the magnetic moments of two neighboring lattice sites point in opposite direction, the energy of those two lattice sites is ε. This way, for a configuration σ of certain s and δ, the energy becomes

$$E_0(\sigma) = (2s + \delta) \cdot \varepsilon \,. \tag{3.9}$$

The energy E_1 of the system corresponding to the magnetic energy of the system in an external applied magnetic field $\vec{B}$ is

$$E_1 = (\nu_2 - \nu_1)B \,. \tag{3.10}$$

Combining equations (3.7), (3.8), (3.9) and (3.10), the partition function Z is obtained as

$$\begin{aligned} Z = \sum_{\nu_1,\nu_2,s,\delta} \Bigg\{ \binom{\nu_1 - 1}{s} \binom{\nu_2 - 1}{s + \delta - 1} + \binom{\nu_2 - 1}{s} \binom{\nu_1 - 1}{s + \delta - 1} \cdot \\ \cdot e^{-\beta((2s+\delta)\varepsilon + (\nu_2 - \nu_1)B)} \Bigg\} \,. \end{aligned} \tag{3.11}$$

In equation (3.11), the sum is over all possible values of the considered variables under the condition of (3.6). In order to solve this sum, the original approach of E. Ising considers following function

$$F(x) = \sum_{N=0}^{\infty} Z(N) x^{\mathrm{N}} \,, \tag{3.12}$$

where x is a variable without physical meaning and $Z(N)$ is regarded as function only depending on the number of lattice sites N. The calculation of (3.12) gives

$$F(x) = \frac{2x\big[\cos\alpha - (1 - \exp(-\beta\epsilon))x\big]}{1 - 2\cos\alpha \cdot x + (1 - \exp(-2\beta\epsilon))x^2} \,, \tag{3.13}$$

with $\alpha = \beta B$. By partial fraction decomposition, (3.13) is developed in orders of x and the coefficients corresponding to x^N are

$$Z(N) = c_1 \Big(\cos(\alpha) + \sqrt{\sin^2(\alpha) + e^{\frac{-2\varepsilon}{k_{\mathrm{B}}T}}} \Big)^N + c_2 \Big(\cos(\alpha) - \sqrt{\sin^2(\alpha) + e^{\frac{-2\varepsilon}{k_{\mathrm{B}}T}}} \Big)^N \,. \tag{3.14}$$

The coefficients c_1 and c_2 do not enter into the solution since $c_1 \in \mathcal{O}(1)$ for all α and the second term $\Big(\cos(\alpha) - \sqrt{\sin^2(\alpha) + e^{\frac{-2\varepsilon}{k_{\mathrm{B}}T}}} \Big) < 1$ vanishes for large N. In this way,

according to (3.5), the magnetization M of the one-dimensional ferromagnet is

$$M = \frac{N \sin(\alpha)}{\sqrt{\sin^2(\alpha) + e^{\frac{-2\varepsilon}{k_B T}}}} \,. \tag{3.15}$$

For the external magnetic field $\vec{B}$ becoming zero, it is clear that $\alpha \to 0$ and the magnetization M therefore vanishes. This implies that the spontaneous magnetization M_0 is zero at any temperature and the Ising model therefore shows no phase transition in one dimension. This result can also be understood qualitatively by following argument [Bru67]: if the linear chain of molecules would be in an ordered state, i.e. all magnetic moments point in the same direction, at finite temperature T, there could always occur a flip of one of the magnetic moments due to thermal fluctuations. A flip of one magnetic moment somewhere in the middle of the chain would allow the magnetic moments on one side or the other to entirely flip simultaneously since the Ising model considers only next neighbor interaction. Hence, in one dimension, a single flip of a magnetic moment can break the communication between one half of the chain and the other and therefore lead to a disordered state even at low (but finite) temperature T.

3.1.2 Transfer matrix formalism

In figure 3.2, a linear chain of molecules or atoms each assigned with a σ_i-value of $+1$ or -1 is shown. The bond strength of the molecular interaction is given by J_1 and the external applied magnetic field is $\vec{B}$. In the following we assume periodic boundary conditions (PBC). In order to examine the thermodynamic properties of the ferromagnet, the partition function Z of the physical system is required. According to

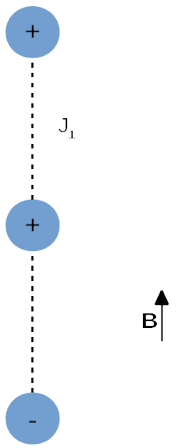

Figure 3.2: Linear chain of $N = 3$ lattice sites. To each lattice site a σ_i-value of $+1$ or -1 is assigned. The intermolecular bond strength is given by J_1. The external applied magnetic field $\vec{B}$ points in the direction of some preferred axis to which the magnetic moment of each lattice site is aligned parallel or anti-parallel.

equations (3.1) and (3.2), the partition function is

$$Z = \sum_{\sigma} \exp[-\beta(E_0(J_1, \sigma) + E_1(B, \sigma))] \,. \tag{3.16}$$

In one dimension, the intermolecular energy E_0 is given by

$$E_0 = -J_1 \sum_i \sigma_i \sigma_{i+1} \,. \tag{3.17}$$

The energy E_1 of the system in a magnetic field $\vec{B}$ is

$$E_1 = -B \sum_i \sigma_i \,. \tag{3.18}$$

From equations (3.17) and (3.18) the partition function can be derived as following expression:

$$Z = \sum_{\sigma} \exp\left(K_1 \sum_i \sigma_i \sigma_{i+1}\right) \exp\left(H \sum_i \sigma_i\right), \tag{3.19}$$

where $K_1 = \beta J_1$ and $H = \beta B$ and the sum is over all possible configurations σ. The idea of the transfer matrix formalism is to express the partition function Z in terms of a matrix, the so called *transfer matrix*. In order to derive the transfer matrix for the partition function in one dimension we rewrite equation (3.19) in the following way:

$$\begin{aligned} Z = \sum_{\sigma} \big[\exp(K_1 \sigma_1 \sigma_2)\big] \big[\exp(0.5H(\sigma_1 + \sigma_2)\big] \cdots \\ \cdots \big[\exp(K_1 \sigma_N \sigma_1)\big] \big[\exp(0.5H(\sigma_N + \sigma_1)\big] \,. \end{aligned} \tag{3.20}$$

Here, for the last terms, the PBC are applied and the N-th lattice site interacts with the first lattice site as if the chain was bound together in a circle. The factor $\big[\exp(K_1 \sigma_i \sigma_{i+1})\big]$ can be represented by the matrix V_1:

$$V_1 = \begin{array}{c} \\ \sigma_i{=}+1 \\ \sigma_i{=}-1 \end{array} \begin{array}{c} \begin{array}{cc} \sigma_i{=}+1 & \sigma_i{=}-1 \end{array} \\ \begin{bmatrix} e^{K_1} & e^{-K_1} \\ e^{-K_1} & e^{K_1} \end{bmatrix} \end{array} . \tag{3.21}$$

The factor $\big[\exp(0.5H(\sigma_i + \sigma_{i+1})\big]$ is represented by the matrix V_2:

$$V_2 = \begin{array}{c} \\ \sigma_i{=}+1 \\ \sigma_i{=}-1 \end{array} \begin{array}{c} \begin{array}{cc} \sigma_i{=}+1 & \sigma_i{=}-1 \end{array} \\ \begin{bmatrix} e^{H} & 0 \\ 0 & e^{-H} \end{bmatrix} \end{array} . \tag{3.22}$$

Plugging V_1 and V_2 in equation (3.20), the partition function Z becomes [Sch64]

$$\begin{aligned} Z &= \mathrm{tr}(V_1 V_2)^N \\ &= \mathrm{tr}(V_2^{\frac{1}{2}} V_1 V_2^{\frac{1}{2}})^N = \mathrm{tr} V^N \end{aligned} \quad . \tag{3.23}$$

This result shows that the partition function Z can be expressed as the trace of N-times the *transfer matrix* V. If Λ_1 and Λ_2 are the eigenvalues of V with

$$\Lambda_1 > \Lambda_2 \,, \tag{3.24}$$

then the partition function Z is

$$Z = \Lambda_1^N + \Lambda_2^N = \Lambda_1^N (1 + (\Lambda_2/\Lambda_1)^N) \tag{3.25}$$

and the smaller eigenvalue Λ_2 is negligible for the thermodynamic limit $N \to \infty$. The transfer matrix formalism in general reduces the problem of calculating the partition function Z to finding the transfer matrix V and determining its largest eigenvalue. In the case of the one-dimensional Ising model, the eigenvalues of the transfer matrix V are

$$\Lambda_{1,2} = e^{K_1} \cosh(H) \pm \sqrt{e^{2K} \sinh^2(H) + e^{-2K}} \,. \tag{3.26}$$

Using equations (3.3) and (3.5) yields the magnetization M as

$$M(H,T) = \frac{e^{K_1} \sinh(H)}{\sqrt{e^{2K_1} \sinh^2(H) + e^{-2K_1}}} \,. \tag{3.27}$$

This result is physically equivalent to E. Isings original solution and shows that the Ising model has no spontaneous magnetization and therefore no phase transition of the ferromagnet in one dimension.

3.2 Two-dimensional Ising model

3.2.1 Transfer matrix formalism

The transfer matrix formalism yielded the partition function Z of the one-dimensional Ising model by finding the transfer matrix V and determining its largest eigenvalue. The transfer matrix V in one dimension is decomposed into the matrices V_1 and V_2:

$$V_1 = \begin{bmatrix} e^{K_1} & e^{-K_1} \\ e^{-K_1} & e^{K_1} \end{bmatrix} , \; V_2 = \begin{bmatrix} e^{H} & 0 \\ 0 & e^{-H} \end{bmatrix} . \tag{3.28}$$

These matrices (3.28) can be expressed in terms of the Pauli matrices 1, τ^x, τ^y and τ^z by

$$V_1 = 1 \cdot e^{K_1} + \tau^x e^{-K_1} \tag{3.29}$$

and

$$V_2 = 1 \cdot \cosh(H) + \tau^z \sinh(H)\,. \tag{3.30}$$

For all Pauli matrices τ^i and any number a

$$\exp(a\tau^i) = 1 \cdot \cosh(a) + \tau^i \sinh(a) \tag{3.31}$$

is valid. Using (3.31), V_1 and V_2 can be rewritten as

$$V_1 = (2\sinh(2K_1))^{\frac{1}{2}} \exp(K_1^*\tau^x) \quad \text{and} \quad V_2 = \exp(H\tau^z)\,, \tag{3.32}$$

whereas K_1^* is defined by

$$\tanh(K_1^*) \equiv e^{-2K_1} \quad \text{and} \quad \sinh(2K_1)\sinh(2K_1^*) \equiv 1\,. \tag{3.33}$$

The formulation of the decomposition matrices V_1 and V_2 of the one dimensional transfer matrix in terms of Pauli matrices τ^i (see (3.32)) allows for the generalization to the two dimensional lattice. For the Ising model in two dimensions, here, two different bond strengths J_1 and J_2 within the lattice are considered (see figure 3.3) which is the reason why the lattice is called a rectangular lattice instead of a square lattice ($J_1 = J_2$). In two dimensions, one has to sum over 2^M possible configurations of each row instead of the two possible orientations of the magnetic moment. Therefore, the decomposition matrices V_1 and V_2 (3.32) in two dimensions become [New53] [Sch64]:

$$V_1^{(2)} = (2\sinh(2K_1))^{\frac{M}{2}} \exp(K_1^* \sum \tau_m^x) \tag{3.34}$$

and

$$V_2^{(2)} = \exp(H \sum \tau_m^z)\,, \tag{3.35}$$

where the τ_m^i are no longer the Pauli matrices, but the direct product

$$\tau_m^i = 1 \times \cdots \times 1 \times \tau^i \times 1 \times \cdots \times 1 \tag{3.36}$$

with the Pauli matrix τ^i at the m-th position. In two dimensions not only the molecular interaction between the N rows but also the interaction between the M columns has to be taken into account. This is done by $V_3^{(2)}$:

$$V_3^{(2)} = \exp(K_2 \sum \tau_m^z \tau_{m+1}^z)\,. \tag{3.37}$$

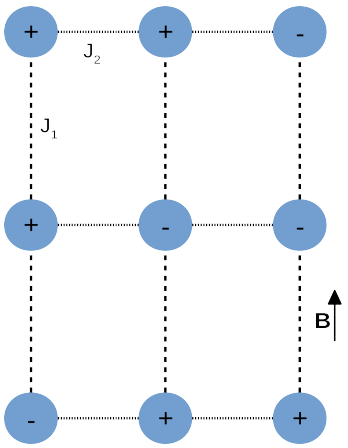

Figure 3.3: Rectangular lattice of $N = 3$ rows and $M = 3$ columns. To each site of the lattice a σ_i-value of $+1$ or -1 is assigned. The intermolecular bond strength is given by J_1 between the rows and J_2 between the columns. The external applied magnetic field $\vec{B}$ points in the direction of some preferred axis to which the magnetic moment of each lattice site is aligned parallel or anti-parallel.

The matrices $V_1^{(2)}$, $V_2^{(2)}$ and $V_3^{(2)}$ are $2^M \times 2^M$ matrices that yield the transfer matrix $V^{(2)}$ for the two-dimensional Ising model as

$$V^{(2)} = (V_2^{(2)} V_3^{(2)})^{\frac{1}{2}} V_1^{(2)} (V_2^{(2)} V_3^{(2)})^{\frac{1}{2}} . \tag{3.38}$$

The partition function is obtained immediately as

$$Z = \mathrm{tr}\left[V^{(2)}\right]^N . \tag{3.39}$$

Although the formulation of the partition function by the transfer matrix formalism is finished, the exact result still has to be calculated. These calculations involve a large amount of higher mathematics [Kra41b] [Kra41a] [Ons44] [New53] [Sch64] and are not shown in this summary.

3.2.2 L. Onsager's exact solution

An exact solution for the Ising model in two dimensions was calculated by L. Onsager [Ons44]. L. Onsager diagonalized the transfer matrix by looking for irreducible representations of the related matrix algebra and showed that the free energy f for the zero-field Ising model in two dimensions in the thermodynamic limit is

$$-\beta f = \ln(2) + \frac{1}{8\pi^2} \int_0^{2\pi} d\theta_1 \int_0^{2\pi} d\theta_2 ln\big[\cosh(2\beta J_1)\cosh(2\beta J_2) - \sinh(2\beta J_1)\cos(\theta_1) - \sinh(2\beta J_2)\cos(\theta_2)\big] . \tag{3.40}$$

The solution reveals that for the Ising model in two dimensions there is a phase transition at the critical temperature T_C defined by

$$\sinh\left(\frac{2J_1}{k_B T_C}\right)\sinh\left(\frac{2J_2}{k_B T_C}\right) = 1\,. \tag{3.41}$$

Equation (3.41) simplifies for a square lattice ($J_1 = J_2 = J$) to

$$T_C = \frac{2J}{k_B \ln(1+\sqrt{2})}\,. \tag{3.42}$$

The spontaneous magnetization M_0 corresponding to the phase transition was published by L. Onsager in 1948 without a rigorous proof:

$$M_0 = \left(1 - [\sinh(2\beta J_1 \sinh(2\beta J_2)]^{-2}\right)^{\frac{1}{8}}\,. \tag{3.43}$$

The first derivation of the spontaneous magnetization M_0 was given later in 1952 by C. N. Yang [Yan52].

4. Numerical simulations of the Ising model

4.1 The Metropolis algorithm

The behavior of a two-dimensional ferromagnet in the description of the Ising model can be numerically simulated by the Metropolis algorithm. The algorithm is also known as the Metropolis-Hastings algorithm named after N. Metropolis who firstly co-published the method in 1953 and W. K. Hastings who extended the algorithm to more general cases in 1970 [Has70]. The algorithm treats the Ising model as a Markov chain which in stochastics is a chain of events whose probabilities each depend only on the state prior to that event. The probabilities $P(\sigma)$ of the system to be in a certain state σ and the probabilities $P(\sigma \to \sigma')$ for the transition from one state σ to another state σ' have to be in a detailed balance:

$$P(\sigma \to \sigma')P(\sigma) = P(\sigma' \to \sigma)P(\sigma')\,. \tag{4.1}$$

The Metropolis algorithm for the Ising model sets the transition probabilities $P(\sigma \to \sigma')$ in dependence of the energies $E(\sigma)$ and $E(\sigma')$ of the corresponding states σ and σ' as

$$P(\sigma \to \sigma') = \begin{cases} 1 & \text{if } E(\sigma') < E(\sigma) \\ \exp(-\frac{E(\sigma')-E(\sigma)}{k_B T}) & \text{if } E(\sigma') \geq E(\sigma) \end{cases}. \tag{4.2}$$

At the beginning of a simulation run, an initial state σ_0 according to a certain configuration of the magnetic moments has to be put into the Metropolis algorithm. In a next step, the algorithm chooses a random number $i \in \{1,...,N_{tot}\}$ with N_{tot} being the total number of lattice sites. For the randomly selected lattice site i, the probability of going from the state $\sigma = (\sigma_1,...,\sigma_i,...,\sigma_{Ntot})$ to the state $\sigma' = (\sigma_1,...,-\sigma_i,...,\sigma_{Ntot})$ by changing the discrete variable σ_i is calculated according to (4.2). Next, another number $r \in [0,1]$ is randomly generated by the algorithm. Due to this property, the Metropolis-Hastings algorithm is specified as a *Marcov chain Monte Carlo* (MCMC) algorithm. By means of the random number r, the Metropolis algorithm decides whether it changes the state in the time step from t_{MC} to $t_{MC}+1$ by

$$\sigma(t_{MC}+1) = \begin{cases} \sigma'(t_{MC}) & \text{if } r < P(\sigma \to \sigma') \\ \sigma(t_{MC}) & \text{if } r \geq P(\sigma \to \sigma') \end{cases}. \tag{4.3}$$

The routine of randomly choosing a lattice site i and attempting a flip of its magnetic moment is repeated for a large amount of time steps t_{MC} in order to simulate the time

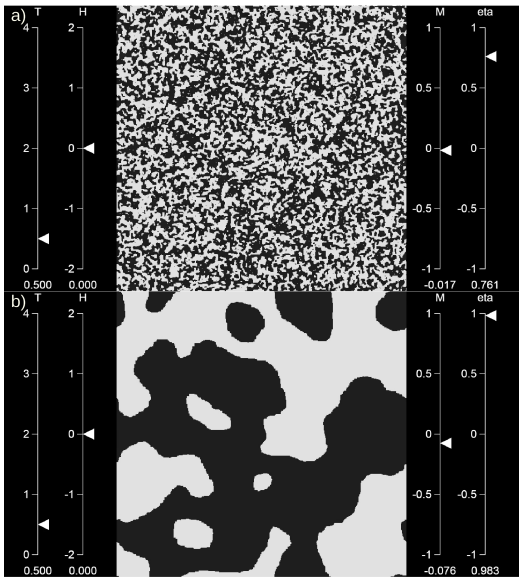

Figure 4.1: Visualization of the orientations of atomic magnetic moments in a ferromagnet simulated by the Metropolis algorithm. The two possible orientations of the magnetic moments are represented by black and white squares. The figure shows a quenched ferromagnet at the beginning ($t_{MC} = 0$) (**a)**) and at the end ($t_{MC} = 3{\cdot}10^8$) (**b)**) of the simulation run. The values of the parameters temperature T, external magnetic field H, magnetization M and order parameter η are indicated at the sides of the pictures.

evolution of the two-dimensional ferromagnet in the description of the Ising model under certain conditions (initial state σ_0, temperature T and external magnetic field H). In figure 4.1[1], the relaxation of the ferromagnet after quenching is visualized. Here, a periodic square lattice of $N \times M = 540 \times 540$ lattice sites is taken at zero magnetic field $H = 0$ and constant temperature $T = \text{const.} < T_C$. Figure 4.1 shows that after the quenching the magnetic moments tend to align themselves in order to reach a lower energetic state. Therefore large regimes of aligned magnetic moments occur.

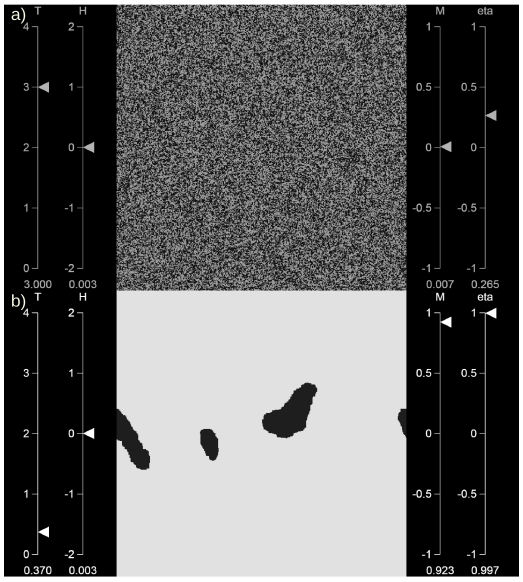

Figure 4.2: Visualization of the orientations of atomic magnetic moments in a ferromagnet simulated by the Metropolis algorithm. The two possible orientations are represented by black and white squares. The figure shows a ferromagnet being cooled down at the beginning ($t_{MC} = 0$) (**a)**) and at the end ($t_{MC} = 3{\cdot}10^8$) (**b)**) of the simulation run. The values of the parameters temperature T, external magnetic field H, magnetization M and order parameter η are indicated at the sides of the pictures.

[1]Source code: https://github.com/CodingPhysics/Ising

In figure 4.2[2], the cooling of a ferromagnet from $T_{\text{init}} = 3J/k_B$ in steps of $T_{\text{step}} = 0.01J/k_B$ to $T_{\text{end}} = 0.01J/k_B$ is visualized. The considered lattice consists again of $N \times M = 540 \times 540$ lattice sites and is located in a weak magnetic field $H = 0.03J/\mu_B$. As one can see, the ferromagnet starts in a disordered state and by passing the critiacl point T_C transitions into an ordered state, where macroscopic regimes of aligned magnetic moments appear and nearly all magnetic moments point in the same direction (white regime).

[2]Source code: https://github.com/CodingPhysics/Ising

5. Summary and Outlook

The Ising model was proposed by Wilhelm Lenz to his PhD student Ernst Ising in 1920 as a theoretical description of ferromagnetism. The assumptions made by the model were the strong simplifications of only nearest neighbor interaction and that only two orientations of the atomic magnetic moments represented by the discrete variable $\sigma_i \in \{\pm 1\}$ are possible. E. Ising was able to solve the problem in one dimension in 1925. In his approach he counted the possible configurations of a linear chain with ν_1 positive and ν_2 negative lattice sites by means of combinatorial methods which led him to the partition function Z. His result did not show the expected phase transition at the critical point T_C but nonetheless was correct which can be proofed by solving the one-dimensional model using the transfer matrix formalism. In the transfer matrix formalism in general, the partition function Z of the physical system is obtained by determining the transfer matrix V and calculating its largest eigenvalue (see section 3.1.2). In one dimension, the transfer matrix formalism yields the partition function Z by applying simple algebra and confirms that there is no phase transition for the linear chain. It was in 1936 that R. Peierls showed that despite the results for the one dimensional model there is a phase transition in two or more dimensions. The first exact solution of the two-dimensional Ising model was calculated by Lars Onsager in 1941. He applied the transfer matrix formalism on the Ising model in two dimensions involving higher mathematics and published an exact formula for the free energy per site f as well as for the critical temperature T_C.

Nowadays, the Ising model is not only relevant in the field of solid state physics but has also found applications in neuroscience, tumor modeling and the description of critical gas-liquid phenomena. The relevance of the Ising model is evident given the approximately 800 papers that are published on it every year [Isi17]. The importance and the success of the Ising model are given by the fact that it is analytically exactly solvable which makes it a powerful tool for benchmarking new models and mathematical approaches. Further, the core of the Ising model that is the binary description of the lattice sites allows for the exportation of it across the boundaries of scientific disciplines and shows that often a scientific field can profit from results of a distinct scientific field.

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