One- and two-dimensional Ising model

Statistical Physics Seminar by Prof. Wolschin

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Abstract

The Ising model is one of the most important models in statistical physics. It is analytically exactly solvable in one and two dimensions. In this extended summary of a seminar presentation, the one- and two-dimensional Ising models are presented and main aspects such as phase transitions are discussed. Further the historical background and modern applications of the Ising model are outlined.

1 Basic idea of the model

The Ising model is a theoretical model in statistical physics that was originally developed to describe ferromagnetism. A system of magnetic particles can be modeled as a linear chain in one dimension or a lattice in two dimension, 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 . Each 'spin' σ can only have a value of $\sigma_i = \pm 1$. The two possible values indicate whether two spins σ_i and σ_j are align and thus parallel $(\sigma_i \cdot \sigma_j = +1)$ or anti-parallel $(\sigma_i \cdot \sigma_j = -1)$.

A system of two spins is considered to be in a lower energetic state if the two magnetic moments are aligned. If the magnetic moments points in opposite directions they are consider to be in a higher energetic state. Due to this interaction the system tends to align all magnetic moments in one direction in order to minimise energy. If nearly all magnetic moments point in the same direction the arrangement of molecules behaves like a macroscopic magnet.

A phase transition in the context of the Ising model is a transition from an ordered state to a disordered state. A ferromagnet above the critical temperature T_C is in a disordered state. In the Ising model this corresponds to a random distribution of the spin values. Below the critical temperature T_C (nearly) all spins are aligned, even in the absence of an external applied magnetic field H. If we heat up a cooled ferromagnet, the magnetization vanishes at T_C and the ferromagnet switches from an ordered to a disordered state. This is a phase transition of second order.

2 Historical Background

The Ising model was invented in 1920 by Wilhelm Lenz, which is why its also referred to as the Lenz-Ising or Ising-Lenz model. Lenz was a German physicist, also notable for his application of the Laplace–Runge–Lenz vector. He was at Rostock University in 1920, but the following year he was appointed ordinary professor at Hamburg. One of his first students was Ernst Ising. Ising started his dissertation on the investigation of ferromagnetism, summarized in a short paper written in 1924 and published 1 in 1925. Ising carried out an exact calculation for the special case of a one-dimensional lattice. His analysis showed that there was no phase transition to a ferromagnetic ordered state at any finite temperature. Ising wrongly predicted, that a phase transition also does not occur in higher dimensions.

This lead to initial rejection of the Lenz-Ising model form the physical community, including Ising himself.



Figure 1: Ernst Ising

When Werner Heisenberg proposed his own theory of ferromagnetism in 1928, he said:

"Ising succeeded in showing that also the assumption of directed sufficiently great forces between two neighboring atoms of a chain is not sufficient to explain ferromagnetism."

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The Lenz-Ising model became more relevant in 1936, when Rudolf Peierl showed that the 2d version must have a phase transition at finite temperature [3]. Finally in 1944 the twodimensional Ising model without an external field was solved analytically by Lars Onsager by a transfer-matrix method.

3 One dimensional Ising model

The one-dimensional Ising model is an chain of spins. Each spin σ can only have a discrete value of $\sigma_i = \pm 1$. The index i marks the position of the spin in the chain.



Figure 2: Ising chain

Like Ising did in 1924 1 we will take a look at the simplest possible case of the onedimensional Ising model. Our goal is to investigate if a phase transition occures, explaining spontaneous magnetisation and thus ferromagnetism. We will introduce two conditions.

- No external magnetic field H
- Each spin can only interact with its neighboring spin.

We will later refer to the second condition as only nears neighboring interactions (NN). The interaction strength between two spins σ_i and σ_{i+1} is characterised by the coupling strength J. The Hamiltonian \mathcal{H} of such a system is than given by

(1)
$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j$$

with the nears neighboring sum $\langle ij \rangle$. For a system with N_{tot} lattice sites and two possible σ_i -values at each lattice site, a total number of $2^{N_{tot}}$ possible configurations of the arrangement of particles exists. Summing over all possible configurations *i* then yields the partition sum Z:

(2)
$$Z = \sum_{\{i\}} e^{-\beta \mathcal{H}}$$
$$= \sum_{\sigma_1 = \pm 1} \sum_{\sigma_2 = \pm 1} \dots \sum_{\sigma_N = \pm 1} e^{\beta J(\sigma_1 \sigma_2 + \sigma_2 \sigma_3 + \sigma_3 \sigma_4 \dots)}$$

In order to simplify eq. (2) we introduce a new variable $\mu_i := \sigma_i \cdot \sigma_{i+1}$, describing whether two neighbouring spins are parallel or anti-parallel. The Hamiltonian (1) and the partition sum (2) can now be rewritten without a NN sum:

(3)
$$\mathcal{H} = -J \sum_{i} \mu_{i} \qquad \Rightarrow \qquad Z = 2 \cdot \sum_{\{\mu\}} e^{\beta J \sum_{i=1}^{N} \mu_{i}}$$

The factor of 2 in the partition function arises from the two possible configurations for the first spin in the chain.

In the thermodynamic limit (N >> 1) we can simplify the partition function:

(4)
$$Z = 2 \cdot \sum_{\{\mu\}} e^{\beta J \sum_{i=1}^{N-1} \mu_i}$$
$$= 2 \cdot \sum_{\mu_1 = \pm 1} \sum_{\mu_2 = \pm 1} \dots \sum_{\mu_{N-1} = \pm 1} e^{\beta J (\mu_1 + \mu_2 + \dots + \mu_{N-1})}$$
$$= 2 \cdot \sum_{\mu_1 = \pm 1} \sum_{\mu_2 = \pm 1} \dots \sum_{\mu_{N-2} = \pm 1} e^{\beta J (\mu_1 + \mu_2 + \dots + \mu_{N-2})} \underbrace{\sum_{\mu_{N-1} = \pm 1} e^{\beta J \mu_{N-1}}}_{(e^{\beta J} + e^{-\beta J})}$$

With the relation $(e^{\beta J} + e^{-\beta J}) = 2\cosh(\beta J)$ it follows:

(5)
$$Z = 2 \cdot \sum_{\mu_1 = \pm 1} \sum_{\mu_2 = \pm 1} \dots \sum_{\mu_{N-2} = \pm 1} e^{\beta J(\mu_1 + \mu_2 + \dots + \mu_{N-2})} 2 \cosh(\beta J)$$

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

This is our final result for the partition function of the one-dimensional Ising model without an external field.

Newt we want to show that in this simple case no phase transition at a finite temperature occurs. The average spin in the chain is given by:

(6)
$$\langle \sigma_i \rangle = \frac{1}{Z} \sum_{\{\sigma\}} \sigma_i e^{-\beta \mathcal{H}}$$

The more interesting case is to average alignment of two spins σ_i and σ_{i+j} , that don not necessarily have to be neighbors.

(7)
$$\langle \sigma_i \sigma_{i+j} \rangle = \frac{1}{Z} \sum_{\{\sigma\}} \sigma_i \sigma_{i+j} e^{-\beta \mathcal{H}}$$

In order to simplefy eq. (7) we introduce a different coupling constant J_i for each spin pair.

(8)
$$\langle \sigma_i \sigma_{i+j} \rangle = \frac{1}{Z} \sum_{\{\sigma\}} \sigma_i \sigma_{i+j} e^{-\beta \mathcal{H}}$$

$$= \frac{1}{Z} \sum_{\sigma_1 = \pm 1} \dots \sum_{\sigma_i = \pm 1} \sum_{\sigma_{i+1} = \pm 1} \dots \sum_{\sigma_N = \pm 1} \sigma_i \sigma_{i+j} e^{\beta (J_1 \sigma_1 \sigma_2 + J_2 \sigma_2 \sigma_3 + J_3 \sigma_3 \sigma_4 \dots)}$$

Next we rewrite the product $\sigma_i \cdot \sigma_{i+j}$ in terms of bonds rather than spins. Note that the product of any spin with itself ($\sigma_i \cdot \sigma_i = 1$) is always equal to one.

(9)
$$\sigma_{i} \cdot \sigma_{i+j} = \sigma_{i} \cdot 1 \cdot \ldots \cdot 1 \cdot \sigma_{i+j}$$
$$= \sigma_{i} \cdot (\sigma_{i+1} \cdot \sigma_{i+1}) \cdot (\sigma_{i+2} \cdot \ldots \cdot \sigma_{i+j-2}) \cdot (\sigma_{i+j-1} \cdot \sigma_{i+j-1}) \cdot \sigma_{i+j}$$
$$= \underbrace{(\sigma_{i} \cdot \sigma_{i+1})}_{\mu_{i}} \cdot \underbrace{(\sigma_{i+1} \cdot \sigma_{i+2})}_{\mu_{i+1}} \cdot \ldots \cdot \underbrace{(\sigma_{i+j-2} \cdot \sigma_{i+j-1})}_{\mu_{i+j-2}} \cdot \underbrace{(\sigma_{i+j-1} \cdot \sigma_{i+j})}_{\mu_{i+j-1}}$$

Combining eq. (8) and eq. (9) yields:

$$(10) < \sigma_i \sigma_{i+j} > = \frac{1}{Z} \sum_{\{\sigma\}} \sigma_i \sigma_{i+j} e^{-\beta \mathcal{H}} = \frac{1}{Z} \left[2\cosh\left(\beta J_1\right) \cdot \ldots \cdot 2\sinh\left(\beta J_i\right) \cdot \ldots \cdot 2\sinh\left(\beta J_{i+j-1}\right) \cdot \ldots \cdot 2\cosh\left(\beta J_{N-1}\right) \right]$$

The partition function Z for different coupling constant J_i for each spin pair can be calculated analogue to eq. (1.5):

$$(11) \Rightarrow \langle \sigma_i \sigma_{i+j} \rangle = \frac{\cosh\left(\beta J_1\right) \cdot \ldots \cdot \sinh\left(\beta J_i\right) \cdot \ldots \cdot \sinh\left(\beta J_{i+j-1}\right) \cdot \ldots \cdot \cosh\left(\beta J_{N-1}\right)}{\cosh\left(\beta J_1\right) \cdot \ldots \cdot \cosh\left(\beta J_i\right) \cdot \ldots \cdot \cosh\left(\beta J_{i+j-1}\right) \cdot \ldots \cdot \cosh\left(\beta J_{N-1}\right)}$$
$$= \prod_{m=1}^{j} \tanh\left(\beta J_{i+m-1}\right)$$

If we go back to a constant coupling constant $J_i = J$ the result becomes:

(12)
$$\langle \sigma_i \sigma_{i+j} \rangle = [tanh (\beta J)]^j$$

All that's left to do is to look at the temperature dependent magnetisation M of the system

(13)
$$M = m N < \sigma >$$

 $M^2 = m^2 N^2 < \sigma >^2 = m^2 N^2 \lim_{j \to \infty} \langle \sigma_i \sigma_{i+j} \rangle = 0 \quad \forall T > 0$

with the magnetic moment of each spin m, the number of spins in the system N and the average spin $< \sigma >$.

Because $tanh(\beta J) \leq 1$ the expression in eq. (12) becomes zero for large j. The only exception is at T = 0, where the $tanh(\beta J)$ diverges. So to be precise one have to say that a phase transition in the one-dimensional Ising model does not occur at a finite temperature.

4 Transfer Matrix

The next question we are going to answer is what happens to our system if we apply an external magnetic field H that can interact with the magnetic moment m of each spin. The Hamiltonian of such a system becomes:

(14)
$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - m H \sum_i \sigma_i$$

It is helpful to assume periodic boundary conditions ($\sigma_{N+1} = \sigma_1$), closing the one-dimensional Ising chain to a ring. We define a transfer matrix in the following way:

(15)
$$e^{-\beta \mathcal{H}(\sigma_1, \sigma_2, \sigma_3, ...)} = \underbrace{e^{\beta E(\sigma_1, \sigma_2)}}_{T_{1,2}} \underbrace{e^{\beta E(\sigma_2, \sigma_3)}}_{T_{2,3}} \dots \underbrace{e^{\beta E(\sigma_N - 1, \sigma_N)}}_{T_{N-1,N}} \underbrace{e^{\beta E(\sigma_N, \sigma_1)}}_{T_{N,1}}$$

So each transfer matrix is given by:

(16)
$$T_{i,i+1} = \exp\left(\beta J \sigma_i \sigma_{i+1} + \frac{1}{2} H (\sigma_i + \sigma_{i+1})\right)$$

Every spin can have two possible values so our transfer matric becomes a 2×2 matrix.

(17)
$$T_{i,i+1} = \begin{pmatrix} T_{+1,+1} & T_{+1,-1} \\ T_{-1,+1} & T_{-1,-1} \end{pmatrix} = \begin{pmatrix} e^{\beta J + H} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J - H} \end{pmatrix}$$

Now we can write down the partition function in terms of the transfer matrices

(18)
$$Z = \sum_{\{i\}} e^{-\beta \mathcal{H}}$$
$$= \sum_{\{i\}} T_{i,i+1}$$
$$= \sum_{\sigma_1 = \pm 1} \sum_{\sigma_2 = \pm 1} \dots \sum_{\sigma_N = \pm 1} T_{1,2} T_{2,3} \dots T_{N-1,N} T_{N,1}$$

Remember that matrix multiplication is defined as $(AB)_{ik} = \sum_j A_{ij}B_{jk}$. If we zoom in on the multiplication between the 1-2 transfer matrix and the 2-3 transfer matrix, we see that the transfer matrices are being multiplied by each other when we sum over their shared index σ_2 :

(19)
$$\sum_{\sigma_2} T_{1,2} T_{2,3} = (T \cdot T)_{\sigma_1 \sigma_3}$$

So when we sum over σ_2 , those two transfer matrices "collapse" together and we're left with a squared transfer matrix between spin σ_1 and spin σ_3 . If we repeat this process of "collapsing" all the transfer matrices together, we end up with

(20)
$$Z = \sum_{\sigma_1} (\underbrace{T \cdot T \cdot T \cdot \dots \cdot T}_{N \text{ times}})_{\sigma_1 \sigma_1},$$

which we recognize as the formula for the trace of T^N ,

(21)
$$Z = \operatorname{tr} \left[T^N \right] = \lambda_1^N + \lambda_2^N$$

The two eigenvalues of the transfer matrix (eq. 17) are

(22)
$$\lambda_{1,2} = e^{\beta J} \left[\cosh(H) \pm \sqrt{\cosh^2(H) - 2 e^{-2\beta J} \sinh(2\beta J)} \right].$$

In the thermodynamic limit the partition function simplifies even further. Only the larger eigenvalues λ_1 is relevant.

(23)
$$Z = \lim_{N \to \infty} \lambda_1^N \left(1 + \left(\frac{\lambda_2}{\lambda_1} \right)^N \right) = \lambda_1^N$$

Thus we have arrived at an exact solution for the one dimension Ising model with external field.

5 Two Dimensional Ising Model and Peirls Proof

The two-dimensional Ising model is defined on a two dimensional lattice. The Hamiltonian of the system is:

(24)
$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - m H \sum_i \sigma_i$$

One of the main differences between the one- and two-dimensional is the amount of nears neighbours. In the two-dimensional case each spin has four NN.

5.1 **Proof of Peirls Theorem**

In contrast to the one-dimensional Ising model, the two-dimensional case does show a phase transition, or to be more precise a phase transitions at a finite temperature. A phase transition means, that our system of spins shows magnetisation without any external field.



Figure 3: Schematic plot of a phase transition in a system of magnets.

In fig. 3 the magnetisation M is plotted against an outer magnetic field. On the left the temperature T is above a critical temperature T_c and on the right temperature T is below a critical temperature T_c . The existence of a phase transition is means that this critical temperature exists.

To proof the existence of a phase transition we have to show that the system tends to be magnetised, even without or with a small external field. Magnetisation means the alignment of spin states. A small, external magnetic field is implemented by fixing all spins on the outer layer into on spin state, lets say to plus spins $(\sigma_1 = +1)$. The idea is visualized in fig. (4). The idea behind Peirls proof is now to look at the spin in the center of our system. If a phase transition occurs and the system tends to magnetise, the probability of the spin in the center of our system being anti-parallel to the outer spins should become zero.



Figure 4: Arrangement of spins

We define ν as a configuration of spins in our system. Further we define two sets of spin configurations. Ω is the set of all configuration, where the outer spins are all spin up. The subset Ω_0 includes all configurations ν , where the outer spins are spin up (+) and the spin in the center of the system is spin down (-). In order to proof the existence of a phase transition we have to show that the probability of any configuration ν lying in Ω_0 diverges to zero in the thermodynamic limit.



Figure 5: different sets of spin configurations

If we take a closer look into any configuration $\nu \in \Omega$, we can see islands of minus spins in a sea of plus spins. As we can see in fig. 6 the island of minus spins can include lakes of plus spins. Note the red lines that separate the lake of plus spins from the islands of minus spins. Those are so called "shorelines". If two spins σ_i and σ_j are separated by a shoreline, their product $\sigma_i \cdot \sigma_j$ is always equal to -1.



Figure 6: Schematic zoom in a spin configuration

With the definition of a shoreline in mind we define a third set of spin configurations Ω_S , where the outer spins are all plus spins, the spin in the center of the system is a minus spin, and we have any fixed shoreline surrounding the spin in the center. Because it is rather hard to estimate the probability of a spin configuration ν lying in Ω_0 directly, we estimate the probability for $\nu \in \Omega_S$ first. To get the probability of $\nu \in \Omega_0$ we than sum over all different shoreline arrangements.

The probability of $\nu \in \Omega_S$ can be obtained by simple counting.

(25) Prob
$$(\nu \in \Omega_S) = \frac{1}{Z_\Omega} \sum_{\nu \in \Omega_S} e^{-\beta \mathcal{H}_{\nu}}$$
$$= \frac{1}{Z_\Omega} \sum_{\nu \in \Omega_S} \exp\left[\beta J \sum_{\langle ij \rangle} \sigma_i \sigma_j\right]$$

Next we separate the NN sum in the exponential function into spin pairs that are separated by the shoreline in the center and into those who are not. The number of spin pairs that are separated by the shoreline is nothing else than just the length of the shoreline n(S).

(26) Prob
$$(\nu \in \Omega_S) = \frac{1}{Z_\Omega} \sum_{\nu \in \Omega_S} \exp\left[-\beta J n(S)\right] \exp\left[\beta J \sum_{\langle ij \rangle \notin S} \sigma_i \sigma_j\right]$$

However the last term is rather hard to calculate. So we need to estimate an more explicit expression. For this we look at a spin configuration $\nu \in \Omega_S$ and flip all spins inside the shoreline surrounding the centering spin. We note this system as Ω'_S .



Figure 7: Flipping spins

The NN sum of two neighboring spins in the flipped system Ω'_S can be split into spin pairs that are separated by the shoreline and those who are not:

(27)
$$\forall \nu' \in \Omega'_S : \sum_{\langle ij \rangle} \sigma'_i \sigma'_j = \sum_{\langle ij \rangle \notin S} \sigma'_i \sigma'_j + \underbrace{\sum_{\langle ij \rangle \in S} \sigma'_i \sigma'_j}_{n(S)}$$

Using the property of the shoreline discussed above ($\sigma_i \cdot \sigma_j = -1$, if the two spins are separated by S), we see that the fallowing statement holds true :

(28)
$$\sum_{\langle ij \rangle \notin S} \sigma'_i \sigma'_j = \sum_{\langle ij \rangle \notin S} \sigma_i \sigma_j$$

Rearranging eq. 27 and using the that the length of the shoreline n(S) is always positive yields:

(29)
$$\sum_{\langle ij \rangle \notin S} \sigma_i \sigma_j = \sum_{\langle ij \rangle} \sigma'_i \sigma'_j - n(S) < \sum_{\langle ij \rangle} \sigma'_i \sigma'_j$$

Now that we found a expression for the sum we can plug eq. 29 in eq. 26

$$(30) \operatorname{Prob} (\nu \in \Omega_S) = \frac{1}{Z_{\Omega}} \sum_{\nu \in \Omega_S} \exp\left[-\beta J n(S)\right] \exp\left[\beta J \sum_{\langle ij \rangle \notin S} \sigma_i \sigma_j\right]$$
$$< \frac{1}{Z_{\Omega}} \sum_{\nu' \in \Omega'_S} \exp\left[-\beta J n(S)\right] \exp\left[\beta J \sum_{\langle ij \rangle} \sigma'_i \sigma'_j\right]$$
$$= e^{-\beta J n(S)} \frac{1}{Z_{\Omega}} \sum_{\nu' \in \Omega_S} \exp\left[\beta J \sum_{\langle ij \rangle} \sigma_i \sigma_j\right]$$
$$= e^{-\beta J n(S)} \frac{1}{Z_{\Omega}} \sum_{\nu \in \Omega_S} \exp\left[\beta J \sum_{\langle ij \rangle} \sigma_i \sigma_j\right]$$
$$< e^{-\beta J n(S)} \frac{1}{Z_{\Omega}} \sum_{\nu \in \Omega} \exp\left[\beta J \sum_{\langle ij \rangle} \sigma_i \sigma_j\right]$$
$$= e^{-\beta J n(S)}$$

So far we have obtained the probability of a spin configuration ν laying in the set Ω_S . To get the wanted probability of a spin configuration ν laying in the set Ω_0 we need to sum

over the set of all possible arrangements of shorelines η .

(31) Prob
$$(\nu \in \Omega_0) = \sum_{S \in \eta} \operatorname{Prob}(\Omega_S)$$

 $< \sum_{S \in \eta} e^{-\beta J n(S)}$

Because the notation of the sum is vague we replace the sum over the set of all possible arrangements of shorelines η by a sum over all shorelines of a certain length s(n).

(32) Prob
$$(\nu \in \Omega_0) < \sum_{n=1}^{\infty} s(n) e^{-\beta J n(S)}$$

The factor s(n) gives the amount of different shoreline configurations for any length n. It can by obtained by looking at closed random walks:

(33)
$$s(n) < \frac{1}{2}n4^n$$

Combining eq. 32 and 33 yields our final result.

(34) Prob
$$(\nu \in \Omega_0) < \sum_{n=1}^{\infty} s(n) e^{-\beta J n(S)}$$

 $< \sum_{n=1}^{\infty} \frac{1}{2} n 4^n e^{-\beta J n(S)}$
 $= \frac{1}{2} \sum_{n=1}^{\infty} n \left(\underbrace{4 e^{-\beta J}}_{x}\right)^n$

Because x < 1 this geometric series converges to $\frac{x}{(1-x)^2}$. To the probability that the spin in the center is a minus spin in a system where the outer spins are all plus spins is given by:

(35) Prob
$$(\nu \in \Omega_0) < \frac{1}{2} \frac{4 e^{-\beta J}}{(1 - 4 e^{-\beta J})^2} \xrightarrow{\beta \to \infty} 0$$

Thus have proven that for sufficiently low temperatures all spins in the systems tend to align even without an external magnetic field.

6 Applications

Due to its rather simple concept and the existence of analytical solutions the Ising model has been successfully applied in many field of science. One example is the description of DNA structures in polymer biology like done in [4].

A recently relevant application of the one-dimensional Ising model is the spread of diseases. In 5 it has been used to model the speed of contamination. The "spin" in this context are infected or non infected people.

In its almost 100 year old history the Ising model has been applied to a vast number of different systems making it to one of the most important models in statistical physics.

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