Insights into tensor network methods for Ising models

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Introduction

The Ising Model

This document presents an introductory work on the Ising model.

The Ising model is a statistical mechanics model. The model consists of discrete variables on a network that can interact with each other. Here, we will study the model as a mathematical model. What the discrete variables represent is therefore irrelevant. However, this model was historically created to study the magnetic properties of systems (invented by Wilhelm Lenz in 1920, and studied by his student, Ernst Ising), and is still used for this purpose. That's why we will use the vocabulary of magnetism to describe the model. But bear in mind that the variable can represent anything, and the result will be the same.

The variables, denoted by σ_i, can take only 2 values : $\sigma_i = +1$ or $\sigma_i = -1$. Although these variables are completely classical, and can represent anything in our model, we will consider that they represent magnetic dipole moments of atomic "spins", and we will call them "spin" for language's sake. The value $+1$ will be called up and will be represented by an arrow pointing upward. The value -1 will be called down and will be represented by an arrow pointing downward.

The state of a system of N spins is given by the value of each spin of the system, and it will be denoted :

$$\{\sigma\} = \{\sigma_0, \sigma_1, ..., \sigma_{N-1}\}$$

The spins can interact with each other and interact with an external field denoted h. Hence, the system is described by the following Hamiltonian :

$$H = -\sum_{i,j} J_{i,j}\sigma_i\sigma_j - h\sum_i \sigma_i$$

Here, we will simplify the problem.

First, we will only take into account the nearest neighbor interactions. It means that $J_{i,j} = 0$ if the spin i and the spin j are not neighbors. Hence, the sum on only the nearest neighbors is denoted by :

$$\sum_{<i,j>} J_{i,j}\sigma_i\sigma_j$$

Then, we will assume that the exchange term $J_{i,j}$ is the same for all the interactions between nearest neighbors and has the value J.

Finally, the Hamiltonian of the system becomes :

$$H = -J\sum_{<i,j>} \sigma_i\sigma_j - h\sum_i \sigma_i$$

Phase Transition

"In a system composed of many particles interacting directly only with their neighbors, a phase transition occurs if a macroscopic property of the system changes abruptly as a relevant parameter (temperature, porosity, density) varies continuously through a critical value". [1]

Ehrenfest classification

A first classification of the phase transitions was made by Paul Ehrenfest. He classified phase transitions on the basis of the behavior of the thermodynamic free energy as a function of other thermodynamic variables. Indeed, an abrupt change of a macroscopic property during a phase transition results in a discontinuity of one of the thermodynamic variables. In this scheme, phase transitions were labeled by the lowest derivative of the free energy that is discontinuous at the transition. First-order phase transitions exhibit a discontinuity in the first derivative of the free energy with respect to some thermodynamic variable. Second-order phase transitions are continuous in the first derivative but exhibit discontinuity in a second derivative of the free energy, etc.

Another way to see it is to say that phase transitions occur when the thermodynamic free energy of a system is non-analytic for some choice of thermodynamic variables.

Modern classifications

In the modern classification scheme, phase transitions are divided into many different categories (topological phase transitions, mixed-order phase transitions, ...), but there are still two categories named similarly to the Ehrenfest classes.

Here, we are only interested in the second-order phase transition category, also called "continuous phase transitions". They are characterized by a critical point that separates the two phases. At the critical point, susceptibility diverges, and the correlation length tends towards infinity. [6]

The aim of this work is to study the 1D and 2D Ising models, their critical point and phase transition.

Chapter 1

The 1D Ising Model

To familiarize ourselves with the various properties of the Ising model, we'll start by studying the simplest possible model: a one-dimensional linear chain.

Most of the model's properties can be deduced from its partition function. We will see how this partition function can be calculated using transfer matrices, and thus tensor networks. This will help us understand how powerful tensor networks can be for calculating partition functions.

We will also look at the conditions under which the 1D Ising model exhibits residual entropy.

Finally, we will check whether the 1D Ising model exhibits a phase transition through its various physical quantities (free energy, magnetization and correlation length).

1.1 Boundary Conditions

When we define a model, we need to define its boundary conditions. There are 3 main types of boundary conditions. We will study the 1D Ising model with these 3 different types of boundary conditions. On the one hand, we'll see that in the thermodynamic limit (when the size of the system tends towards infinity), the behavior of the system is the same with all boundary conditions. On the other hand, we will also look at some of the consequences of boundary conditions on a system of finite (small) size.

1. Open Boundary Conditions (OBC)

   For a system with Open Boundary Conditions, the first spin labelled 0 and the last spin labelled $N-1$ can each take the value $+1$ or -1.

   Here is a graphical representation of the system :

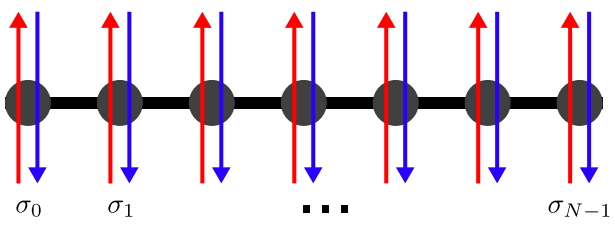


Figure 1.1: 1D Ising Model with Open Boundary Conditions.

2. Fixed Boundary Conditions (FBC)

   For a system with Fixed Boundary Conditions, the first spin labelled 0 and the last spin labelled $N-1$ have a fixed value, for instance $\sigma_0 = -1$ and $\sigma_{N-1} = +1$, or $\sigma_0 = +1$ and $\sigma_{N-1} = +1$.

   Here is a graphical representation of the system :

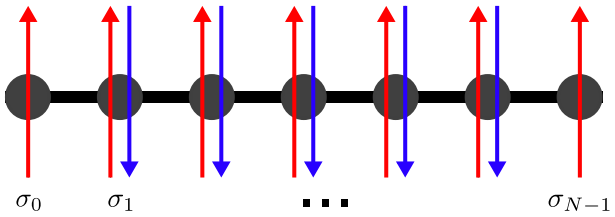


Figure 1.2: 1D Ising Model with Fixed Boundary Conditions.

3. Periodic Boundary Conditions (PBC)

   For a system with Periodic Boundary Conditions, the last spin labelled $N-1$ is linked to the first one labelled 0. One way to see it is to identify the N^{th} spin with the first one (labelled 0).

   Here are two ways to visualize the system :

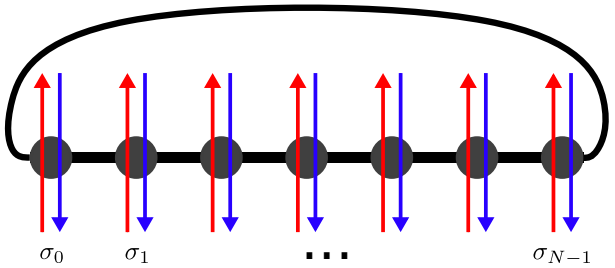


Figure 1.3: 1D Ising Model with Periodic Boundary Conditions. First visualization.

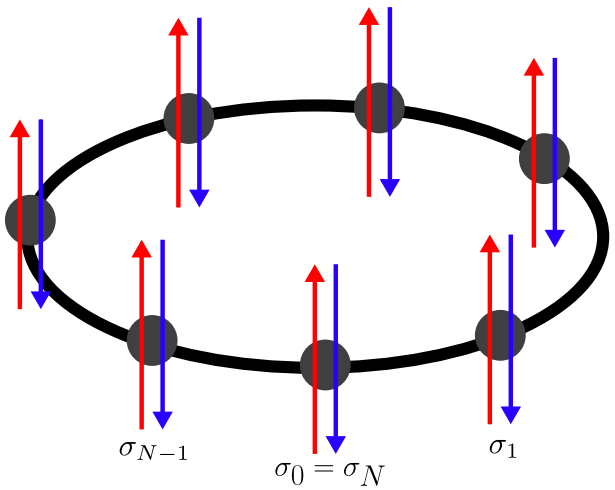


Figure 1.4: 1D Ising Model with Periodic Boundary Conditions. Second visualization.

1.2 Partition Function

1.2.1 Transfer matrix [9]

The partition function is a fundamental variable in statistical mechanics. It describes the statistical properties of a system in thermodynamic equilibrium. Most thermodynamic variables of a system can be calculated from the partition function.

We will calculate the partition function of the 1D Ising model with the 3 different boundary conditions, then show how it can be calculated with tensor networks.

The partition function is given by :

$$Z_N = \sum_{\{\sigma\}} e^{-\beta H(\{\sigma\})} \qquad \text{with} \quad \beta = \frac{1}{k_b T}$$

where the sum is done over every possible configurations.

1. Periodic Boundary Conditions

   Here we will use the identification $\sigma_N = \sigma_0$.

   $$Z_N^{PBC} = \sum_{\{\sigma\}} e^{\beta J(\sigma_0\sigma_1+\sigma_1\sigma_2+...+\sigma_{N-1}\sigma_0)+\beta h(\sigma_0+\sigma_1+...+\sigma_{N-1})}$$
   $$Z_N^{PBC} = \sum_{\{\sigma\}} e^{\beta J\sigma_0\sigma_1+\beta h\frac{1}{2}(\sigma_0+\sigma_1)} e^{\beta J\sigma_1\sigma_2+\beta h\frac{1}{2}(\sigma_1+\sigma_2)} ... e^{\beta J\sigma_{N-1}\sigma_0+\beta h\frac{1}{2}(\sigma_{N-1}+\sigma_0)}$$
   $$Z_N^{PBC} = \sum_{\{\sigma\}} T_{0,1}T_{1,2}...T_{N-1,0}$$

   Where $T_{i,j}$ is defined by :

   $$T_{i,j} = \begin{pmatrix} \overset{\sigma_j=+1}{e^{\beta(J+h)}} & \overset{\sigma_j=-1}{e^{-\beta J}} \\ e^{-\beta J} & e^{\beta(J-h)} \end{pmatrix} \begin{matrix} \sigma_i = +1 \\ \sigma_i = -1 \end{matrix}$$

   T is called the **transfer matrix** of the system.

2. Open Boundary Conditions

   $$Z_N^{OBC} = \sum_{\{\sigma\}} e^{\beta J(\sigma_0\sigma_1+\sigma_1\sigma_2+...+\sigma_{N-2}\sigma_{N-1})+\beta h(\sigma_0+\sigma_1+...+\sigma_{N-1})}$$
   $$Z_N^{OBC} = \sum_{\{\sigma\}} e^{\beta J\sigma_0\sigma_1+\beta h\frac{1}{2}(2\sigma_0+\sigma_1)} e^{\beta J\sigma_1\sigma_2+\beta h\frac{1}{2}(\sigma_1+\sigma_2)} ... e^{\beta J\sigma_{N-2}\sigma_{N-1}+\beta h\frac{1}{2}(\sigma_{N-2}+2\sigma_{N-1})}$$
   $$Z_N^{OBC} = \sum_{\{\sigma\}} T'_{0,1}T_{1,2}T_{2,3}...T_{N-3,N-2}T'^{\intercal}_{N-2,N-1}$$

Where $T'_{i,j}$ is defined by :

$$T'_{i,j} = \begin{matrix} \\ \sigma_i = +1 \\ \sigma_i = -1 \end{matrix} \overset{\begin{matrix} \sigma_j = +1 & \sigma_j = -1 \end{matrix}}{\begin{pmatrix} e^{\beta(J+\frac{3}{2}h)} & e^{\beta(-J+\frac{h}{2})} \\ e^{-\beta(J+\frac{h}{2})} & e^{\beta(J-\frac{3}{2}h)} \end{pmatrix}}$$

3. Fixed Boundary Conditions

   Here, the only difference with the previous case is that the value of the first and last spin is fixed. It means that the sum over all the possible configurations are done only over the spin 1, 2, ..., $N-2$ instead a sum over the spin 0, 1, ..., $N-1$. With $\sigma_0 = s_0$ and $\sigma_{N-1} = s_{N-1}$, we can write :

$$Z_N^{FBC} = \sum_{\substack{\sigma_1,\sigma_2,...,\sigma_{N-2} \\ \sigma_0=s_0 \\ \sigma_{N-1}=s_{N-1}}} e^{\beta J(\sigma_0\sigma_1+\sigma_1\sigma_2+...+\sigma_{N-2}\sigma_{N-1})+\beta h(\sigma_0+\sigma_1+...+\sigma_{N-1})}$$

$$Z_N^{FBC} = \sum_{\substack{\sigma_1,\sigma_2,...,\sigma_{N-2} \\ \sigma_0=s_0 \\ \sigma_{N-1}=s_{N-1}}} T'_{0,1}T_{1,2}T_{2,3}...T_{N-3,N-2}T'^{\intercal}_{N-2,N-1}$$

1.2.2 Tensor Network

Tensors can be seen as a mathematical concept that encapsulates and generalizes the idea of multilinear maps, i.e. functions of multiple parameters that are linear with respect to each parameter. From a numerical point of view, tensors can be considered simply as a multidimensional array of complex numbers. Tensor networks can then be seen as factorizations of very large tensors into smaller ones.

Tensor network methods are new computational methods that extend the range of models that can be simulated with a conventional computer in new and unprecedented directions. This is why tensor networks are finding applications in applied mathematics, chemistry, physics, machine learning and many other fields.

Moreover, tensor networks come with an intuitive graphical language to help us reason about them.

The expression of the partition function as a product of transfer matrices is in fact a tensor network. We will see that this is also the case in two dimensions. And it is because we can represent the partition function of an Ising model by a tensor network, that tensor networks are particularly useful for studying the Ising model [4].

Here, we will express the partition function of the 1D Ising model with the 3 possible boundary conditions as a tensor network.

We define a tensor as an array with n indices and we represent it by a shape (a disk) with n legs (see figure 1.5).

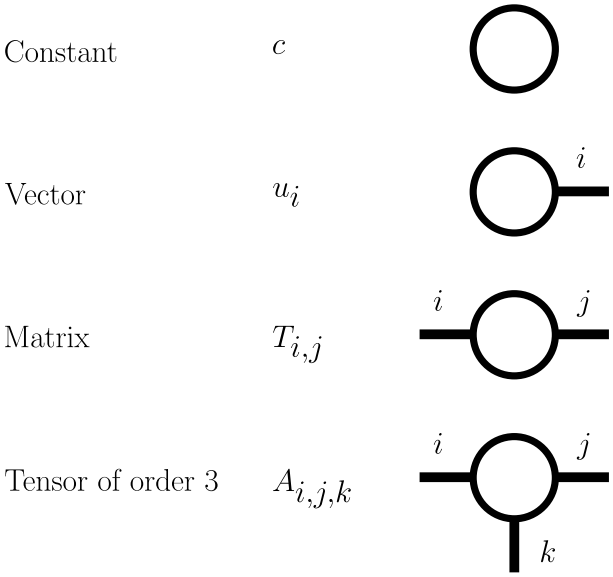


Figure 1.5: Tensor Network representation.

The total number of indices is called the order, degree or rank of a tensor, although the term "rank" generally has another meaning in the context of matrices and tensors.

You can contract tensors by connecting them. The rule is to sum over the indices which are connected, as illustrated below :

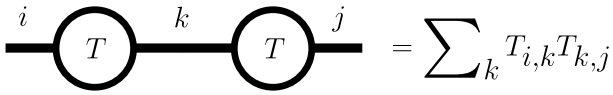


Figure 1.6: Tensor Network contraction rule.

1. Periodic Boundary Conditions

   The partition function of the 1D Ising model with periodic boundary conditions can be represented by the following tensor network :

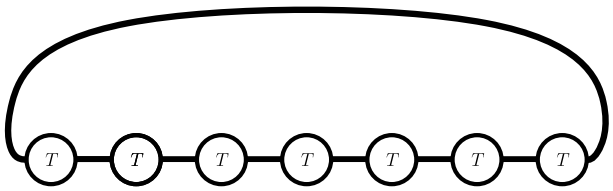


Figure 1.7: Periodic Boundary Conditions Tensor Network representation.

2. Open Boundary Conditions

We define the vector : $I = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$.

If $N \geq 3$, then the partition function of the 1D Ising model with Open Boundary Conditions can be represented by the following tensor network :

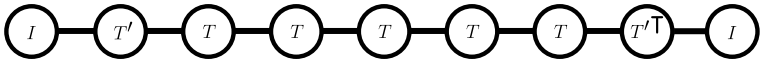


Figure 1.8: Open Boundary Conditions Tensor Network representation 1.

We have :

$$Z_N^{OBC} = \sum_{\{\sigma\}} I_0 T'_{0,1} T_{1,2} T_{2,3} ... T_{N-3,N-2} T'^{\intercal}_{N-2,N-1} I_{N-1}$$

$$Z_N^{OBC} = \sum_{\{\sigma\}} T_{1,2} T_{2,3} ... T_{N-3,N-2} T'^{\intercal}_{N-2,N-1} I_{N-1} I_0 T'_{0,1}$$

$$Z_N^{OBC} = \sum_{\sigma_1, \sigma_2, ..., \sigma_{N-2}} T_{1,2} T_{2,3} ... T_{N-3,N-2} A_{N-2,1}$$

Where :

$$A_{N-2,1} = \sum_{\substack{\sigma_0 \\ \sigma_{N-1}}} T'^{\intercal}_{N-2,N-1} I_{N-1} I_0 T'_{0,1}$$

$$A_{N-2,1} = \begin{pmatrix} e^{\beta(2J+3h)} + 2e^{\beta h} + e^{\beta(-2J-h)} & e^{2\beta h} + e^{-2\beta J} + e^{2\beta J} + e^{-2\beta h} \\ e^{2\beta h} + e^{-2\beta J} + e^{2\beta J} + e^{-2\beta h} & e^{\beta(2J-3h)} + 2e^{-\beta h} + e^{\beta(-2J+h)} \end{pmatrix}$$

The Tensor Network representation of Z_N^{OBC} becomes :

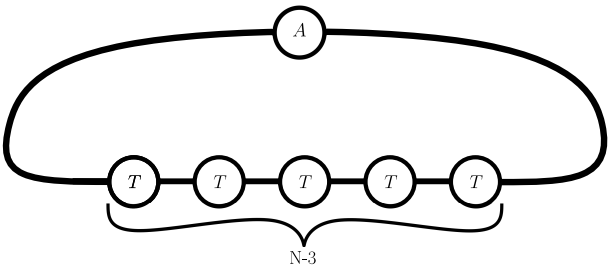


Figure 1.9: Open Boundary Conditions Tensor Network representation.

3. Fixed Boundary Conditions

If $N \geq 3$, then, we have :

$$Z_N^{FBC} = \sum_{\substack{\sigma_1,\sigma_2,...,\sigma_{N-2} \\ \sigma_0=s_0 \\ \sigma_{N-1}=s_{N-1}}} T'_{0,1} T_{1,2} T_{2,3} ... T_{N-3,N-2} T'^{\intercal}_{N-2,N-1}$$

$$Z_N^{FBC} = \sum_{\substack{\sigma_1,\sigma_2,...,\sigma_{N-2} \\ \sigma_0=s_0 \\ \sigma_{N-1}=s_{N-1}}} T_{1,2} T_{2,3} ... T_{N-3,N-2} T'^{\intercal}_{N-2,N-1} T'_{0,1}$$

$$Z_N^{FBC} = \sum_{\sigma_1,\sigma_2,...,\sigma_{N-2}} T_{1,2} T_{2,3} ... T_{N-3,N-2} B_{N-2,1}$$

where

$$B_{N-2,1} = T'^{\intercal}_{N-2,N-1} T'_{0,1}$$

$$B_{N-2,1} = \begin{pmatrix} \overset{\sigma_1=+1}{e^{\beta(s_{N-1}J+(\frac{1}{2}+s_{N-1})h)} e^{\beta(s_0 J+(\frac{1}{2}+s_0)h)}} & \overset{\sigma_1=-1}{e^{\beta(s_{N-1}J+(\frac{1}{2}+s_{N-1}))} e^{\beta(-s_0 J+(-\frac{1}{2}+s_0)h)}} \\ e^{\beta(-s_{N-1}J+(-\frac{1}{2}+s_{N-1})h)} e^{\beta(s_0 J+(\frac{1}{2}+s_0)h)} & e^{\beta(-s_{N-1}J+(-\frac{1}{2}+s_{N-1})h)} e^{\beta(-s_0 J+(-\frac{1}{2}+s_0)h)} \end{pmatrix} \begin{matrix} \sigma_{N-2}=+1 \\ \sigma_{N-2}=-1 \end{matrix}$$

$$B_{N-2,1} = \begin{pmatrix} \overset{\sigma_1=+1}{e^{\beta[(s_0+s_{N-1})J+(s_0+s_{N-1}+1)h]}} & \overset{\sigma_1=-1}{e^{\beta[(s_{N-1}-s_0)J+(s_0+s_{N-1})h]}} \\ e^{\beta[(s_0-s_{N-1})J+(s_0+s_{N-1})h]} & e^{\beta[-(s_0+s_{N-1})J+(s_0+s_{N-1}-1)h]} \end{pmatrix} \begin{matrix} \sigma_{N-2}=+1 \\ \sigma_{N-2}=-1 \end{matrix}$$

The Tensor Network representation of Z_N^{FBC} becomes :

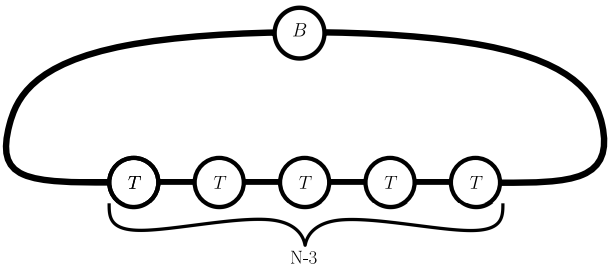


Figure 1.10: Fixed Boundary Conditions Tensor Network representation.

Note that the 3 boundary conditions can be represented by a tensor network of the same form, with only one tensor needed to define the boundary conditions (T^3, A or B).

1.2.3 Diagonalization

Now, we want to express the partition function as a function of the eigenvalues of the transfer matrix. Indeed, let be P a matrix such that :

$$T = P \begin{pmatrix} \lambda_0 & 0 \\ 0 & \lambda_1 \end{pmatrix} P^{-1}$$

Then, the partition function with Periodic Boundary Conditions becomes :

$$Z_N^{PBC} = \sum_{\{\sigma\}} T_{0,1} T_{1,2} ... T_{N-1,0} = Tr(T^N) = \sum_{i=0}^{1} \lambda_i^N$$

We define :

$$\alpha_+^2 = \frac{1}{2} \left(1 + \frac{e^{\beta J} \sinh(\beta h)}{\sqrt{e^{-2\beta J} + e^{2\beta J} \sinh(\beta h)^2}} \right)$$

$$\alpha_-^2 = \frac{1}{2} \left(1 - \frac{e^{\beta J} \sinh(\beta h)}{\sqrt{e^{-2\beta J} + e^{2\beta J} \sinh(\beta h)^2}} \right)$$

We can note that :

$$0 < \alpha_+ \leq 1$$

and

$$\alpha_+^2 + \alpha_-^2 = 1$$

Hence, the eigenvalues of T are :

$$\lambda_0 = e^{\beta J} \cosh(\beta h) + \sqrt{e^{-2\beta J} + e^{2\beta J} \sinh(\beta h)^2}$$

$$\lambda_1 = e^{\beta J} \cosh(\beta h) - \sqrt{e^{-2\beta J} + e^{2\beta J} \sinh(\beta h)^2}$$

And its eigenvectors are :

$u_0 = \begin{pmatrix} \alpha_+ \\ \alpha_- \end{pmatrix}$ and $u_1 = \begin{pmatrix} \alpha_- \\ -\alpha_+ \end{pmatrix}$

Then,

$$P = \begin{pmatrix} \alpha_+ & \alpha_- \\ \alpha_- & -\alpha_+ \end{pmatrix}$$

And

$$P^{-1} = \begin{pmatrix} \alpha_+ & \alpha_- \\ \alpha_- & -\alpha_+ \end{pmatrix}$$

Now we can give the expression of the partition function for the 3 Boundary Conditions :

1. Periodic Boundary Conditions

   The main goal of this diagonalization was to be able to compute Z_N^{PBC} as :

$$Z_N^{PBC} = \sum_{\{\sigma\}} T_{0,1}T_{1,2}...T_{N-1,0} = Tr(T^N) = \lambda_0^N + \lambda_1^N$$

2. Open Boundary Conditions

   In the case of Open Boundary Conditions, if $N \geq 3$, then we have :

   $Z_N^{OBC} = \sum_{\sigma_1,\sigma_2,...,\sigma_{N-2}} T_{1,2}T_{2,3}...T_{N-3,N-2}A_{N-2,1}$

   $Z_N^{OBC} = Tr(T^{N-3}A)$

   $Z_N^{OBC} = Tr(P \begin{pmatrix} \lambda_0^{N-3} & 0 \\ 0 & \lambda_1^{N-3} \end{pmatrix} P^{-1}A)$

   $Z_N^{OBC} = Tr(\begin{pmatrix} A_{1,1}(\alpha_+^2\lambda_0^{N-3}+\alpha_-^2\lambda_1^{N-3})+A_{2,1}\alpha_+\alpha_-(\lambda_0^{N-3}-\lambda_1^{N-3}) & A_{1,2}(\alpha_+^2\lambda_0^{N-3}+\alpha_-^2\lambda_1^{N-3})+A_{2,2}\alpha_+\alpha_-(\lambda_0^{N-3}-\lambda_1^{N-3}) \\ A_{2,1}(\alpha_-^2\lambda_0^{N-3}+\alpha_+^2\lambda_1^{N-3})+A_{1,1}\alpha_+\alpha_-(\lambda_0^{N-3}-\lambda_1^{N-3}) & A_{2,2}(\alpha_-^2\lambda_0^{N-3}+\alpha_+^2\lambda_1^{N-3})+A_{1,2}\alpha_+\alpha_-(\lambda_0^{N-3}-\lambda_1^{N-3}) \end{pmatrix})$

   $Z_N^{OBC} = A_{1,1}(\alpha_+^2\lambda_0^{N-3}+\alpha_-^2\lambda_1^{N-3})+A_{2,2}(\alpha_-^2\lambda_0^{N-3}+\alpha_+^2\lambda_1^{N-3})+(A_{2,1}+A_{1,2})\alpha_+\alpha_-(\lambda_0^{N-3}-\lambda_1^{N-3})$

3. Fixed Boundary Conditions

   In a similar way, if $N \geq 3$, then :

   $Z_N^{FBC} = Tr(P \begin{pmatrix} \lambda_0^{N-3} & 0 \\ 0 & \lambda_1^{N-3} \end{pmatrix} P^{-1}B)$

   $Z_N^{FBC} = Tr(\begin{pmatrix} B_{1,1}(\alpha_+^2\lambda_0^{N-3}+\alpha_-^2\lambda_1^{N-3})+B_{2,1}\alpha_+\alpha_-(\lambda_0^{N-3}-\lambda_1^{N-3}) & B_{1,2}(\alpha_+^2\lambda_0^{N-3}+\alpha_-^2\lambda_1^{N-3})+B_{2,2}\alpha_+\alpha_-(\lambda_0^{N-3}-\lambda_1^{N-3}) \\ B_{2,1}(\alpha_-^2\lambda_0^{N-3}+\alpha_+^2\lambda_1^{N-3})+B_{1,1}\alpha_+\alpha_-(\lambda_0^{N-3}-\lambda_1^{N-3}) & B_{2,2}(\alpha_-^2\lambda_0^{N-3}+\alpha_+^2\lambda_1^{N-3})+B_{1,2}\alpha_+\alpha_-(\lambda_0^{N-3}-\lambda_1^{N-3}) \end{pmatrix})$

   $Z_N^{FBC} = B_{1,1}(\alpha_+^2\lambda_0^{N-3}+\alpha_-^2\lambda_1^{N-3})+B_{2,2}(\alpha_-^2\lambda_0^{N-3}+\alpha_+^2\lambda_1^{N-3})+(B_{2,1}+B_{1,2})\alpha_+\alpha_-(\lambda_0^{N-3}-\lambda_1^{N-3})$

1.3 The Free Energy

Helmholtz free energy (referred to here simply as free energy) is an important thermodynamic potential that measures the useful work that can be obtained from a closed thermodynamic system at a constant temperature. Moreover, at constant temperature, free energy is minimized at equilibrium.

The total free energy of a system can be related to the partition function by the following formula :

$$F = -kTln(Z)$$

And we can define the free energy per site :

$$f_N = \frac{F}{N}$$

We want to calculate thermodynamic quantities in the thermodynamic limit, which is the limit when the number of particles N tends towards infinity.

N.B: In practice, there is no such thing as a physical system with an infinite number of particles. In this case, the thermodynamic limit is a priori never reached. However, it is important to bear in mind that the characteristic number of particles in a macroscopic system is the Avogadro number $N \sim 10^{23} >> 1$. This is why the thermodynamic limit should help us understand macroscopic systems.

Furthermore, quantities such as the total magnetic moment can tend towards infinity when N tends towards infinity. Because of the previous explanation, the laws of thermodynamics remain valid with a finite number of particles, and therefore finite quantities, when this number of particles is very large compared with 1.

In our case, the expression of the free energy per site becomes simpler when N tends towards infinity.

1. Periodic Boundary Conditions

   For the Periodic Boundary Conditions, the free energy is :

$$F_N^{PBC} = -kTln(\lambda_0^N + \lambda_1^N)$$

   And

$$f^{PBC} = \lim_{N\to\infty} f_N^{PBC} = -kTln(\lambda_0)$$

To illustrate the convergence of the free energy with the number of sites N towards the thermodynamic limit, here is the plot of the free energy per site for different number of site N :

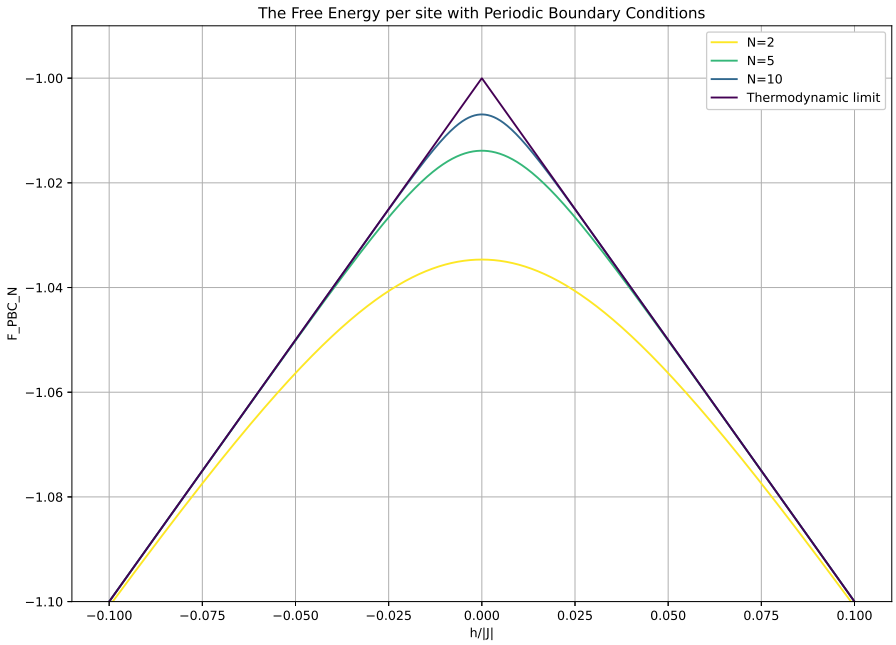


Figure 1.11: The free energy per site with Periodic Boundary Conditions (Ferromagnetic).

Here is how f^{PBC} looks as a function of the external field h for different temperature T :

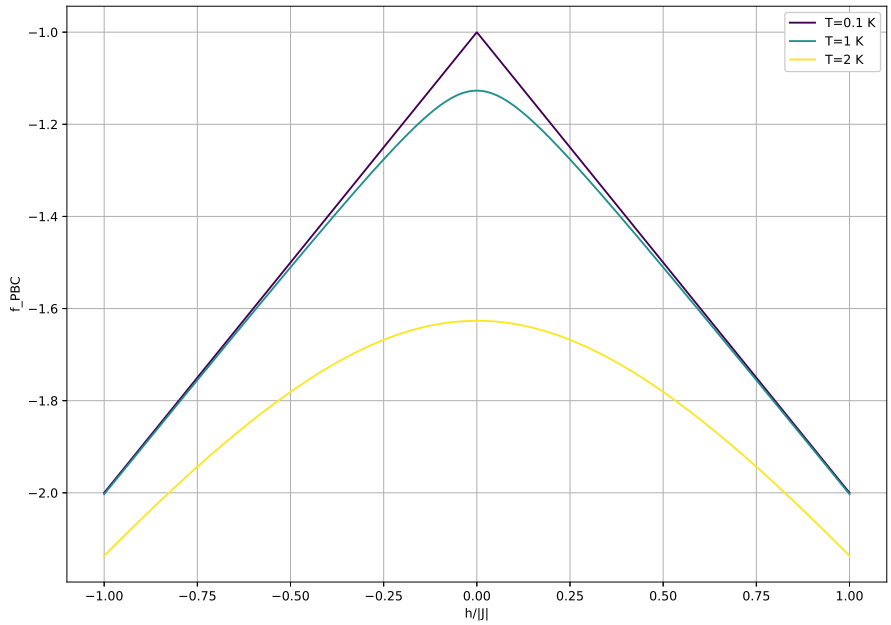


Figure 1.12: The free energy per site with Periodic Boundary Conditions in the thermodynamic limit (Ferromagnetic).

On figure 1.12, we see that when the temperature T tends towards 0, the curve for the free energy f^{PBC} becomes sharp at $h = 0$. It means that the derivative of f^{PBC} as a function of h has a discontinuity at $h = 0$. So, for the first time, we see that the Ising 1D model has a critical point at $T = 0$.

On figure 1.11, we see that when N tends toward infinity, the free energy per site tends toward the free energy per site in the thermodynamic limit. A crucial point is that with a finite number of particles N, all the quantity are completely smooth. It means that, in theory, there is no critical point in a finite system. However, for real systems with a number of particles of the order of magnitude of the Avogadro number, the thermodynamic limit should be a good description, and we can expect to see critical points.

2. Open Boundary Conditions

$f^{OBC} = \lim_{N\to\infty} f_N^{OBC} = \lim_{N\to\infty} -\frac{1}{N}kTln(Z_N^{OBC})$

$f^{OBC} = \lim_{N\to\infty} -\frac{1}{N}kTln\big(A_{1,1}(\alpha_+^2\lambda_0^{N-3}+\alpha_-^2\lambda_1^{N-3})+A_{2,2}(\alpha_-^2\lambda_0^{N-3}+\alpha_+^2\lambda_1^{N-3})+(A_{2,1}+A_{1,2})\alpha_+\alpha_-(\lambda_0^{N-3}-\lambda_1^{N-3})\big)$

$f^{OBC} = \lim_{N\to\infty} -\frac{N-3}{N}kTln(\lambda_0) - \frac{1}{N}kTln(A_{1,1}\alpha_+^2 + A_{2,2}\alpha_-^2 + (A_{2,1}+A_{1,2})\alpha_+\alpha_-)$

Hence :

$$f^{OBC} = -kTln(\lambda_0) = f^{PBC}$$

3. Fixed Boundary Conditions

It is the same thing for the fixed boundary conditions :

$$f^{FBC} = -kTln(\lambda_0) = f^{PBC}$$

We note that in the thermodynamic limit, the free energy per site is the same for all 3 possible boundary conditions. This means that the behavior of the system in the thermodynamic limit will be the same with all 3 boundary conditions. The difference between the 3 boundary conditions will only exist for systems of finite size.

1.4 The thermal average

We define the thermal average of any physical quantity A denoted $\langle A\rangle$ by :

$$\langle A\rangle = \frac{\sum_r A_r e^{-\beta E_r}}{\sum_r e^{-\beta E_r}}$$

Where the sum run over all the possible configurations.
For instance, we define the thermal average of the i^{th} spin by :

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

1.5 The magnetization

Historically, the Ising model was a mathematical model for studying ferromagnetism. That's why we're interested in the "magnetization" of the model. But we must bear in mind that the variables in the model do not necessarily describe the magnetic dipole moments of atomic "spins", and can represent anything with 2 states interacting with each other.

The sum of the values of all the variables (here, magnetization), is useful for studying the collective behavior of the model, and its phase transition. That's why it's an important physical quantity that we're going to study.

1.5.1 Definition

Here, the total magnetic moment of the system is :

$$M = \sum_i \sigma_i$$

We have :

$$kT\left(\frac{\partial ln(Z)}{\partial h}\right)_T = \frac{kT}{Z}\frac{\partial}{\partial h}\sum_{\{\sigma\}} e^{-\beta(-J\sum \sigma_i\sigma_{i+1} - h\sum \sigma_i)} = kT\sum_{\{\sigma\}} \beta(\sum_i \sigma_i)\frac{e^{-\beta(-J\sum \sigma_i\sigma_{i+1} - h\sum \sigma_i)}}{Z}$$

i.e.

$$\left(-\frac{\partial F}{\partial h}\right)_T = \sum_{\{\sigma\}}(\sum_i \sigma_i)\frac{e^{-\beta H(\{\sigma\})}}{Z} = \langle M\rangle$$

In the thermodynamic limit, this result can also be found as follows: :

$$dU = TdS - \langle M\rangle dh - PdV$$

where U is the energy, T the temperature, S the entropy, M the total magnetic moment, h the magnetic field, P the pressure and V the volume of the system. We assume the volume is constant, hence :

$$dU = TdS - \langle M\rangle dh$$

$$F = U - TS$$

$$dF = dU - TdS - SdT = TdS - \langle M\rangle dh - TdS - SdT = -\langle M\rangle dh - SdT$$

Then, the total magnetic moment is given by :

$$\langle M \rangle = (-\frac{\partial F}{\partial h})_T$$

The magnetization m is defined as the magnetic moment per unit volume [2] and M is the integral of the magnetization over the sample. Here, we have :

$$m = \frac{M}{N} = \frac{1}{N}\sum_i \sigma_i$$

$$\langle m \rangle = \frac{1}{N}(-\frac{\partial F}{\partial h})_T = (-\frac{\partial f}{\partial h})_T$$

1.5.2 Magnetization in the Periodic Boundary Conditions

In the periodic boundary conditions, we have :

$\langle M_N^{PBC} \rangle = (-\frac{\partial F_N^{PBC}}{\partial h})_T$

$= (\frac{\partial}{\partial h} kTln(\lambda_0^N + \lambda_1^N))_T$

$= \frac{kT}{\lambda_0^N + \lambda_1^N}[N(\frac{\partial \lambda_0}{\partial h})_T \lambda_0^{N-1} + N(\frac{\partial \lambda_1}{\partial h})_T \lambda_1^{N-1}]$

where

$(\frac{\partial \lambda_{0,1}}{\partial h})_T = \beta e^{\beta J} sinh(\beta h) \pm \frac{2\beta e^{2\beta J} cosh(\beta h) sinh(\beta h)}{2\sqrt{e^{-2\beta J} + e^{2\beta J} sinh(\beta h)^2}} = \beta e^{\beta J} sinh(\beta h)[1 \pm \frac{e^{\beta J} cosh(\beta h)}{\sqrt{e^{-2\beta J} + e^{2\beta J} sinh(\beta h)^2}}]$

In the thermodynamic limit, we have :

$$\langle m^{PBC} \rangle = (-\frac{\partial f}{\partial h})_T$$

$$\langle m^{PBC} \rangle = \frac{kT}{\lambda_0}(\frac{\partial \lambda_0}{\partial h})_T$$

$$\langle m^{PBC} \rangle = \frac{e^{\beta J} sinh(\beta h)}{\sqrt{e^{-2\beta J} + e^{2\beta J} sinh(\beta h)^2}}$$

The figure 1.13 shows how $\langle m^{PBC} \rangle$ looks as a function of h.

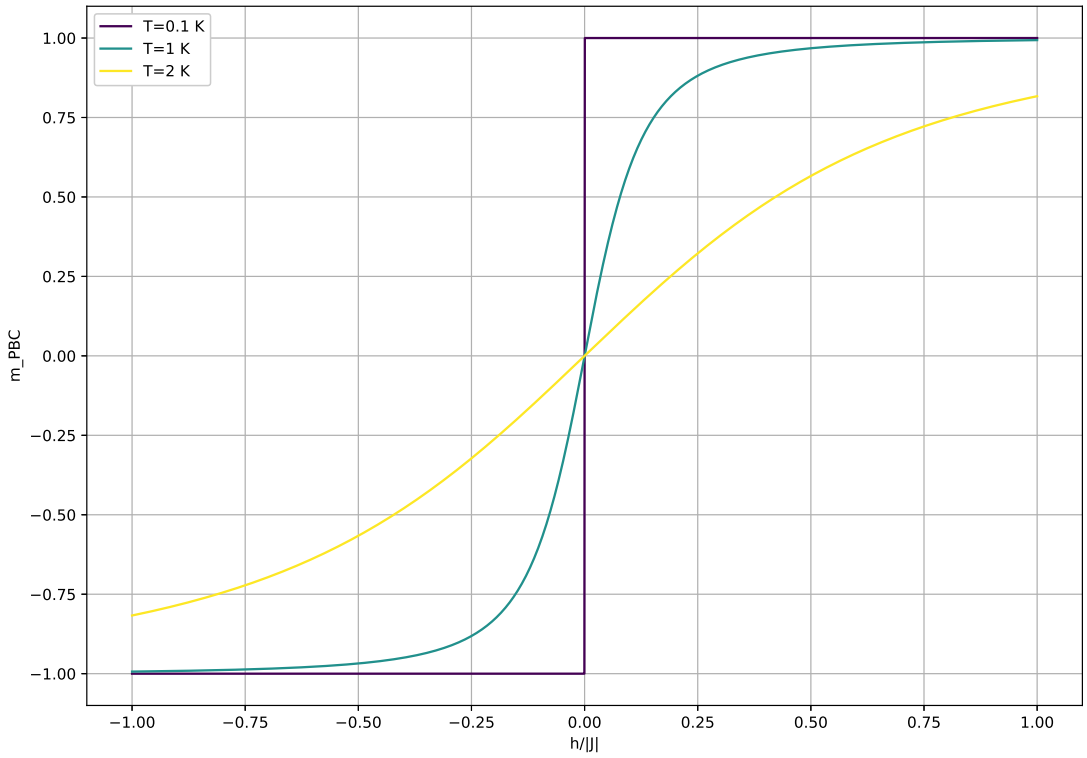


Figure 1.13: The thermal average of magnetization with Periodic Boundary Conditions in the thermodynamic limit (Ferromagnetic).

Here it is clear that when the temperature T tends towards 0, a discontinuity in the magnetization $\langle m^{PBC} \rangle$ appears at $h = 0$. The magnetization is the first derivative of the free energy as a function of the external field h. Hence, in the thermodynamic limit, the 1D Ising Model exhibits a critical point at $T = 0$.

We can check that when T tends towards 0:

$$\langle m^{PBC} \rangle \sim \frac{e^{\beta J} sinh(\beta h)}{\sqrt{e^{2\beta J} sinh(\beta h)^2}} \sim \frac{e^{\beta J} sinh(\beta h)}{|e^{\beta J} sinh(\beta h)|} \sim sgn(sinh(\beta h)) = \begin{cases} -1 & \text{if} \quad h < 0 \\ +1 & \text{if} \quad h > 0 \end{cases}$$

1.5.3 Magnetization with Fixed Boundary Conditions

We have seen that in the thermodynamic limit $f^{FBC} = f^{PBC}$, hence in the thermodynamic limit $\langle m^{FBC} \rangle = \langle m^{PBC} \rangle$.

But, it is interesting to see what happens for small N with Fixed Boundary Conditions. Indeed, let assume that we impose the first and the last spin to be up in the ferromagnetic case ($J > 0$), then intuitively we tend to think that the spins in the middle will tend to be up. Here is the thermal average of the mean magnetic moment per site $m_N^{FBC} = \frac{M_N^{FBC}}{N}$ for $N = 3$:

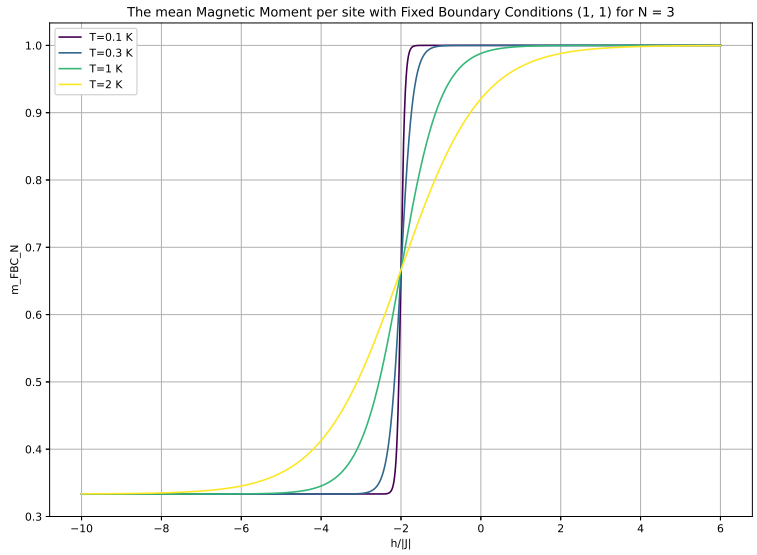


Figure 1.14: The thermal average of the mean magnetic moment per site with Fixed Boundary Conditions for $N = 3$ (Ferromagnetic).

We see that the mean magnetic moment per site is between $\frac{1}{3}$ and 1. Indeed, there are 2 spins up, and only the spin in the middle is free. So, if the spin in the middle is up, $m_3^{FBC} = \frac{3}{3} = 1$, and if it is down, $m_3^{FBC} = \frac{1}{3}$.

What it is remarkable is the external field h must be twice as strong as the exchange term J to flip the spin in the middle. Indeed, flip the spin in the middle from top to bottom induced a change in the energy of the system of $4J - 2h$.

It can also be seen that with increasing chain length, the curve profile tends towards the thermodynamic limit profile, with the total magnetic moment tilting at $h = 0$.

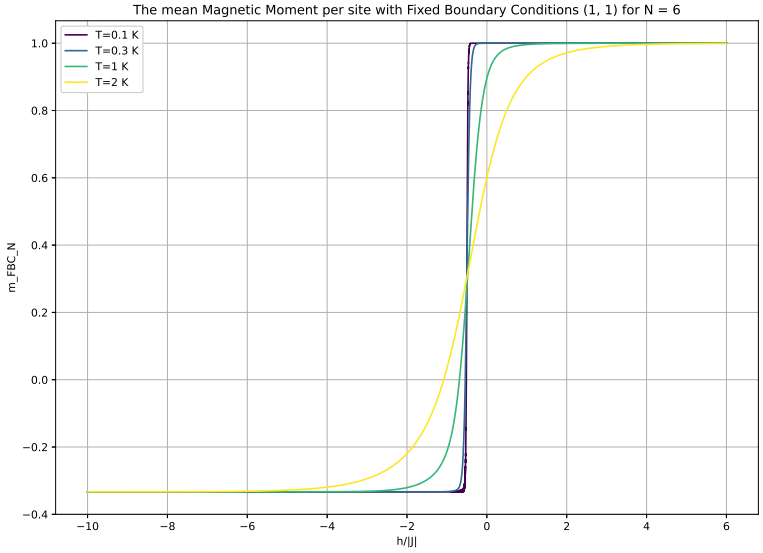


Figure 1.15: The thermal average of the mean magnetic moment per site with Fixed Boundary Conditions for $N = 6$ (Ferromagnetic).

1.6 Residual entropy

Usually, a microstate is defined as a state in which all the molecular details of the system, including the position and momentum of each molecule, are specified. Here, a microstate will be a state in which the orientation of each spin of the system is specified.

According to the fundamental postulate of statistical mechanics, among the system's microstates with the same energy (i.e. degenerate microstates), each microstate is assumed to be populated with equal probability (in general, this assumption is justified for an isolated system in thermodynamic equilibrium). Then, the entropy is proportional to the natural logarithm of the number of microstates likely to cause the observed macroscopic state (macrostate) of the system and is defined as $S = k_B \ln(\Omega)$ (where Ω is the number of microstates whose energy equals to the one of the system). The more such states are available to the system with appreciable probability, the higher the entropy.

In general, there is a single microstate (called the ground state) with minimum energy. In this case, at absolute zero, the system will be in the unique ground state and entropy will be exactly zero. In some cases, a finite amount of entropy may remain when the system is brought to very low temperatures: this is the residual entropy of the system.

In this section, we will look at the particular conditions under which the 1D Ising model exhibits residual entropy.

What happens in the antiferromagnetic case (J<0) when |h|=|2J| ?

Antiferromagnetic case (J<0)

In the antiferromagnetic case ($J < 0$), there is a competition between the exchange term J and the external field h. This is because the exchange term pushes neighboring spins to align in the opposite direction, whereas the external field always pushes spins to align in the same direction. We can see it on the following plot :

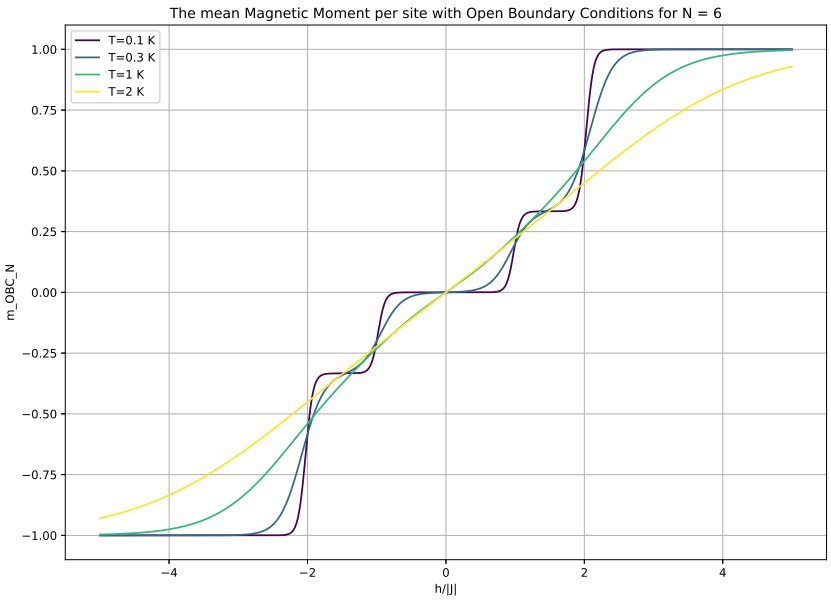


Figure 1.16: The thermal average of the mean magnetic moment per site with Open Boundary Conditions for $N = 6$ (Antiferromagnetic).

At $h = 0$, the configurations with the lowest energy are $|+-+-+-\rangle$ and $|-+-+-+\rangle$. As $\frac{h}{|J|}$ increases, there is a change in the total magnetic moment at $\frac{h}{|J|} = 1$. Changing the orientation of the first or last spin only modifies the interaction with 1 neighbor. The 'energy cost' is therefore only $2J - 2h$. When $1 < \frac{h}{|J|} < 2$, the configurations with the lowest energy are $|+-+-++\rangle$ and $|++-+-+\rangle$.

Then, there is another change of the total magnetic moment at $\frac{h}{|J|} = 2$. Here, the external field succeeds to flip all the spin of the chain. The 'energy cost' to flip a spin which is in the middle of the chain is $4J - 2h$. When $2 < \frac{h}{|J|}$, the configurations with the lowest energy is $|++++++\rangle$.

With Periodic Boundary Conditions, there are only the steps for $|\frac{h}{J}| = 2$:

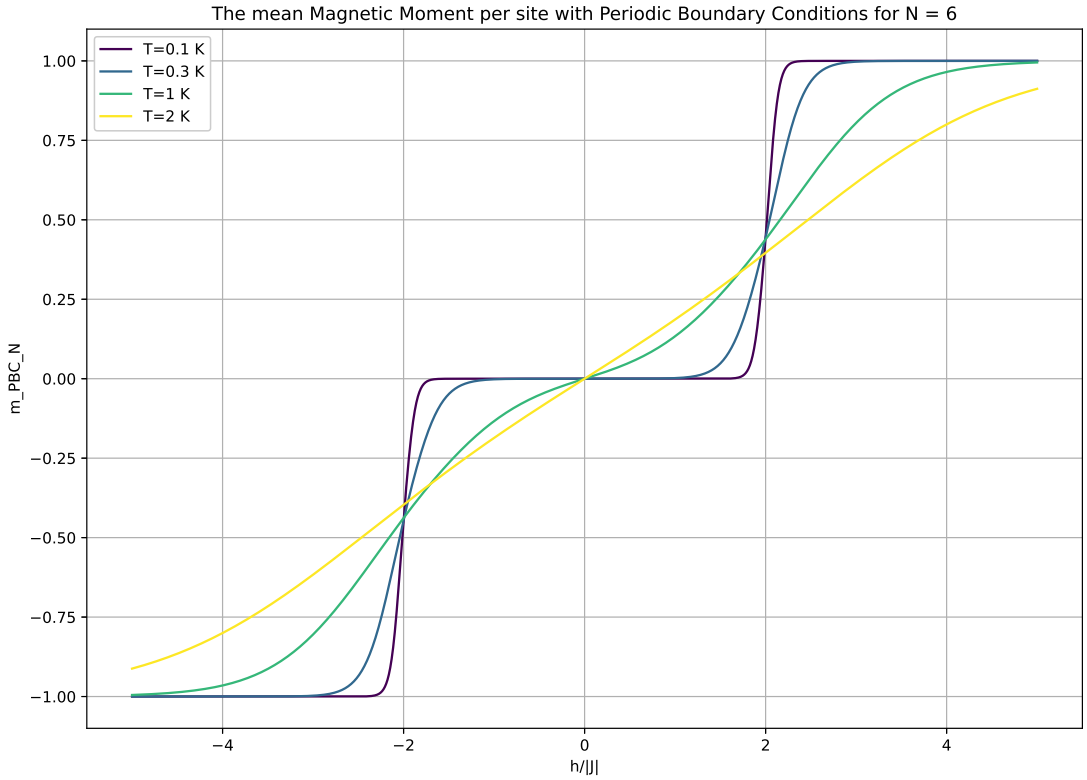


Figure 1.17: The thermal average of the mean magnetic moment with Periodic Boundary Conditions for $N = 6$ (Antiferromagnetic).

In fact, the step between $|\frac{h}{J}| = 1$ and $|\frac{h}{J}| = 2$ in the figure 1.16 is a finite size effect. We see below that this step fades as the size of the system N increases :

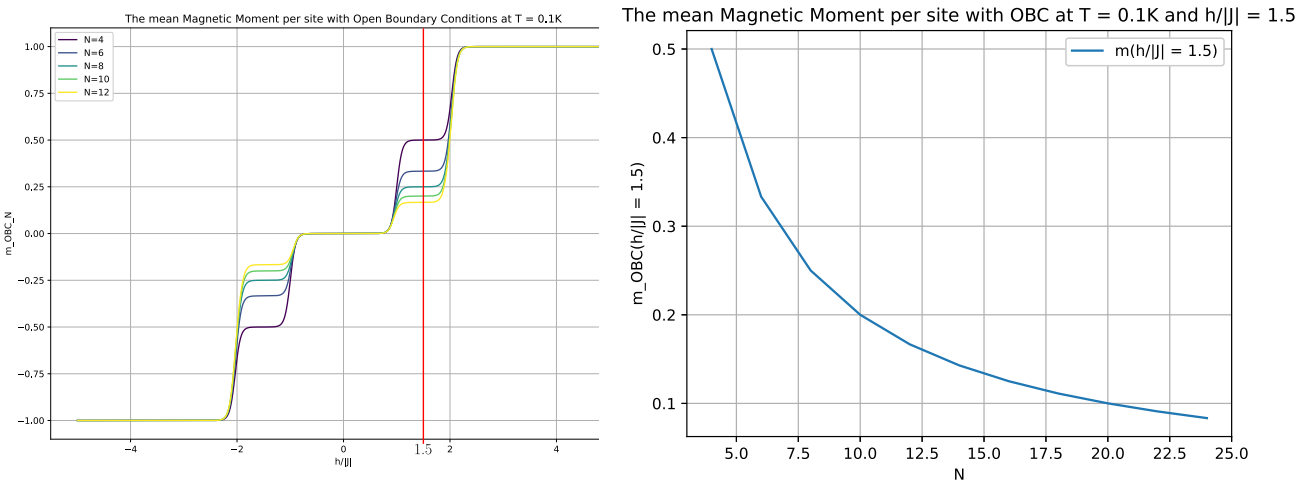


Figure 1.18: The thermal average of the mean magnetic moment with Periodic Boundary Conditions for $T = 0.1K$ (Antiferromagnetic).

As we saw in the Free Energy part 1.3, the free energy per site is the same for the 3 Boundary Conditions in the thermodynamic limit. Hence, we expected that the thermal average of the mean magnetic moment to be the same for the 3 Boundary Conditions in the thermodynamic limit.

Antiferromagnetic case (J<0) when |h|=|2J|

In this section, we will only study the cases where N is even.

Here is the plot of the energy per site as a function of h/J of all the possible configurations with Periodic Boundary Conditions for $N = 8$ in the antiferromagnetic case ($J = -1$).

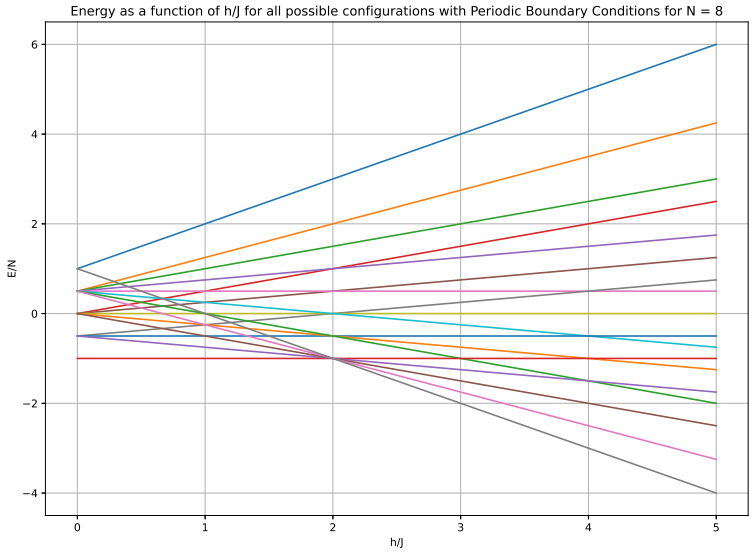


Figure 1.19: The energy per site as a function of h/J of all the possible configurations with Periodic Boundary Conditions for $N = 8$ in the antiferromagnetic case ($J = -1$).

We can see that something interesting happens when $|\frac{h}{J}| = 2$. Let us analyze this graph.

Here, this is the antiferromagnetic case ($J = -1$), it means that without external field, the energy is minimum when the neighbors spins are in opposite direction. So the y-intercept is defined by the number of boundaries between spin up and spin down. The upper point corresponds to the configurations with zero frontier, meaning the configuration where all the spins are up or all are down. The lowest point corresponds to the configuration with alternating spin-up and spin-down, i.e this configuration $|+-+-+-+-\rangle$ or this one $|-+-+-+-+\rangle$.

The slope of the energy is given by : $a = N^+ - N^-$ where N^+ and N^- are respectively the number of spins up and of spins down in the configurations.

We can see that for any y-intercept, all the configurations with the smallest slope intersect at the same point at $\frac{h}{J} = 2$. In fact, for each y-intercept, the configurations with the smallest slope are the configurations with n spins up in which there are not 2 spins up next to each other. For $N = 8$, the 5 "types" of configurations which intersect at $\frac{h}{J} = 2$ are (from top to bottom) :

$$|--------\rangle\,,\ |+-------\rangle\,,\ |+-+------\rangle\,,\ |+-+-+---\rangle\,,\ |+-+-+-+-\rangle$$

For this type of configuration with $n \leq \frac{N}{2}$ spins up, we have :

$$E = -(N - 4n)J - (2n - N)h$$

Then, it intersects the ground state of energy $E_0 = NJ$ when :

$$-(N - 4n)J - (2n - N)h = NJ$$

i.e.

$$h = 2J$$

We should remark that for $|\frac{h}{J}| < 2$, there are only two configurations with the ground state energy, for $|\frac{h}{J}| > 2$ there is only one configuration with the ground state energy ($|-----\rangle$). How many configurations there are with the minimum energy at $|\frac{h}{J}| = 2$?

For the Open Boundary Conditions, we find that the number of configurations with the minmium energy, denoted $u_{OBC}(N)$, is (see Appendix A.1) :

$$u_{OBC}(N) = \frac{\sqrt{5}+3}{2\sqrt{5}}\phi^N + \frac{\sqrt{5}-3}{2\sqrt{5}}\psi^N$$

The key point is that the number of valid configurations is exponential to the size of the system. Indeed, the mean residual entropy per site is given by $s = \frac{S}{N} = \frac{1}{N}k_B \ln(\Omega)$. So, if the number of configurations grows less quickly than exponentially with the size of the system, the average residual entropy per site tends towards 0.

This means that at $T = 0$, the 1D Ising model in the antiferromagnetic case ($J < 0$) has a residual entropy when $|h| = |2J|$.

Calculation of the residual entropy with the partition function

We can use the partition function to compute the number of configurations with the minimal energy at $T = 0K$ in the antiferromagnetic case ($J < 0$) when $h = |2J|$.

We denote E_0 the lowest energy that the system can take. We can shift all the energies by E_0. The Hamiltonian becomes :

$$H = -J \sum_{<i,j>} \sigma_i \sigma_j - h \sum_i \sigma_i - E_0$$

And the partition function becomes :

$$Z_N = \sum_{\{\sigma\}} e^{-\beta(H(\{\sigma\})-E_0)}$$

For any configuration $\{\sigma\}$ with the lowest energy, we have :

$$e^{-\beta(H(\{\sigma\})-E_0)} = e^0 = 1$$

And for any configuration $\{\sigma\}$ with an energy $H(\{\sigma\})$ higher than E_0, we have :

$$\lim_{T\to 0} e^{-\beta(H(\{\sigma\})-E_0)} = 0$$

Then :

$$\lim_{T\to 0} Z_N = \#\text{ configurations with energy equal to } E_0 = u_{PBC}(N)$$

Let us work on the Periodic Boundary Conditions. The new partition function is :

$Z_N^{PBC} = \sum_{\{\sigma\}} e^{\beta(J(\sigma_0\sigma_1+\sigma_1\sigma_2+...+\sigma_{N-1}\sigma_0)+h(\sigma_0+\sigma_1+...+\sigma_{N-1})+E_0)}$
$Z_N^{PBC} = \sum_{\{\sigma\}} e^{\beta(J\sigma_0\sigma_1+h\frac{1}{2}(\sigma_0+\sigma_1)+\frac{E_0}{N})} e^{\beta(J\sigma_1\sigma_2+h\frac{1}{2}(\sigma_1+\sigma_2)+\frac{E_0}{N})} ... e^{\beta(J\sigma_{N-1}\sigma_0+h\frac{1}{2}(\sigma_{N-1}+\sigma_0)+\frac{E_0}{N})}$
$Z_N^{PBC} = \sum_{\{\sigma\}} T_{0,1}^{shifted} T_{1,2}^{shifted} ... T_{N-1,0}^{shifted}$

Where $T_{i,j}^{shifted}$ is defined by :

$$T_{i,j}^{shifted} = \begin{matrix} \\ \sigma_i = +1 \\ \sigma_i = -1 \end{matrix} \begin{matrix} \begin{matrix} \sigma_j = +1 & \sigma_j = -1 \end{matrix} \\ \begin{pmatrix} e^{\beta(J+h+\frac{E_0}{N})} & e^{\beta(-J+\frac{E_0}{N})} \\ e^{\beta(-J+\frac{E_0}{N})} & e^{\beta(J-h+\frac{E_0}{N})} \end{pmatrix} \end{matrix}$$

And

$$Z_N^{PBC} = Tr(T^{shifted^N}) = \sum_{i=0}^{1} \lambda_i^{shifted^N}$$

A configuration with the minimum energy E_0 is the configuration where all spins are alternated, denoted $|E_0\rangle$, with $|E_0\rangle = |+-+-...+-\rangle$.

Case when N is even

When N is even, in $|E_0\rangle$ the last and the first spin are in an opposite direction.
Thus, when N is even :

$$E_0 = -J \sum_{<i,j>} (-1) - h \times 0 = NJ$$

Case when N is odd

When N is odd, in $|E_0\rangle$, the last and the first spin are in the same direction.
Thus, when N is odd :

$$E_0 = -J(-(N-1)+1) - h = -J(-N+2) - h = (N-2)J - h$$

At the precise point $h = -2J$ where we work, we have :

$$E_0 = (N-2)J + 2J = NJ$$

The value of the minimum energy is therefore the same when N is odd as when N is even.

Then,

$$T^{shifted} = \begin{pmatrix} e^{\beta(2J+h)} & 1 \\ 1 & e^{\beta(2J-h)} \end{pmatrix}$$

And $(h = -2J)$:

$$T^{shifted} = \begin{pmatrix} 1 & 1 \\ 1 & e^{4\beta J} \end{pmatrix}$$

We diagonalize $T^{shifted}$. Its eigenvalues are :

$$\lambda_{0,1}^{shifted} = \frac{1}{2}(1 + e^{4\beta J} \pm \sqrt{4 + (1 - e^{4\beta J})^2})$$

Hence

$$\lim_{T \to 0} Z_N = u_{PBC}(N) = (\frac{1+\sqrt{5}}{2})^N + (\frac{1-\sqrt{5}}{2})^N$$

The Fibonacci sequence recurrence formula is back !

The magnetization

At the point $h = |2J|$, all the configurations that we have just counted has the same Boltzmann weight. Hence, the mean magnetization per site is the average of the magnetization of all these configurations.

We denote $c(k, N)$ the number of configurations with k spins up in which there are not 2 spins up next to each other. The magnetization of a configuration with k spins up is $k - (N - k) = 2k - N$. Then, the mean magnetization per site at the point $h = |2J|$ is given by :

$$\langle m_N \rangle = \frac{1}{N \times u_{PBC}(N)} \sum_{k=0}^{\lfloor N/2 \rfloor} c(k, N)(2k - N)$$

We can show that (see Appendix A.2) that :

$$\langle m_N \rangle = -\frac{1}{\sqrt{5}} \frac{\phi^N - \psi^N}{\phi^N + (-\phi)^{-N}}$$

And in the thermodynamic limit :

$$\langle m \rangle = \lim_{N \to \infty} \langle m_N \rangle = -\frac{1}{\sqrt{5}}$$

1.7 Correlation

The correlation between different sites (or spins) is a tool to study the collective behavior of the system. In the Ising model under study here, only the nearest neighbor interact between each other. In a way, you could think that 2 sites that aren't directly adjacent wouldn't "see" each other. However, there is an influence between "long-distance" sites. We will even see that at the critical point, the influence between spin has an infinite range ! This is a characteristic of critical point and phase transition.

1.7.1 The spin-spin correlation function

The spin-spin correlation function $\Gamma(\vec{r_i}, \vec{r_j})$ measure the correlation between the spin i and the spin j. It is defined by :

$$\Gamma(\vec{r_i}, \vec{r_j}) = \langle (\sigma_i - \langle \sigma_j \rangle)(\sigma_j - \langle \sigma_j \rangle) \rangle$$

It will be positive when the differences between the spin values and their averages tend to be of the same sign, negative otherwise.

If the system is translationally invariant ($\langle \sigma_i \rangle = \langle \sigma_j \rangle = \langle \sigma \rangle$ for any (i, j)), then :

$$\Gamma(\vec{r_i}, \vec{r_j}) = \Gamma(\vec{r}) = \Gamma(\vec{r_0}, \vec{r_r}) = \langle \sigma_0 \sigma_r \rangle - \langle \sigma \rangle^2$$

Away from the critical point, the spins become uncorrelated as r tends towards infinity, hence the correlation function decays to zero. The correlations decay to zero exponentially with the distance between the spins [9]. We can write :

$$|\Gamma(\vec{r})| \sim r^{-\tau} e^{-\frac{r}{\xi}}$$

where τ is some number and ξ is the correlation length.

1.7.2 The correlation length

Definition

The above formula can be written as follows :

$$-\frac{1}{r}ln(|\Gamma(\vec{r})|) = \tau\frac{ln(r)}{r} + \frac{r}{r\xi}$$

Then :

$$\lim_{r\to\infty} -\frac{1}{r}ln(|\Gamma(\vec{r})|) = \frac{1}{\xi}$$

And we can define the correlation length by :

$$\xi = \frac{1}{\lim_{r\to\infty} -\frac{1}{r}ln(|\Gamma(\vec{r})|)}$$

The correlation length for Periodic Boundary Conditions

The correlation length is defined by:

$$\xi_N^{PBC} = \frac{1}{\lim_{r\to\infty} -\frac{1}{r}ln(|\langle\sigma_0\sigma_r\rangle_N - \langle\sigma\rangle_N{}^2|)}$$

With :

$$\langle\sigma_0\sigma_r\rangle_N = \frac{\sum_{\{\sigma\}}\sigma_0\sigma_r e^{-\beta H(\{\sigma\})}}{Z_N^{PBC}}$$

We can show (see Appendix B) that :

$$\xi^{PBC^{-1}} = ln(|\frac{\lambda_0}{\lambda_1}|) = ln(|\frac{e^{\beta J}cosh(\beta h) + \sqrt{e^{-2\beta J} + e^{2\beta J}sinh(\beta h)^2}}{e^{\beta J}cosh(\beta h) - \sqrt{e^{-2\beta J} + e^{2\beta J}sinh(\beta h)^2}}|)$$

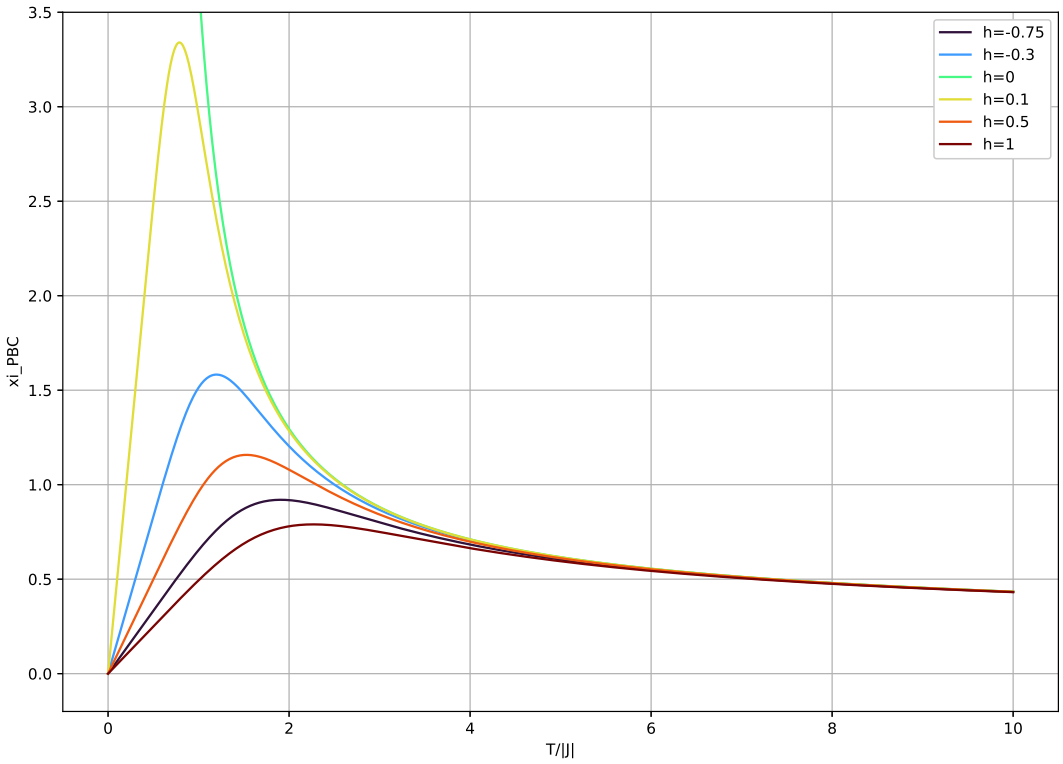


Figure 1.20: The correlation length as a function of the temperature in the ferromagnetic case ($J = +1$) for Periodic Boundary Conditions in the thermodynamic limit.

Here, the first thing to say is that for $h = 0$, the correlation length tends towards infinity when T tends towards 0. For $h = 0$, there is no symmetry breaking, and the thermal average of each spin is 0. But, at $T = 0$, the system is either in the state with all the spins up or all the spins down. Then, when on spin deviates from its mean value, all the other spins deviate in the same manner. This means that the correlation length is infinite.

The second thing to say is that for $h \neq 0$, at $T = 0K$, the correlation length is 0. Indeed, a non-zero external field breaks the symmetry of the system. Then, if $h > 0$, at $T = 0K$, all the spins are up (and if $h < 0$, all the spins are down). It means that the spin don't deviate from their mean value. The correlation length is therefore zero.

The third thing to say is that the correlation length tends towards 0 when the temperature T tends towards infinity. In fact, as thermal agitation increases, the distance at which two spins feel each other's influence decreases.

Finally, the 1D ferromagnetic case ($J > 0$) Ising model shows one and only one critical point at $T = 0$.

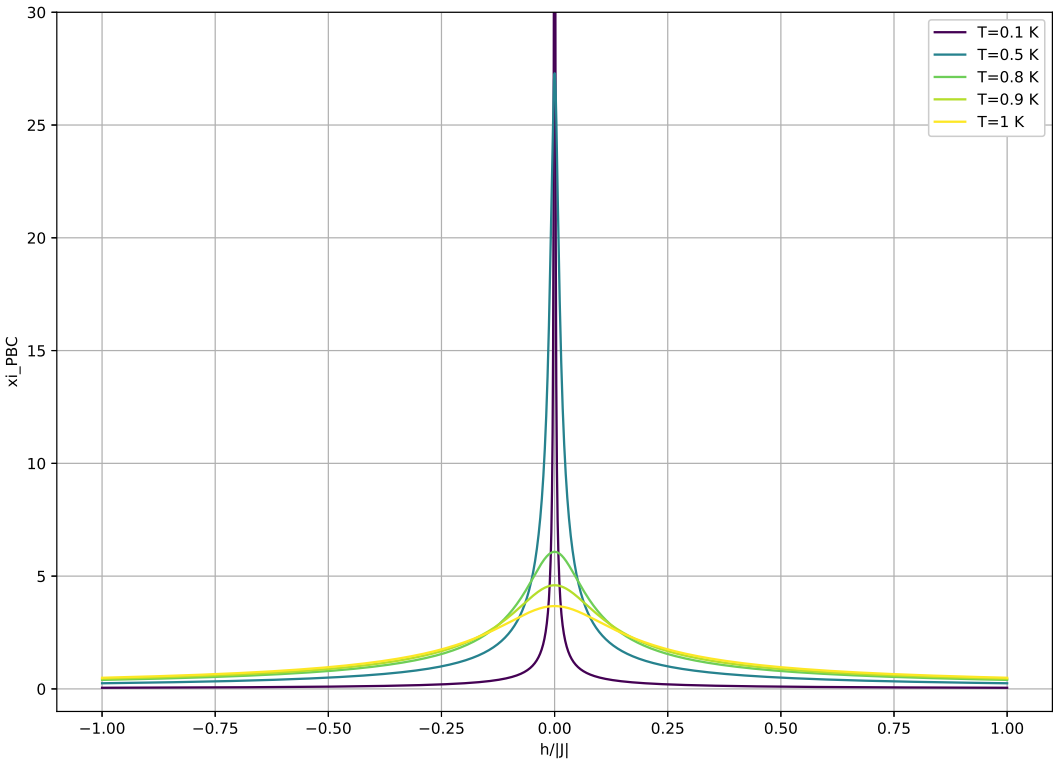


Figure 1.21: The correlation length as a function of the external field in the ferromagnetic case ($J = +1$) with Periodic Boundary Conditions in the thermodynamic limit.

Here, we see again that when $h = 0$, the correlation length tends towards infinity when T tends towards 0.

We also see that the correlation length tends towards 0 when $|h|$ tends towards infinity. In fact, when the external field is very strong, all the spins are aligned with it. In this case, the spins do not deviate much from their mean value. It means that the correlation length tends towards 0.

1.8 Conclusion

In conclusion, the 1D Ising model does show the presence of a critical point at T=0, but on the one hand this point cannot be reached experimentally, and on the other, it cannot be “crossed” to change phase. In the end, therefore, the 1D Ising model shows no phase transition.

Chapter 2

The Kagome Chain

The Ising model can exhibit an interesting property in the antiferromagnetic case: frustration.

The Kagome chain is one of the simplest cases where frustration is observed. It will therefore be a useful case for studying this property.

2.1 Description of the system

In this section, we will work on the 1D Kagome Chain.

Here is a graphical representation of the system :

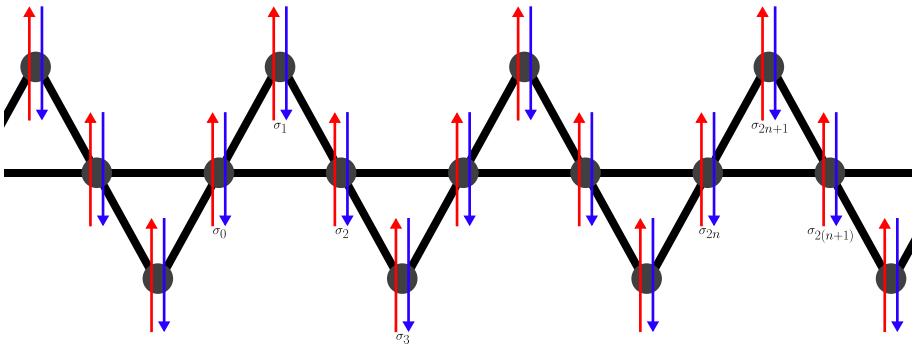


Figure 2.1: The Kagome Chain with Periodic Boundary Condition.

The Hamiltonian of the system has still the same expression :

$$H = -J \sum_{<i,j>} \sigma_i \sigma_j - h \sum_i \sigma_i$$

2.2 Partition Function

To calculate the partition function of the Kagome Chain, we can express it as a product of tensors:

$$Z_N = \sum_{\{\sigma\}} e^{\beta J(\sigma_0\sigma_1+\sigma_1\sigma_2+\sigma_2\sigma_0+\sigma_2\sigma_3+\sigma_3\sigma_4+\sigma_4\sigma_2+...\sigma_{N-4}\sigma_{N-3}+\sigma_{N-3}\sigma_{N-2}+\sigma_{N-2}\sigma_{N-4}+\sigma_{N-2}\sigma_{N-1}+\sigma_{N-1}\sigma_0+\sigma_0\sigma_{N-2})}$$

$$= \sum_{\{\sigma\}} e^{\beta(J(\sigma_0\sigma_1+\sigma_1\sigma_2+\sigma_2\sigma_0)+\frac{1}{2}h(\sigma_0+2\sigma_1+\sigma_2))} e^{\beta(J(\sigma_2\sigma_3+\sigma_3\sigma_4+\sigma_4\sigma_2)+\frac{1}{2}h(\sigma_2+2\sigma_3+\sigma_4))} ... e^{\beta(J(\sigma_{N-2}\sigma_{N-1}+\sigma_{N-1}\sigma_0+\sigma_0\sigma_{N-2})+\frac{1}{2}h(\sigma_{N-2}+2\sigma_{N-1}+\sigma_0))}$$

$$Z_N = \sum_{\{\sigma\}} T_{0,1,2} T_{2,3,4} ... T_{N-4,N-3,N-2} T_{N-2,N-1,0}$$

with :

$$T_{i,j,k} = e^{\beta(J(\sigma_i\sigma_j+\sigma_i\sigma_k+\sigma_j\sigma_k)+\frac{1}{2}h(\sigma_i+2\sigma_j+\sigma_k))}$$

We have defined a tensor for each triangle of the chain. Because there are 3 spins on each triangle, this tensor has 3 indices.

Here is a graphical representation of the tensor network which represent the partition function of the Kagome Chain before the contraction :

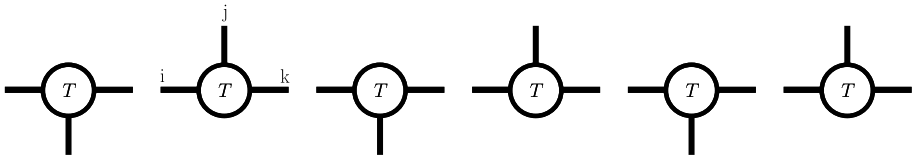


Figure 2.2: Tensor network of the Kagome Chain before contraction.

And here is the graphical representation of the tensor network which represent the partition function of the Kagome Chain after the contraction :

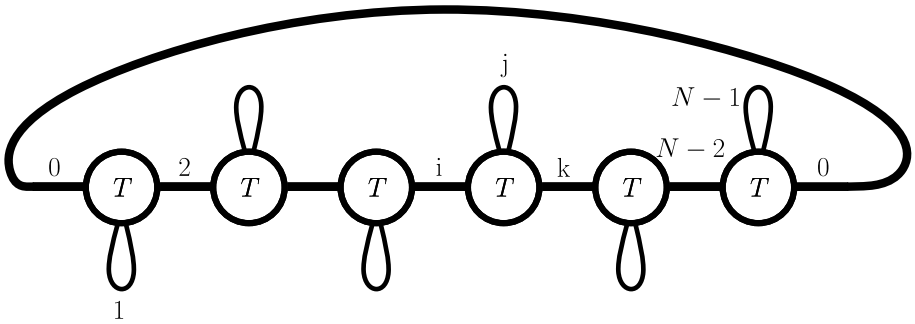


Figure 2.3: Tensor network of the Kagome Chain after contraction.

2.3 Frustration

In condensed matter physics, frustration is a phenomenon where the combination of contradictory constraints leads to complex structures. This can happen in magnetic systems when the geometry of the system prevents all local constraints from being satisfied simultaneously.

We will see that frustration can involve a plenitude of distinct ground states at zero temperature, and thus be responsible for residual entropy.

Here, in order to study frustration, we will work on the Kagome Chain in the antiferromagnetic case ($J < 0$).

2.3.1 Without external field

Here, we will assume that $h = 0$.

Let us focus on one triangle of the chain and try to minimize the energy of this triangle. Let us assume that the first spin is up, then the second spin should be down because of the antiferromagnetic condition. If the third spin is up, then the link with the first spin will be "unsatisfied" (because the spins tend to be in opposite direction). If the third spin is down, then the link with the second spin will be "unsatisfied". It is impossible to minimize simultaneously the energy of the 3 link of the system. The system is frustrated !

For one triangle, there are 6 configurations with the minimal energy :

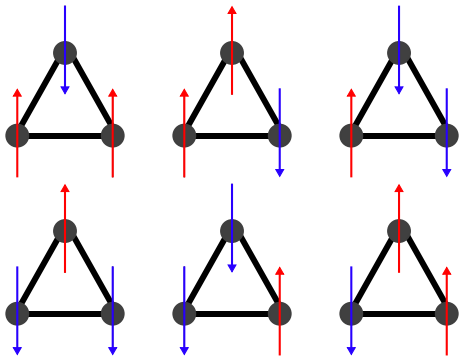


Figure 2.4: Configurations of one triangle with minimal energy.

Therefore, even at $T = 0K$, there are many different configurations with the minimal energy.

Let us count this number of configurations for a chain with N_t triangles. We will use the partition function. We denote E_0 the lowest energy the system can take, and we shift all the energy by E_0 as we did in section 1.6.

Here, this is a special case where $\frac{E_0}{N_t}$ is equal to the lowest energy E_0^t that the system can take on one triangle.

In the case where $h = 0$, the lowest energy of one triangle is :

$$E_0^t = \frac{E_0}{N_t} = -J(-1 - 1 + 1) = J$$

Then, we define :

$$T_{i,j,k}^{shifted} = e^{\beta(J(\sigma_i\sigma_j+\sigma_j\sigma_k+\sigma_k\sigma_i)+J)} = e^{\beta J(\sigma_i\sigma_j+\sigma_j\sigma_k+\sigma_k\sigma_i+1)}$$

We can then define the transfer matrix :

$$M_{i,k} = \sum_{\sigma_j} T^{shifted}_{i,j,k} = 2e^{\beta J(\sigma_k\sigma_i+1)}\cosh(\beta J(\sigma_i+\sigma_k))$$

$$M_{i,k} = \begin{pmatrix} \overset{\sigma_k=+1}{2e^{2\beta J}\cosh(2\beta J)} & \overset{\sigma_k=-1}{2} \\ 2 & 2e^{2\beta J}\cosh(2\beta J) \end{pmatrix} \begin{matrix} \sigma_i = +1 \\ \sigma_i = -1 \end{matrix}$$

When the temperature T tends toward $0K$, β tends toward infinity, and remembering that $J < 0$:

$$\lim_{T\to\infty} 2e^{2\beta J}\cosh(2\beta J) = 1$$

Thus, at $T = 0K$:

$$M = \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix}$$

We diagonalize M, its eigenvalues are 3 and -1.
Finally :

$$Z^{shifted}_N = \sum_{\{\sigma\}} T^{shifted}_{0,1,2} T^{shifted}_{2,3,4} ... T^{shifted}_{N-4,N-3,N-2} T^{shifted}_{N-2,N-1,0}$$

$$Z^{shifted}_N = \sum_{\{\sigma_{2i}\}} M_{0,2}M_{2,4}...M_{N-4,N-2}M_{N-2,0} = Tr(M^{N_t})$$

And

$$\lim_{T\to 0} Z^{shifted}_N = 3^{N_t} + (-1)^{N_t}$$

The number of configurations with the lowest energy at $T = 0K$ growths exponentially with the size of the system ! There is a residual entropy !

2.3.2 Case where 0<h<|J/2|

When $h > 0$, the 6 configurations of figure 2.4 haven't got the same energy. Indeed, the one with 2 spins up and 1 spin down have a lower energy than the other. Their energy is :

$$E_0^t = -J(-1-1+1) - h(1+1-1) = J - h$$

With an external field, we have to check if the configuration with 3 spins aligned with the field (here 3 spins up) has a lower energy than the previous ones or not :

$$\frac{E_0}{N_t} = -J(1+1+1) - h(1+1+1) = -3J - 3h$$

Then,

$$J - h < -3J - 3h \iff h < \frac{-J}{2}$$

Here, we will study the case where $0 < h < \frac{-J}{2}$.

We have to be careful, because in this case, the lowest total energy of the system divided by the number of triangles is not equal to the lowest energy of a single triangle :

$$E_0^t \neq \frac{E_0}{N_t}$$

Moreover, we can no longer reason in terms of isolated triangles. Indeed, when the triangles are placed side by side to build the Kagome Chain, the 3 configurations with 2 spins up and 1 spin down are no longer equivalent. We can see it with the 2 following configurations :

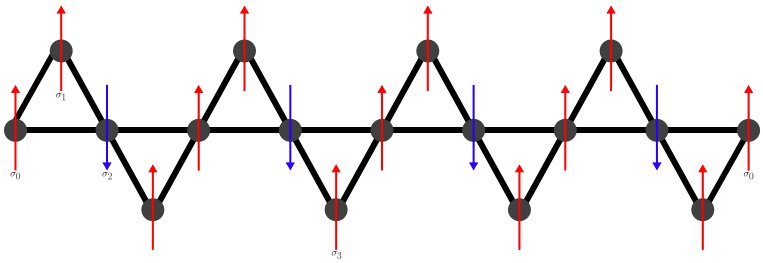


Figure 2.5

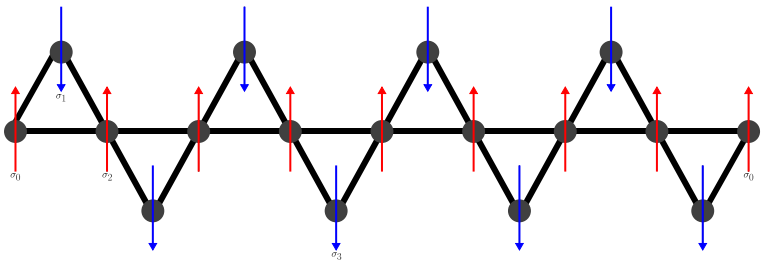


Figure 2.6

The energy of the configuration of figure 2.5 ($N_t = 8$) is :

$$-8J(-1-1+1) - h(12-4) = 8J - 8h$$

The energy of the configuration of figure 2.6 ($N_t = 8$) is :

$$-8J(-1-1+1) - h(8-8) = 8J$$

We see that the energy of the first configuration is lower than the energy of the second one. In fact, when N_t is even, there are only 2 configurations with minimal energy. The configuration of the figure 2.5 and the configuration of the figure 2.7.

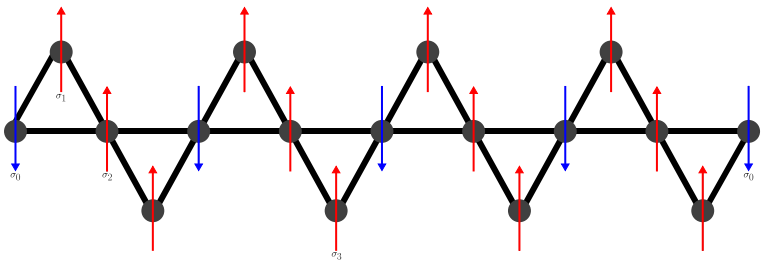


Figure 2.7

Let us try to find this result with the partition function. We want to define E_0^t such that $T_{i,j,k}^{shifted} = 1$ if we are in one of the 2 configurations with the lowest energy, and $T_{i,j,k}^{shifted} < 1$ otherwise. Thus, we define:

$$E_0^t = -J(-1-1+1) - \frac{h}{2}(1+2-1) = J - h$$

And :

$$T_{i,j,k}^{shifted} = e^{\beta(J(\sigma_i\sigma_j+\sigma_j\sigma_k+\sigma_k\sigma_i)+\frac{h}{2}(\sigma_i+2\sigma_j+\sigma_k)+J-h)} = e^{\beta(J(\sigma_i\sigma_j+\sigma_j\sigma_k+\sigma_k\sigma_i+1)+\frac{h}{2}(\sigma_i+2\sigma_j+\sigma_k-2))}$$

We can then define the transfer matrix :

$$M_{i,k} = \sum_{\sigma_j} T_{i,j,k}^{shifted} = 2e^{\beta(J(\sigma_k\sigma_i+1)+\frac{h}{2}(\sigma_i+\sigma_k-2))}\cosh(\beta(J(\sigma_i+\sigma_k)+h))$$

$$M_{i,k} = \begin{matrix} \\ \sigma_i=+1 \\ \sigma_i=-1 \end{matrix} \overset{\begin{matrix} \sigma_k=+1 & \sigma_k=-1 \end{matrix}}{\begin{pmatrix} 2e^{\beta 2J}\cosh(\beta(2J+h)) & 2e^{-\beta h}\cosh(\beta h) \\ 2e^{-\beta h}\cosh(\beta h) & 2e^{\beta(2J-2h)}\cosh(\beta(-2J+h)) \end{pmatrix}}$$

Thus, at $T = 0K$:

$$M = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

The characteristic polynomial of M is :

$$\chi_M = X^2 - 1 = (X-1)(X+1)$$

And

$$\lim_{T \to 0} Z_N^{shifted} = (1)^{N_t} + (-1)^{N_t} = 1 + (-1)^{N_t}$$

This is the expected result for N_t even !

For N_t odd, this result is obviously false. For N_t odd, the configurations with the lowest energy are the configurations similar to the one of the figure 2.8. So, there are N_t configurations with the lowest energy (there are N_t possible positions for the triangle with 2 spins down).

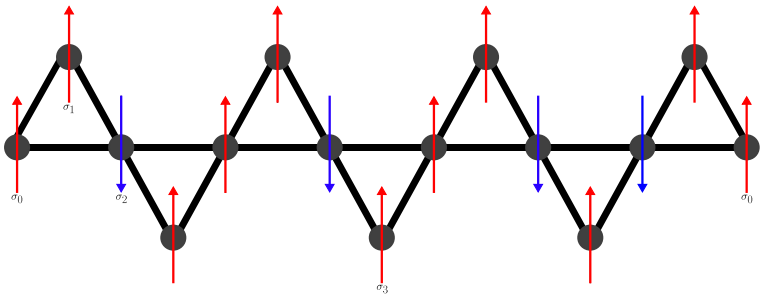


Figure 2.8

The issue is that the shifted tensor associated to the triangle with 2 spins down tends toward 0 when the temperature T tends toward 0. This is why the limit of the shifted partition function equals 0 when N_t is odd.

2.4 Conclusion

In the case without an external field (part 2.3.1), we have seen how frustration can create residual entropy.

In the case of an external field (part 2.3.2), we were able to gain an initial insight into the importance of being able to reason or not to reason about elementary tiles in the presence of frustration.

Finally, this example is a first approach to frustration in the Ising model, a phenomenon that gives rise to rich and exciting physics in more complex cases.

Chapter 3

Tensor Renormalization Group Algorithm

3.1 Why is TRG necessary ?

We have seen that to compute a partition function with tensor networks, there are 2 steps :

1. First, translate the partition function into a tensor network.
2. Second, contract the tensor network to get the partition function.

In 1D, the second step is easy. We have a 1D chain of tensors, and we can contract them successively by multiplying or contracting a tensor to the intermediate result of the calculation at each step. Graphically, this can be represented as follows :

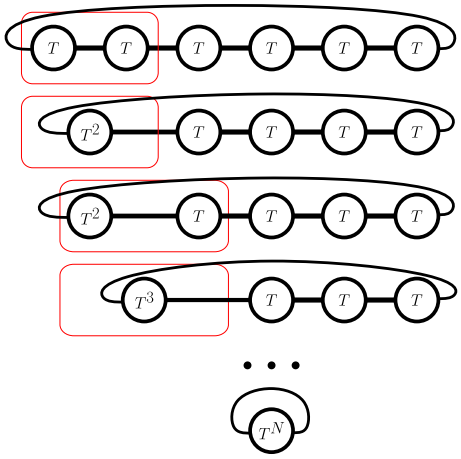


Figure 3.1: Contraction of the 1D chain tensor network.

The important thing to notice is that at each step of the contraction, the intermediate result of the calculation is a tensor with only 2 legs. Hence, if each index is of dimension 2 for instance, there are only 4 values to store during the calculation.

Let us now try to apply the same naive method to a 2D lattice, such as the square lattice :

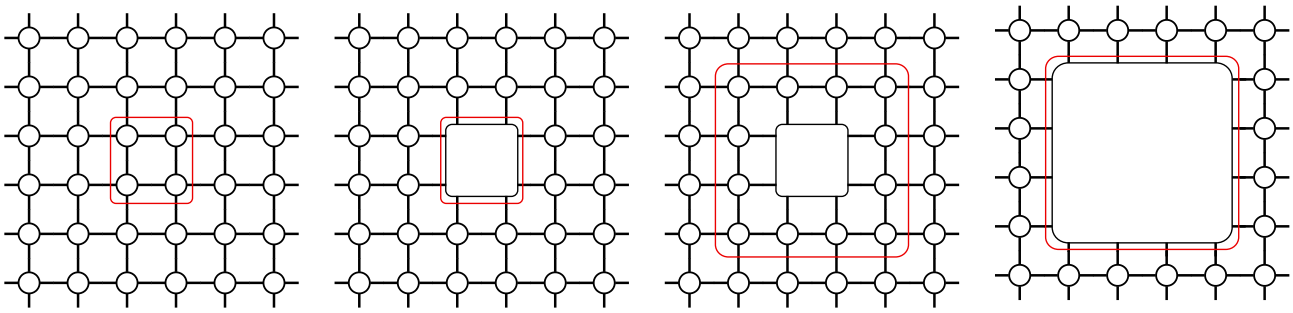


Figure 3.2: Contraction of the 2D square lattice tensor network.

Here, we see that the intermediate tensor gains 8 additional legs at each stage of contraction (from left to right on the figure 3.2). Hence, if each index is of dimension 2 for instance, there are 2^{8n} values to store at the n^{th} step of the calculation. So, if we want to contract a large 2D square lattice tensor network, we will quickly reach the limit of digital memory.

This shows intuitively why another method is needed to contract a large 2D tensor network. A solution to this problem was presented by Levin and Nave in 2007 : the Tensor Renormalization Group (TRG) [3].

3.2 Description of the algorithm

The Tensor Renormalization Group (TRG) algorithm was presented by Levin and Nave in their 2007 article [3].

Here I will focus on only two points :

1. Why the first step of the algorithm is an approximation
2. Applying the TRG algorithm to the square lattice Ising model.

3.3 First step of the TRG algorithm

Problem statement

Let $T_{i,j,k}$ be a tensor with bond dimensions equal to D, i.e $0 < i, j, k < D - 1$.

The first step of the TRG method is to find a tensor $S_{i,j,k}$ such that :

$$\sum_m S_{l,i,n} S_{j,k,n} \approx \sum_m T_{i,j,m} T_{k,l,m} \tag{3.1}$$

Geometrically, we can illustrate this equation like this :

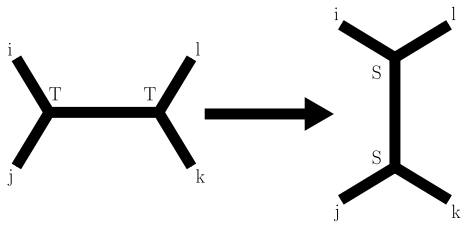


Figure 3.3: Geometrical representation of the first step of the TRG.

First, by looking to figure 3.3, we see that the bond dimension of the two first indices l and i of the tensor $S_{l,i,n}$ is equal to D. But, there is a priori no constraint on the bond dimension of the third index n. We denote this bond dimension by N.

Let us try to understand why in general there is no tensor $S_{l,i,n}$ with all the 3 bond dimensions equal to D such that equation 3.1 is exact.

Dimer model on the honeycomb lattice

To study the problem defined above, we will use a dimer model on the honeycomb lattice. The aim is to count the number of ways in which edges can be covered, so that each vertex is covered exactly once. This means that for each vertex, there is exactly one covered edge whose end is that vertex.

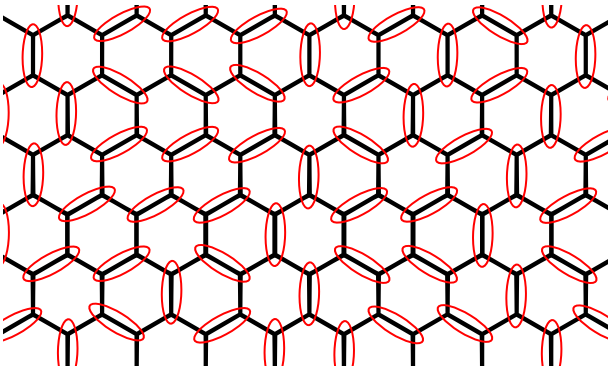


Figure 3.4: Example of one dimer covering of the honeycomb lattice.

We define a tensor at each vertex of the honeycomb lattice, whose indices represent the edge linked to that vertex. Let us say that the index 0 means there is no dimer on the edge, and the index 1 means there is a dimer on the edge (here, $D = 2$). Then, the tensor T is defined by :

$$T_{1,0,0} = T_{0,1,0} = T_{0,0,1} = 1$$
$$T_{i,j,k} = 0 \quad \text{otherwise}$$

This defines a simple and useful model for our purpose.

In order to do the transformation of the figure 3.3, first, we define a matrix $M_{li,jk}$ of dimension $D^2 \times D^2 = 2^2 \times 2^2 = 4 \times 4$ by :

$$M_{li,jk} = \sum_m T_{i,j,m} T_{k,l,m}$$

We can see the tensor S as a vector $S_{li,n}$ of dimensions $D^2 \times N = 4 \times N$. Then, we have to find a vector S such that :

$$M_{li,jk} \approx SS^T$$

The maximum rank of the vector S is $\min(D^2, N) = \min(4, N)$, then the maximum rank of the product SS^T is $\min(D^2, N) = \min(4, N)$.

But the dimensions of the matrix M is $D^2 \times D^2 = 4 \times 4$ and the maximum rank of a matrix with this dimension is $D^2 = 4$.

However, the matrix M is not a random matrix, it is build from a tensor $T_{i,j,k}$ of dimension $D \times D \times D = 2 \times 2 \times 2$. So, maybe we can see T as a vector $T_{ij,k}$ of dimension $D^2 \times D = 4 \times 2$ and express M as TT^T.

We have :

$$T_{ij,k} = \begin{array}{c} \begin{matrix} k{=}0 & k{=}1 \end{matrix} \\ \begin{pmatrix} 0 & 1 \\ 1 & 0 \\ 1 & 0 \\ 0 & 0 \end{pmatrix} \end{array} \begin{matrix} ij = 00 \\ ij = 01 \\ ij = 10 \\ ij = 11 \end{matrix}$$

And

$$TT^T = \sum_m T_{ij,m} T_{m,kl}$$

$$TT^T = \begin{array}{c} \begin{matrix} kl{=}00 & kl{=}01 & kl{=}10 & kl{=}11 \end{matrix} \\ \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \end{array} \begin{matrix} ij = 00 \\ ij = 01 \\ ij = 10 \\ ij = 11 \end{matrix}$$

The product TT^T has a rank equal to $2 < D^2 = 4$. So maybe we can hope to find a tensor S with bond dimension $D \times D \times N = 2 \times 2 \times 2$.

But we have to be careful ! The product TT^T is not equal to the matrix $M_{li,jk}$! Indeed, the product TT^T is equal to $M_{ij,kl}$!

Then, we can calculate the matrix $M_{li,jk}$ (and check that it is consistent with the matrix $M_{ij,kl}$). We find :

$$M_{li,jk} = \begin{array}{c} \begin{matrix} jk{=}00 & jk{=}01 & jk{=}10 & jk{=}11 \end{matrix} \\ \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \end{array} \begin{matrix} li = 00 \\ li = 01 \\ li = 10 \\ li = 11 \end{matrix}$$

Graphically, the only non-zero terms are :

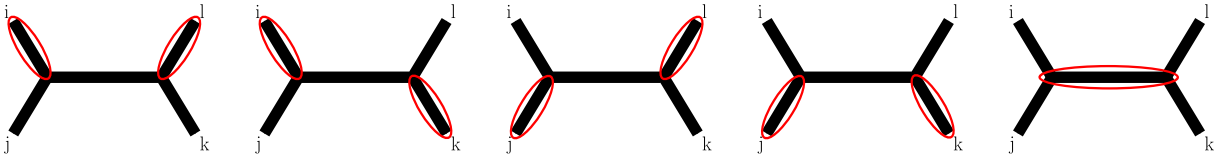


Figure 3.5: Geometrical representation of the 5 non-zero terms of the matrix M.

With this example, we understand that even if the matrix $M_{li,jk}$ is build from the tensor T of dimensions $D \times D \times D$, because of the permutation, in general, this matrix has a rank equal to D^2. Then, if we want to find an exact solution of equation 3.1, we need to take a tensor S with bond dimensions $D \times D \times D^2$.

In the TRG method, we don't want the bond dimensions to grow exponentially larger and larger. That is the reason why we fix a maximal bond dimension denoted D_{max}.
And if at a given step $D^2 > D_{max}$, then we cut the third bond dimension of S to $N = D_{max}$.

This is why the first step of the TRG is an approximation.

In practice, we use a singular value decomposition (SVD) of M to find a satisfactory S tensor. This decomposition allows us to retain the D_{max} largest singular values in the decomposition when we cut the third bond dimension of S. Thus, it yields the optimal tensor S that minimizes the approximation error (see [3]).

3.4 The square lattice

In their paper, Levin and Nave present an application of the TRG to the triangular lattice Ising model [3].
Here, I have worked on the square lattice Ising Model (figure 3.6).

First, we will look at different ways of translating the model's partition function into a tensor network. This will be an opportunity to introduce a property of tensor networks that we haven't yet encountered: an index cannot be common to more than 2 tensors.
Then, we will look at the result of the TRG on this model.

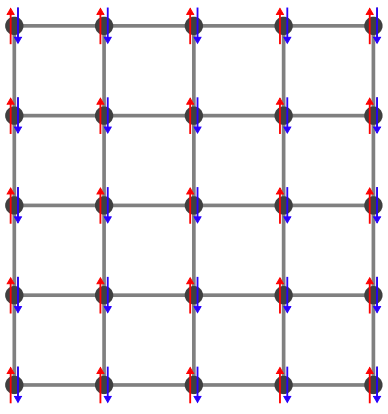


Figure 3.6: 2D square lattice.

3.4.1 Translation of the partition function into a tensor network

There are several possibilities to implement the partition function of the classical Ising Model on the 2D square lattice.

Tensors in the squares connected to the spin

One option is to put the tensors in the squares and connect them to the 4 sites of the square :

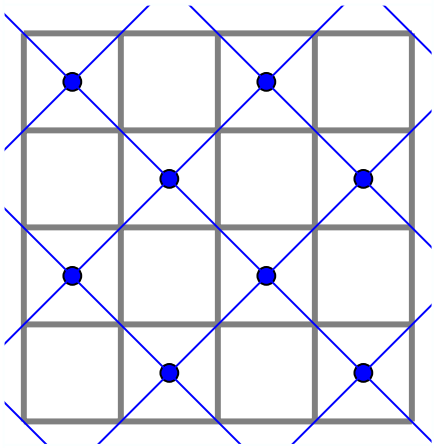


Figure 3.7: Tensor network of the 2D square lattice with tensor in the squares connected to the sites.

Here, each tensor has 4 legs and is defined by :

$$T_{i,j,k,l} = e^{\beta(J(\sigma_i\sigma_j+\sigma_j\sigma_k+\sigma_k\sigma_l+\sigma_l\sigma_i)+\frac{h}{2}(\sigma_i+\sigma_j+\sigma_k+\sigma_l))}$$

This is the choice I made to apply the TRG algorithm to the Ising square lattice model.

Tensors on the bonds

Another option is to put the tensor on the bonds of the lattice :

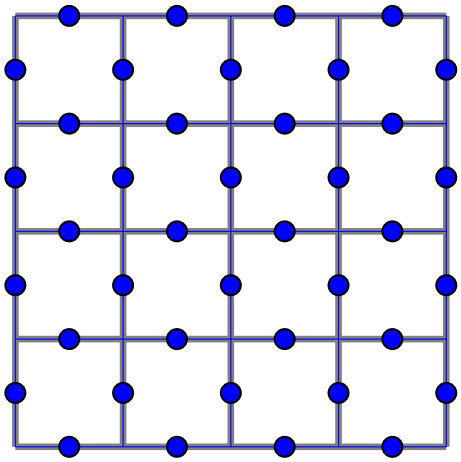


Figure 3.8: Tensors on the bonds of the 2D square lattice.

Here each tensor has 2 indices and is defined by :

$$T_{i,j} = e^{\beta(J\sigma_i\sigma_j + \frac{h}{4}(\sigma_i+\sigma_j))}$$

However, the figure 3.8 is not a tensor network because in this diagram, there are points where 4 legs are connected to each other. This is not allowed in a tensor network. Let us try to justify why in a tensor network, a leg (or index) can't be connected to more than 2 tensors.

Index common to more than 2 tensors ?

A tensor can be viewed as a multilinear function. A part of the legs of the tensor represents the input of the function, and the other part represents the output of the function. From this point of view, the connection of two tensors is essentially the composition of the two corresponding functions [8]. Then, it makes no sense to connect more than 2 tensors through the same leg.

The advantage of this point of view is that, numerically, linear operations are very well optimized and efficient. This gives tensor networks good numerical performance.

Another explanation is practical. Consider the following graphs :

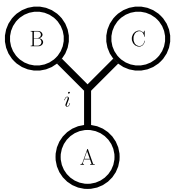


Figure 3.9: 3 tensors connected by the same leg.

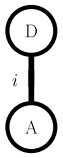


Figure 3.10: An attempt at contraction.

The figure 3.9 could be interpreted as :

$$\sum_i A_i B_i C_i$$

But, if we want to contract the tensors B and C to get the figure 3.10, there is no way to contract them using the contraction rule. To do that, we should define the tensor D as $D_i = B_i C_i$, which is not a valid contraction.

This is why, in a tensor network, a leg can only be connected to a maximum of two tensors.

How do you transform figure 3.8 into a tensor network?

To transform the diagram of the figure 3.8 into a tensor network, we can add a delta tensor at each interaction of 4 legs. A delta tensor is defined by :

$$\delta_{i,j,k,l} = \begin{cases} 1 & \text{if} \quad i = j = k = l \\ 0 & \text{if} \quad \text{otherwise} \end{cases}$$

The diagram become :

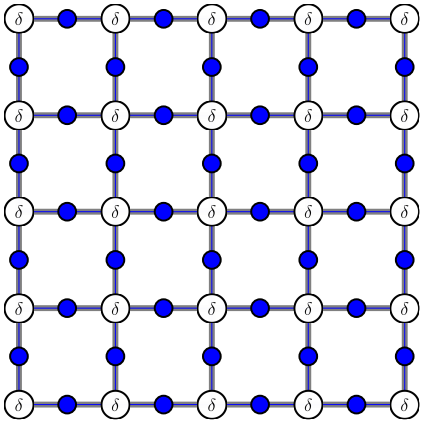


Figure 3.11: Tensor network with tensor on the bonds of the 2D square lattice.

The figure 3.11 is a tensor network. But there are 2 different type of tensors (T and δ) in this network. To apply the TRG algorithm, it may be simpler to have a network with only one type of tensor. There are several possibilities to transform the diagram of figure 3.11 to get what we want.

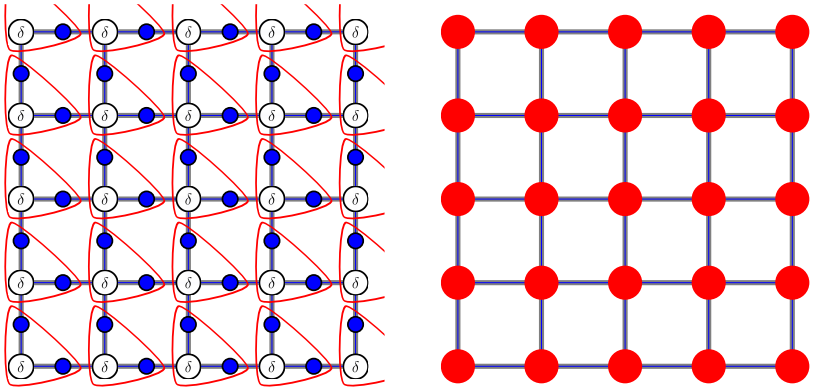


Figure 3.12: First Option : Contraction of 3-tensor pack

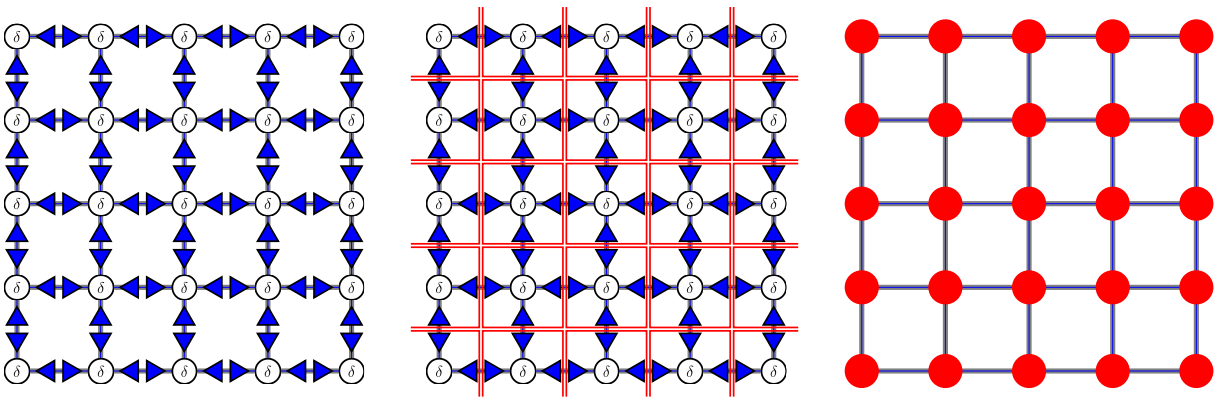


Figure 3.13: Second Option

To build the second option, first we split the tensor T in two. Then, we contract 4 "half" of the tensor T with a delta tensor to get a tensor network with only one type of tensor.

3.4.2 Result of the TRG on the square lattice Ising model

The phase transition of the square lattice Ising model

In 1925, Ernst Ising solved the 1-dimensional model, showing that it had no phase transition. In his thesis, he also asserted that Ising's higher-dimensional model (2D and 3D) would show no phase transition. In 1936, Peierls showed that, in fact, the 2D and a fortiori the 3D Ising model must have a phase transition at finite non-zero temperature [5]. Then, in 1944, Onsager presented an analytical solution for the partition function of the square lattice Ising model. He also proposed a formula for spontaneous magnetization, which was demonstrated by Yang in 1952.

So the 2-dimensional model behaves radically differently from the 1-dimensional model: there's a critical temperature where a phase transition takes place.

Spontaneous magnetization of the square lattice Ising model computed by TRG algorithm

In the appendix C, I present drawings detailing the various steps in the practical implementation of the algorithm with ITensor in Julia. You can find my code on my github repository.

Here is the spontaneous magnetization of the square lattice Ising model we obtain with TRG for different maximum bond dimensions :

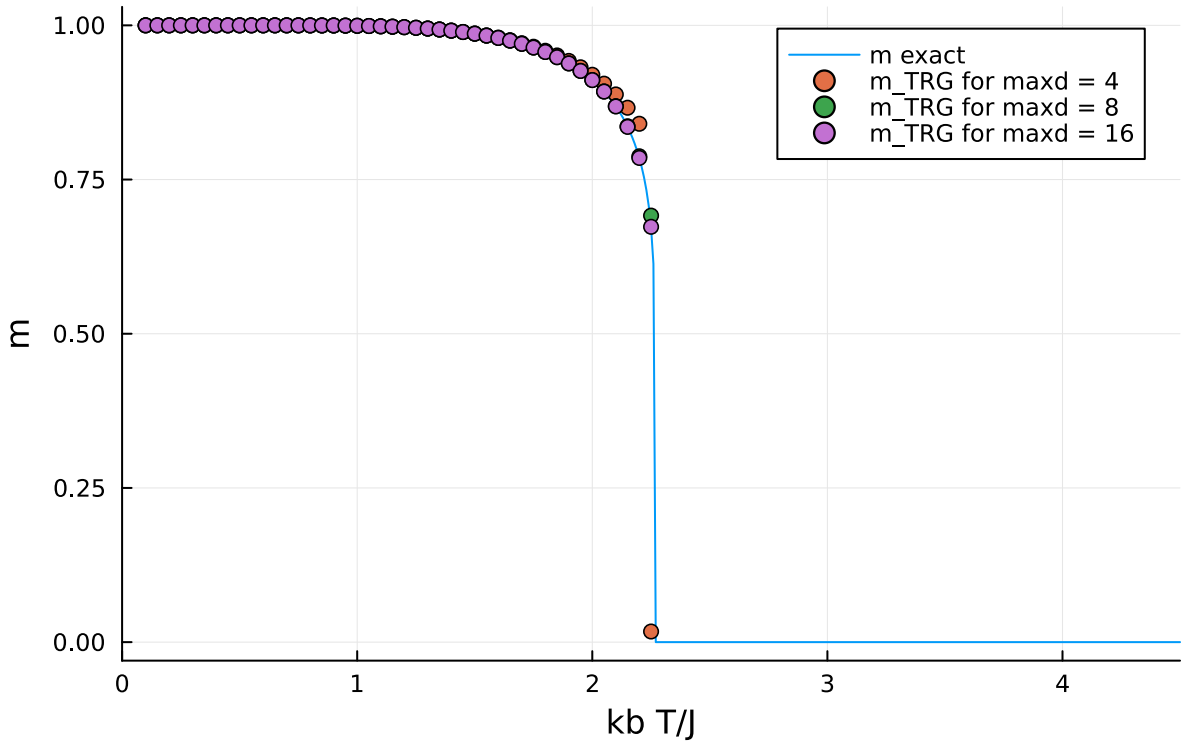


Figure 3.14: The mean spontaneous magnetization per site of the square lattice Ising model.

We note that the result seems to be in good agreement with the theoretical value. But let us change scale and take a closer look at what happens near the phase transition (see Figure 6 of [3]).

We define $\alpha = e^{-2\beta J}$, and we plot the spontaneous magnetization as a function of $\frac{\alpha_c - \alpha}{\alpha_c}$ where $\alpha_c = e^{-2\beta_c J} = e^{\frac{-2J}{k_B T_c}}$ with T_c the critical temperature of the model.

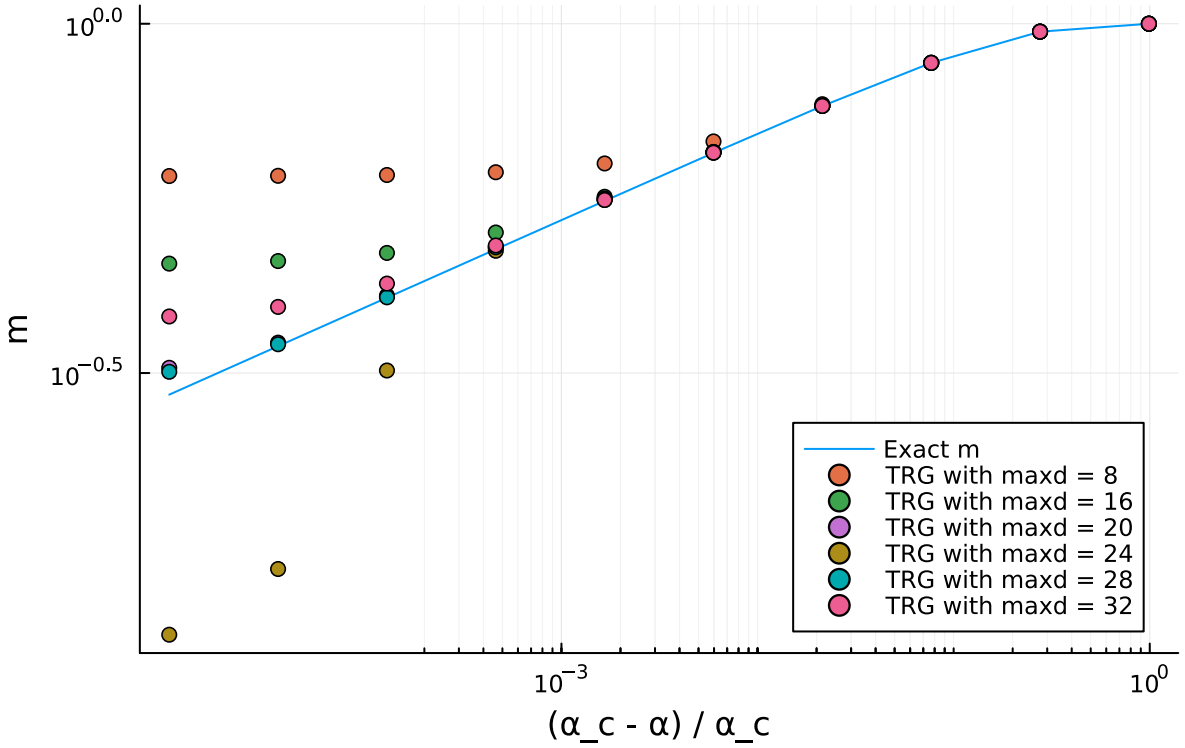


Figure 3.15: The mean spontaneous magnetization per site of the square lattice Ising model.

The result is similar to that obtained by Levin and Nave in the case of the triangular network: the result obtained with the TRG algorithm agrees with the theoretical value far from the critical point, and deviates from the theoretical value when approaching the critical point.

An explanation to this result is presented in their paper [3].

Conclusion

In one hand, the Ising model is a toy model with many applications (magnetism, lattice gas description, neuroscience, artificial neural network, etc.).

In condensed matter physics, Onsager's 1944 solution, the study of spin glasses and other developments have opened up a rich and exciting new field of study.

In the other hand, the tensor networks offer a new numerical method to study these systems.

The aim of this project was to discover these fascinating subjects, and these notes are intended to present a conclusion to this work.

Further developments of this work could be :

- Better understand why the renormalization group in real space (the TRG algorithm) fails to calculate the properties of the system close to the critical point. Investigate whether other methods can overcome this problem.
- Test the TRG algorithm on the triangular lattice in the antiferromagnetic case, which is prone to frustration, and study its behavior.

Appendices

Appendix A

A.1

Here we will count how many configurations of the 1D Ising model there are with the minimum energy in the antiferromagnetic case ($J < 0$) when $|h| = |2J|$ (see part 1.6).

For this, we will think with Open Boundary Conditions. The aim is to count the number of possible configurations in which there are no two spins up next to each other, denoted by $u_{OBC}(N)$. We are going to reason by recurrence :

For $N = 2$ there are 3 valid configurations.
For $N = 3$ there are 5 valid configurations.

Let us take $N > 0$. To build a valid configuration, there are two options. First, we can take any valid configuration with $N - 1$ spins and add one spin down. Secondly, we can take any valid configuration with $N - 2$ spins, and add 1 spin down and 1 spin up. Hence :

$$u_{OBC}(N) = u(N-1) + u(N-2)$$

We recognize the recurrence relation of the Fibonacci. Hence :

$$u_{OBC}(N) = a\phi^N + b\psi^N$$

where $\phi = \frac{1+\sqrt{5}}{2}$ and $\psi = \frac{1-\sqrt{5}}{2}$

With the initial conditions, we find :

$$u_{OBC}(N) = \frac{\sqrt{5}+3}{2\sqrt{5}}\phi^N + \frac{\sqrt{5}-3}{2\sqrt{5}}\psi^N$$

A.2

We recall that work here on the 1D Ising model with Periodic Boundary Conditions in the antiferromagnetic case ($J < 0$) when $h = |2J|$ (see part 1.6).

We denote $c(k, N)$ the number of configurations with k spins up in which there are not 2 spins up next to each other. Then the magnetization of a configuration with k spins up is $k - (N - k) = 2k - N$. Thus, the mean magnetization per site at the point $h = |2J|$ is given by :

$$\langle m_N \rangle = \frac{1}{N \times u_{PBC}(N)} \sum_{k=0}^{\lfloor N/2 \rfloor} c(k, N)(2k - N)$$

How to count $c(k, N)$ in the Periodic Boundary Conditions ?

Let us choose one spin, for instance, the spin labeled 0. There are two cases : either it is up, or it is down.

If the spin 0 is up, then the spin $N - 1$ and the spin 1 should be down. So, we can remove these 3 spins, and now we have to choose $(k - 1)$ spins up on a linear chain of $(N - 3)$ spins with Open Boundary Conditions.

If the spin 0 is down, we can remove it, and now we have to choose k spins up on a linear chain of $(N - 1)$ spins with Open Boundary Conditions.

The new question is : How to choose k spin up on a linear chain of N spins with Open Boundary Conditions. This question is the same to choose k integers $a_0, a_1, ..., a_{k-1}$ such that :

$$1 \leq a_0 < a_1 < ... < a_{k-1} \leq N$$

Let us define $b_i = a_i - i$ for all $0 \leq i \leq k - 1$.
We have $b_0 = a_0$, and :
$b_1 = a_1 - 1 > a_0 - 1 \geq a_0 = b_0$
$b_2 = a_2 - 2 > a_1 - 2 \geq a_1 - 1 = b_1$
etc.

Finally :

$$1 \leq b_0 \leq b_1 \leq b_2 \leq ... \leq b_{k-1} \leq N - (k - 1)$$

There is a one-to-one correspondence between $\{a_i\}_{0 \leq i \leq k-1}$ and $\{b_i\}_{0 \leq i \leq k-1}$.
There are $\binom{N-k+1}{k}$ ways to choose a valid set of $\{b_i\}_{0 \leq i \leq k-1}$.
Then, there are $\binom{N-k+1}{k}$ ways to choose k spins up on a linear chain of N spins with Open Boundary Conditions in which there are not 2 spins up next to each other.

We find the previous result for the number of possible configurations with Open Boundary Conditions :

$$u_{OBC}(N) = \sum_{k=0}^{\lfloor N/2 \rfloor} \binom{N - k + 1}{k} = F(N + 2) = \frac{\sqrt{5} + 3}{2\sqrt{5}} \phi^N + \frac{\sqrt{5} - 3}{2\sqrt{5}} \psi^N$$

with $F(N) = \frac{1}{\sqrt{5}}(\phi^N - \psi^N)$ the n^{th} Fibonacci number.

We have shown that :

$$c(k,N) = \binom{N-k-1}{k-1} + \binom{N-k}{k}$$

We find the previous result for the number of possible configurations with Periodic Boundary Conditions :

$$u_{PBC}(N) = \sum_{k=0}^{\lfloor N/2 \rfloor} c(k,N) = \sum_{k=1}^{\lfloor N/2 \rfloor} \binom{N-k-1}{k-1} + \sum_{k=0}^{\lfloor N/2 \rfloor} \binom{N-k}{k}$$

$$u_{PBC}(N) = \sum_{k=0}^{\lfloor N/2 \rfloor} \binom{N-k-2}{k} + \sum_{k=0}^{\lfloor N/2 \rfloor} \binom{N-k}{k} = F(N-1) + F(N+1) = L(N)$$

where $L(N) = (\frac{1+\sqrt{5}}{2})^N + (\frac{1-\sqrt{5}}{2})^N$ is the n^{th} Lucas number [7].

Now, we can calculate :

$$\sum_{k=0}^{\lfloor N/2 \rfloor} c(k,N)(2k-N) = 2\sum_{k=0}^{\lfloor N/2 \rfloor} kc(k,N) - N\sum_{k=0}^{\lfloor N/2 \rfloor} c(k,N)$$

We define

$$U(N) = \sum_{k=0}^{\lfloor N/2 \rfloor} kc(k,N)$$

Now comes a key symmetry argument: In the Periodic Boundary Conditions, each spin is equivalent by symmetry. Then, counting the number of spins up in all the set of valid configuration, is equivalent to count the number of valid configuration where one given spin is up, for instance the spin labelled 0, and multiply this by N. And we have already counted the number of valid configurations where the spin 0 is up, this is $F(N-1)$.

Then :

$$U(N) = NF(N-1)$$

And

$$\langle m_N \rangle = \frac{1}{N \times L(N)}(2NF(N-1) - NL(N)) = \frac{2F(N-1) - L(N)}{L(N)} = -\frac{F(N)}{L(N)}$$

Finally :

$$\langle m_N \rangle = -\frac{1}{\sqrt{5}} \frac{\phi^N - \psi^N}{\phi^N + (-\phi)^{-N}}$$

And in the thermodynamic limit :

$$\langle m \rangle = \lim_{N\to\infty} \langle m_N \rangle = -\frac{1}{\sqrt{5}}$$

Appendix B

The goal is to find a formula for the correlation length of the 1D Ising Model with Periodic Boundary Conditions given by (see 1.7.2) :

$$\xi_N^{PBC} = \frac{1}{\lim_{r\to\infty} -\frac{1}{r} ln(|\langle\sigma_0\sigma_r\rangle_N - \langle\sigma\rangle_N{}^2|)}$$

With :

$$\langle\sigma_0\sigma_r\rangle_N = \frac{\sum_{\{\sigma\}} \sigma_0\sigma_r e^{-\beta H(\{\sigma\})}}{Z_N^{PBC}}$$

Where :

$\sum_{\{\sigma\}} \sigma_0\sigma_r e^{-\beta H(\{\sigma\})} = \sum_{\{\sigma\}} \sigma_0 T_{0,1}T_{1,2}...T_{r-1,r}\sigma_r T_{r,r+1}...T_{N-1,0}$

$= \sum_{\sigma_0,\sigma_r} \sigma_0 (T^r)_{0,r}\sigma_r (T^{N-r})_{r,0}$

We will use the Dirac notation. With $\lambda_{0,1}$ the eigenvalues of T and $\langle u_{0,1}|$ its eigenvectors, we write :

$$T = \sum_{i=0}^{1} |u_i\rangle\lambda_i\langle u_i|$$

We denote σ_k the two values that can take the spin k, it means that $\sigma_k = +1$ or $\sigma_k = -1$. Then we define the two vectors $\langle +1| = \begin{pmatrix}1\\0\end{pmatrix}$ and $\langle -1| = \begin{pmatrix}0\\1\end{pmatrix}$ and the matrix :

$$S_k = \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix} = \sum_{\sigma_k} |\sigma_k\rangle\sigma_k\langle\sigma_k| = S$$

With this notation, we have :

$$(T^k)_{p,q} = \sum_{i=0}^{1} \langle\sigma_p|u_i\rangle\lambda_i^k\langle u_i|\sigma_q\rangle$$

And

$\sum_{\{\sigma\}} \sigma_0\sigma_r e^{-\beta H(\{\sigma\})} = \sum_{\sigma_0,\sigma_r} \sigma_0(\sum_{i=0}^{1}\langle\sigma_0|u_i\rangle\lambda_i^r\langle u_i|\sigma_r\rangle)\sigma_r(\sum_{j=0}^{1}\langle\sigma_r|u_j\rangle\lambda_j^{N-r}\langle u_j|\sigma_0\rangle)$

$\sum_{\{\sigma\}} \sigma_0\sigma_r e^{-\beta H(\{\sigma\})} = \sum_{i,j} \lambda_i^r \lambda_j^{N-r} (\sum_{\sigma_0} \langle u_j|\sigma_0\rangle \sigma_0 \langle \sigma_0|u_i\rangle)(\sum_{\sigma_r} \langle u_i|\sigma_r\rangle \sigma_r \langle \sigma_r|u_j\rangle)$

$\sum_{\{\sigma\}} \sigma_0\sigma_r e^{-\beta H(\{\sigma\})} = \sum_{i,j} \lambda_i^r \lambda_j^{N-r} \langle u_j|S_0|u_i\rangle\langle u_i|S_r|u_j\rangle$

Hence

$\langle\sigma_0\sigma_r\rangle_N = \frac{1}{\sum_k \lambda_k^N} \sum_{i,j} \lambda_i^r \lambda_j^{N-r} \langle u_j|S_0|u_i\rangle\langle u_i|S_r|u_j\rangle$

$\langle\sigma_0\sigma_r\rangle_N = \frac{1}{\sum_k (\frac{\lambda_k}{\lambda_0})^N} \sum_{i,j} (\frac{\lambda_i}{\lambda_0})^r (\frac{\lambda_j}{\lambda_0})^{N-r} \langle u_j|S_0|u_i\rangle\langle u_i|S_r|u_j\rangle$

In the thermodynamic limit (remember that $|\frac{\lambda_1}{\lambda_0}| < 1$):

$\langle\sigma_0\sigma_r\rangle = \lim_{N\to\infty} \langle\sigma_0\sigma_r\rangle_N = \sum_i (\frac{\lambda_i}{\lambda_0})^r \langle u_0|S_0|u_i\rangle\langle u_i|S_r|u_0\rangle$

Similarly, let us show that $\langle\sigma_l\rangle = \langle u_0|S_l|u_0\rangle$.

$\langle\sigma_l\rangle_N = \frac{1}{Z_N} \sum_{\{\sigma\}} \sigma_l e^{-\beta H_N(\sigma)}$

$= \frac{1}{Z_N} \sum_{\{\sigma\}} \sigma_l T_{l,l+1} T_{l+2,l+3} ... T_{N-1,0} T_{0,1} T_{1,2} ... T_{l-1,l} = \frac{1}{Z_N} \sum_{\sigma_l} \sigma_l (T^N)_{l,l}$

$= \frac{1}{Z_N} \sum_{\sigma_l} \sigma_l \sum_i \langle\sigma_l|u_i\rangle \lambda_i^N \langle u_i|\sigma_l\rangle = \frac{1}{Z_N} \sum_i \lambda_i^N \langle u_i|(\sum_{\sigma_l} |\sigma_l\rangle\sigma_l\langle\sigma_l|)|u_i\rangle$

$= \frac{1}{Z_N} \sum_i \lambda_i^N \langle u_i|S_l|u_i\rangle = \frac{1}{\sum_i (\frac{\lambda_i}{\lambda_0})^N} \sum_i (\frac{\lambda_i}{\lambda_0})^N \langle u_i|S_l|u_i\rangle$

In the thermodynamic limit :

$$\langle\sigma_l\rangle = \lim_{N\to\infty} \langle\sigma_l\rangle_N = \langle u_0|S_l|u_0\rangle$$

Hence (remember that $S_0 = S_r = S$) :

$\langle\sigma_0\sigma_r\rangle - \langle\sigma\rangle^2 = \sum_{i=0}^{1} (\frac{\lambda_i}{\lambda_0})^r \langle u_0|S_0|u_i\rangle\langle u_i|S_r|u_0\rangle - (\langle u_0|S|u_0\rangle)^2$

$\langle\sigma_0\sigma_r\rangle - \langle\sigma\rangle^2 = (\frac{\lambda_1}{\lambda_0})^r \langle u_0|S_0|u_1\rangle\langle u_1|S_r|u_0\rangle$

And

$-\frac{1}{r} ln(|\Gamma(\vec{r})|) = -ln(|\frac{\lambda_1}{\lambda_0}|) - \frac{1}{r} ln(|\langle u_0|S_0|u_1\rangle\langle u_1|S_r|u_0\rangle|)$

Then

$\lim_{r\to\infty} -\frac{1}{r} ln(|\Gamma(\vec{r})|) = -ln(|\frac{\lambda_1}{\lambda_0}|)$

Finally :

$$\xi^{PBC^{-1}} = ln(|\frac{\lambda_0}{\lambda_1}|) = ln(|\frac{e^{\beta J} cosh(\beta h) + \sqrt{e^{-2\beta J} + e^{2\beta J} sinh(\beta h)^2}}{e^{\beta J} cosh(\beta h) - \sqrt{e^{-2\beta J} + e^{2\beta J} sinh(\beta h)^2}}|)$$

Appendix C

Implementation of the TRG algorithm with ITensor on the Square Lattice

The package ITensor in Julia is a usefull package to implement Tensor Network Algorithm.

In this package, there is 3 steps to define a tensor :

1. Define the indices

   In ITensor, each index has a unique identity. So we have to be careful to the indices that we use.

2. Assign the indices to the tensor

   A tensor is first defined by its indices.

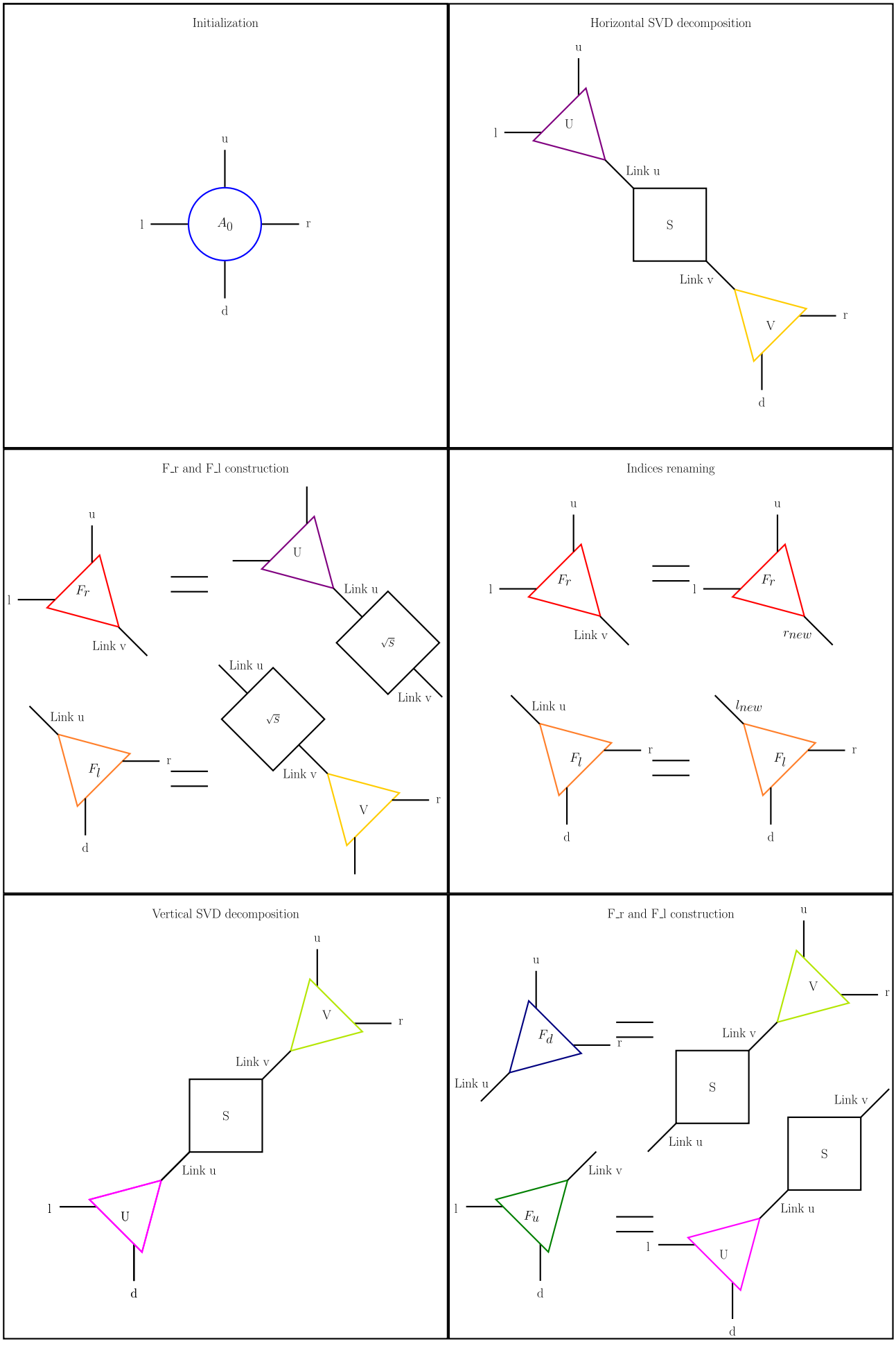
3. Define the values of the tensor

   Then a tensor is defined by the value it takes for each value of its indices.

In their paper, Levin and Nave detail the algorithm for the Honeycomb Lattice [3].

Here is a detailed graphical representation of the different steps of the TRG algorithm on the Square Lattice.

You can find my code on my github repository.


Initialization
u
l
A_0
r
d
Horizontal SVD decomposition
u
l
U
Link u
S
Link v
V
r
d
F_r and F_l construction
u
l
F_r
Link v
U
Link u
$\sqrt{s}$
Link v
Link u
F_l
r
d
Link u
$\sqrt{s}$
Link v
V
r
Indices renaming
u
l
F_r
Link v
u
l
F_r
r_{new}
Link u
F_l
r
d
l_{new}
F_l
r
d
Vertical SVD decomposition
u
V
r
Link v
S
Link u
l
U
d
F_r and F_l construction
u
F_d
r
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F_u
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Link v
l
U
d

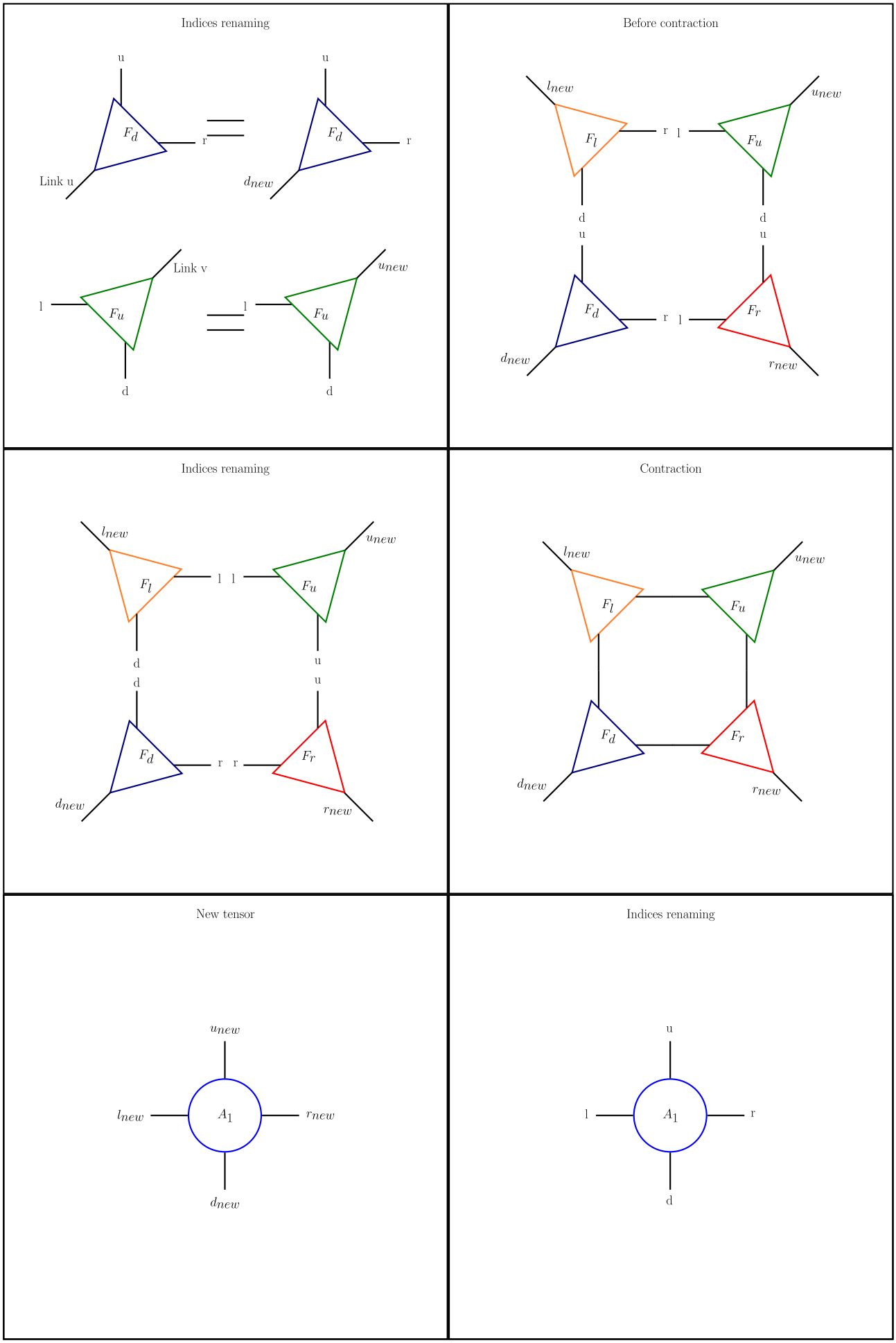

Figure C.1: Graphical representation of the TRG algorithm.

Bibliography

[1] H. Duminil-Copin – *Parafermionic observables and their applications to planar statistical physics models*, 2014.

[2] C. Kittel – *Introduction to solid state physics*, 8 éd., Wiley, 2004.

[3] M. Levin & C. P. Nave – "Tensor renormalization group approach to two-dimensional classical lattice models", *Physical Review Letters* **99** (2007), no. 12.

[4] R. Orús – "A practical introduction to tensor networks: Matrix product states and projected entangled pair states", *Annals of Physics* **349** (2014), p. 117–158.

[5] R. Peierls – "On ising's model of ferromagnetism", *Mathematical Proceedings of the Cambridge Philosophical Society* **32** (1936), no. 3, p. 477–481.

[6] Wikipedia – "Phase transition".

[7] — , "Lucas number — Wikipedia, the free encyclopedia", http://en.wikipedia.org/w/index.php?title=Lucas%20number&oldid=1269138323, 2025, [Online; accessed 23-March-2025].

[8] — , "Penrose graphical notation — Wikipedia, the free encyclopedia", http://en.wikipedia.org/w/index.php?title=Penrose%20graphical%20notation&oldid=1272901405, 2025, [Online; accessed 22-April-2025].

[9] J. M. Yeomans – "Introduction", in *Statistical Mechanics of Phase Transitions*, Oxford University Press, 05 1992.