FYS3150
Project 4 -

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Abstract

Contents

Introduction

Chapter 1

Theory

1.1 The Ising model

1.1.1 The general model

The Ising model is a mathematical model used in statistical mechanics. It consists of discrete variables, which represent the magnetic moment of the spin, which can take the value $+1$ or -1. The spins will only interact with their direct neighbors. With this model, we can study the phase transitions at finite temperature for magnetic systems. We can expressed the energy as

$$E = -J \sum_{\langle kl \rangle}^{N} s_k s_l - B \sum_{k}^{N} s_k \tag{1}$$

with J a constant expressing the strength of the interaction between the neighboring spins, $\langle kl \rangle$ indicating the fact that we only sum the nearest neighbors, N the number of spins, $s_{k,l} = \pm 1$ and B an external magnetic field interacting with the magnetic moment set up by the spins.

This is the general expression of the Ising model. For our use, we will only focus on the case where $B = 0$.
Then, we will be able to calculate expectation values of the mean energy $\langle E \rangle$ and magnetization $\langle M \rangle$ at a given temperature. To do this, we will use a Boltzmann distribution

$$P_i(\beta) = \frac{e^{-\beta E_i}}{Z} \tag{2}$$

where P_i is the probability of finding the system in the state i, $\beta = \frac{1}{kT}$, T being the temperature and k the Boltzmann constant, E_i is the energy of a state i and Z is the partition function defined by $Z = \sum_{i=1}^{M} e^{-\beta E_i}$ with M the number of states. E_i, which is the energy in the state i, is given by

$$E_i = -J \sum_{\langle kl \rangle}^{N} s_k s_l \tag{3}$$

with k, l the different spins of the state i.

A simple particular case of the Ising model, the two-dimensional square lattice model, allows us to have an analytical solution.

1.1.2 Two-dimensional square lattice model

This particular case is one of the simplest models to show a phase transition. It is defined by conditions : the external magnetic field $B = 0$, this is a two-dimensional lattice with N sites, with periodic boundary conditions. Let's take the case with $N = 2 \times 2$ spins. We have $2^4 = 16$ different states with those conditions. We reuse the equation (3) to find the energy of each configuration with the spins-up taking the value $+1$ and the spins-down taking the value -1. Let's take for example the case where three spins are pointing up (and so one is pointing down) numbered from 1 to 4 : $\begin{matrix}\downarrow^{(1)} & \uparrow^{(2)} \\ \uparrow^{(3)} & \uparrow^{(4)}\end{matrix}$.

$$
\begin{aligned}
E &= -J \sum_{\langle kl \rangle}^{4} s_k s_l \\
&= -J(s_1 s_2 + s_2 s_1 + s_1 s_3 + s_3 s_1 + s_2 s_4 + s_4 s_2 + s_3 s_4 + s_4 s_3) \\
&= -J\left[(-1) + (-1) + (-1) + (-1) + 1 + 1 + 1 + 1\right] = -J \times 0 \\
E &= 0
\end{aligned}
$$

The magnetization formula is $M = \sum_{k}^{N} s_k$. So in our example, we have

$$
\begin{aligned}
M &= s_1 + s_2 + s_3 + s_4 \\
&= (-1) + 1 + 1 + 1 \\
M &= 2
\end{aligned}
$$

The following table sums up all the possible states of a two-dimensional square lattice model.

Number of spins-up	Possible configurations	Degeneracy	Energy	Magnetization
4	$\begin{matrix}\uparrow & \uparrow \\ \uparrow & \uparrow\end{matrix}$	1	$-8J$	4
3	$\begin{matrix}\downarrow & \uparrow \\ \uparrow & \uparrow\end{matrix}$ $\begin{matrix}\uparrow & \downarrow \\ \uparrow & \uparrow\end{matrix}$ $\begin{matrix}\uparrow & \uparrow \\ \downarrow & \uparrow\end{matrix}$ $\begin{matrix}\uparrow & \uparrow \\ \uparrow & \downarrow\end{matrix}$	4	0	2
2	$\begin{matrix}\uparrow & \uparrow \\ \downarrow & \downarrow\end{matrix}$ $\begin{matrix}\downarrow & \downarrow \\ \uparrow & \uparrow\end{matrix}$ $\begin{matrix}\uparrow & \downarrow \\ \uparrow & \downarrow\end{matrix}$ $\begin{matrix}\downarrow & \uparrow \\ \downarrow & \uparrow\end{matrix}$	4	0	0
2	$\begin{matrix}\uparrow & \downarrow \\ \downarrow & \uparrow\end{matrix}$ $\begin{matrix}\downarrow & \uparrow \\ \uparrow & \downarrow\end{matrix}$	2	$8J$	0
1	$\begin{matrix}\downarrow & \downarrow \\ \downarrow & \uparrow\end{matrix}$ $\begin{matrix}\downarrow & \downarrow \\ \uparrow & \downarrow\end{matrix}$ $\begin{matrix}\downarrow & \uparrow \\ \downarrow & \downarrow\end{matrix}$ $\begin{matrix}\uparrow & \downarrow \\ \downarrow & \downarrow\end{matrix}$	4	0	-2
0	$\begin{matrix}\downarrow & \downarrow \\ \downarrow & \downarrow\end{matrix}$	1	$-8J$	-4

Table : Energy and magnetization for a $N = 2 \times 2$-spin Ising model with periodic boundary conditions.

The 16 configurations known, we can calculate the partition function in its analytic form.

$$Z = \sum_{i=1}^{16} e^{-\beta E_i}$$
$$Z = (1 \times e^{-\beta\times(-8J)}) + (4 \times e^{-\beta\times 0}) + (4 \times e^{-\beta\times 0}) + (2 \times e^{-\beta\times 8J}) + (4 \times e^{-\beta\times 0}) + (1 \times e^{-\beta\times(-8J)})$$

$$Z = 2(e^{8J\beta} + e^{-8J\beta} + 6) \tag{4}$$
$$Z = 4[\cosh(8J\beta) + 3] \tag{4'}$$

Let's now compute the expectation value of the energy, defined by

$$\langle E \rangle = \sum_{i=1}^{M} E_i P_i(\beta)$$

From (2), we can write :

$$\langle E \rangle = \frac{1}{Z} \sum_{i=1}^{M} E_i e^{-\beta E_i}$$
$$\langle E \rangle = \frac{1}{Z} \left(2 \times (-8J) e^{8J\beta} + 2 \times 8J e^{-8J\beta} \right)$$

$$\langle E \rangle = -\frac{J}{Z} \left(16 e^{8J\beta} - 16 e^{-8J\beta} \right) \tag{5}$$
$$\langle E \rangle = -8J \frac{e^{8J\beta} - e^{-8J\beta}}{e^{8J\beta} + e^{-8J\beta} + 6}$$

So

$$\langle E \rangle = -J \frac{32(\sinh(8J\beta))}{4(\cosh(8J\beta) + 3)}$$
$$\langle E \rangle = -8J \frac{\sinh(8J\beta)}{\cosh(8J\beta) + 3} \tag{5'}$$

Similarly, we compute the mean value of the magnetic moment (or mean magnetization) $\langle M \rangle$:

$$\langle M \rangle = \sum_{i=1}^{M} M_i P_i(\beta) = \frac{1}{Z} \sum_{i=1}^{M} M_i e^{-\beta E_i}$$
$$\langle M \rangle = \frac{1}{Z} \left(4e^{8J\beta} + 4 \times 2e^{0} + 4 \times (-2) e^{0} + (-4) e^{8J\beta} \right)$$

$$\langle M \rangle = 0 \tag{6}$$

which match with the fact that we have taken the external magnetic field $B = 0$.

We can use the expression of the expectation value of the energy to find the specific heat C_V which is defined by

$$C_V = \frac{\langle E^2\rangle - \langle E\rangle^2}{kT^2}$$

The specific heat capacity represents the amount of energy requiered to raise the temperature of a unit of mass by a unit of temperature.

We need to compute $\langle E^2\rangle$:

$$\begin{aligned}\langle E^2\rangle &= \sum_{i=1}^{M} E_i^2 P_i(\beta) = \frac{1}{Z}\sum_{i=1}^{M} E_i^2 e^{-\beta E_i} \\ &= \frac{1}{Z}\left(2\times(-8J)^2 e^{8J\beta} + 2\times(8J)^2 e^{-8J\beta}\right)\end{aligned}$$

$$\langle E^2\rangle = \frac{J^2}{Z}\left(128e^{8J\beta} + 128e^{-8J\beta}\right) \tag{7}$$

$$\langle E^2\rangle = 64J^2\frac{e^{8J\beta} + e^{-8J\beta}}{e^{8J\beta} + e^{-8J\beta} + 6}$$

$$\langle E^2\rangle = J^2\frac{256\cosh(8J\beta)}{4[\cosh(8J\beta)+3]}$$

$$\langle E^2\rangle = 64J^2\frac{\cosh(8J\beta)}{\cosh(8J\beta)+3} \tag{7'}$$

Then, with (5), we have

$$C_V = \frac{J^2}{ZkT^2}\left[\left[128\left(e^{8J\beta} + e^{-8J\beta}\right)\right] - \frac{1}{Z}\left[16\left(e^{8J\beta} - e^{-8J\beta}\right)\right]^2\right]$$

$$C_V = \frac{256J^2}{ZkT^2}\left[\cosh(8J\beta) - \frac{4}{Z}\sinh^2(8J\beta)\right] \tag{8}$$

Similarly, to have the susceptibility χ, which is its capacity to be attracted or not into a magnetic field, defined by

$$\chi = \frac{\langle M^2\rangle - \langle M\rangle^2}{kT^2},$$

we start by computing $\langle M^2\rangle$:

$$\begin{aligned}\langle M^2\rangle &= \sum_{i=1}^{M} M_i^2 P_i(\beta) = \frac{1}{Z}\sum_{i=1}^{M} M_i^2 e^{-\beta E_i} \\ &= \frac{1}{Z}\left(4^2 e^{8J\beta} + 4\times 2^2 e^0 + 4\times(-2)^2 e^0 + (-4)^2 e^{8J\beta}\right)\end{aligned}$$

$$\langle M^2 \rangle = \frac{1}{Z}\left(32e^{8J\beta} + 32\right) \tag{9}$$
$$\langle M^2 \rangle = 16\frac{e^{8J\beta} + 1}{e^{8J\beta} + e^{-8J\beta} + 6}$$

Using (6), we can write

$$\chi = \frac{32(e^{8J\beta} + 1)}{ZkT^2} \tag{10}$$

1.2

1.3

Chapter 2

Implementation

Chapter 3

Results

Conclusion

Bibliography

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