

Project 3

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Abstract

1 Introduction

In this report, we will study the Ising model by applying

2 Theory

2.1 The problem

WRITE a bit about the system we want to solve! What is it?

2.2 2×2 lattice, analytical expressions

To get started we will find the analytical expression for the partition function and the corresponding expectation values for the energy E , the mean absolute value of the magnetic moment $|M|$ (which we will refer to as magnetization), the specific heat C_V and the susceptibility χ as function of T using periodic boundary conditions. These calculations will serve as benchmarks for our next steps.

Partition function, Z

The partition function in the canonical ensemble is defined as:

$$Z = \sum_{i=1}^M e^{-\beta E_i}$$

Where $\beta = \frac{1}{k_B T}$ and E_i is the energy of the system in the microstate i and M is the number of microstates ($= 2^N$ if N is number of electrons).

We therefore have to find E_i which is defined as:

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

Where $\langle kl \rangle$ indicates that we sum only over the nearest neighbors and J is a constant for the bonding strenght. For our two dimensional system the equation reads:

$$E_{i,2D} = -J \sum_i^N \sum_j^N (s_{i,j} s_{i,j+1} + s_{i,j} s_{i+1,j})$$

Four our two-spin-state system with two dimensions we get the following table if we use periodic boundary conditions:

Number of spins up	Degeneracy	Energy	Magnetization
4	1	-8J	4
3	4	0	2
2	4	0	0
2	2	8J	0
1	4	0	-2
0	1	-8J	-4

Table 1: Number of spins up, degeneracy, energy and magnetization of the two-dimensional benchmark scenario.

Where the magnetization is found by subtracting the number of spins down from the number of spins up, or in other words the sum of the spins:

$$\mathcal{M} = \sum_{j=1}^N s_j$$

Getting back to the partition function, we insert all 16 of the E_i respectively. For the degeneracies, we just multiply one iteration of the respective E_i with the amount of degeneracies. When the energy E_i is zero, we will just add one to the sum since $e^0 = 1$. Thus we get the following:

$$Z = e^{-\beta(-8J)} + 2 \cdot e^{-\beta(8J)} + e^{-\beta(-8J)} + 12 = 2e^{-\beta 8J} + 2e^{\beta 8J} + 12$$

$$Z = 4cosh(\beta 8J) + 12$$

Energy expectation value, $\langle E \rangle$

The expectation value of the energy is defined as:

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

Where M is the sum over all microstates. P_i is the Boltzmann probability distribution which reads:

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

For our system, this is easily calculated by inserting the partition function and the microstate energy E_i . The mean energy is then (calculations are shown in appendix, equation (3)):

$$\langle E \rangle = -8J \frac{\sinh(\beta 8J)}{\cosh(\beta 8J) + 3}$$

Since the variance of the mean energy (σ_E) is needed for the heat capacity later, we will calculate this as well. Full calculation is found in the appendix, equation (4).

$$\sigma_E^2 = 64J^2 \left(\frac{\cosh(\beta 8J)}{\cosh(\beta 8J) + 3} - \left(\frac{\sinh(\beta 8J)}{\cosh(\beta 8J) + 3} \right)^2 \right)$$

Magnetization, \mathcal{M}

In the canonical ensemble the mean absolute magnetization can be described as

$$\langle |\mathcal{M}| \rangle = \sum_i^M |\mathcal{M}_i| P_i(\beta) = \frac{1}{Z} \sum_i^M |\mathcal{M}_i| e^{-\beta E_i}$$

We can now simply insert the magnetization and the energies for each respective microstate. This is found in table 2. Using this, we find (shown in the appendix, equation (6.2)):

$$\langle |\mathcal{M}| \rangle = \frac{2e^{\beta 8J} + 4}{\cosh(\beta 8J) + 3}$$

Since the variance of the mean magnetization (σ_M) is needed for the susceptibility later, we will calculate this here. For this we will need $\langle \mathcal{M}^2 \rangle$, and the regular mean absolute $\langle \mathcal{M} \rangle$.

$$\begin{aligned}
\langle \mathcal{M} \rangle &= \frac{1}{4\cosh(\beta 8J) + 12} (4 \cdot e^{\beta 8J} + 4 \cdot 2 \cdot e^0 + 4 \cdot -2 \cdot e^0 + -4 \cdot e^{\beta 8J}) \\
&= \frac{1}{\cosh(\beta 8J) + 3} (4e^{\beta 8J} - 4e^{\beta 8J} + 8 - 8) \\
&= \frac{1}{\cosh(\beta 8J) + 3} (0) \\
\langle \mathcal{M} \rangle &= 0
\end{aligned}$$

$$\begin{aligned}
\langle \mathcal{M}^2 \rangle &= \frac{1}{Z} \sum |\mathcal{M}_i|^2 e^{-\beta E_i} \\
&= \frac{1}{4\cosh(\beta 8J) + 12} (4^2 \cdot e^{\beta 8J} + 4 \cdot 2^2 \cdot e^0 + 4 \cdot |-2|^2 \cdot e^0 + |-4|^2 \cdot e^{\beta 8J}) \\
&= \frac{1}{4\cosh(\beta 8J) + 12} (16 \cdot e^{\beta 8J} + 16 \cdot e^0 + 16 \cdot e^0 + 16 \cdot e^{\beta 8J}) \\
&= \frac{4}{\cosh(\beta 8J) + 3} (2e^{\beta 8J} + 2) \\
\langle \mathcal{M}^2 \rangle &= \frac{8e^{\beta 8J} + 8}{\cosh(\beta 8J) + 3}
\end{aligned}$$

And we get the variance:

$$\begin{aligned}
\sigma_{\mathcal{M}}^2 &= \langle \mathcal{M}^2 \rangle - \langle \mathcal{M} \rangle^2 \\
&= \frac{8e^{\beta 8J} + 8}{\cosh(\beta 8J) + 3} - (0)^2 \\
\sigma_{\mathcal{M}}^2 &= \frac{8e^{\beta 8J} + 8}{\cosh(\beta 8J) + 3}
\end{aligned}$$

Specific heat capacity, C_V

The specific heat capacity is defined as

$$C_V = \frac{\sigma_E^2}{k_B T^2}$$

Inserting the value σ_E^2 we get

$$C_V = \frac{1}{k_B T^2} 64J^2 \left(\frac{\cosh(\beta 8J)}{\cosh(\beta 8J) + 3} - \left(\frac{-\sinh(\beta 8J)}{\cosh(\beta 8J) + 3} \right)^2 \right)$$

This is the main function we will be comparing to the values from our computations later.

Susceptibility, χ

The susceptibility is defined as

$$\chi = \frac{\sigma_{\mathcal{M}}^2}{k_B T^2}$$

Inserting the value $\sigma_{\mathcal{M}}^2$ we get

$$\chi = \frac{1}{k_B T^2} \frac{8e^{\beta 8J} + 8}{\cosh(\beta 8J) + 3}$$

Note that these four characteristics are temperature dependent through $\beta = \frac{1}{k_B T}$. Ref [1].

2.3 Ising model

The Ising model is applied for the study of phase transitions at finite temperatures for magnetic systems. Energy is expressed as:

$$E = -J \sum_{\langle kl \rangle}^N s_k s_l \quad s_k = \pm 1 \quad (1)$$

N is the number of spins and J is a constant expressing the interaction between neighboring spins. The sum is over the nearest neighbours only, indicated by $\langle kl \rangle$ in the above equation. For $J > 0$ it is energetically favorable for neighboring spins to align. Leading to, at low temperatures, T, spontaneous magnetisation.

A probability distribution is needed in order to calculate the mean energy $\langle E \rangle$ and magnetization $\langle M \rangle$ at a given temperature. The distribution is given by:

$$P_i(\beta) = \sum_{i=1}^M s_k s_l \exp -\beta E_i, \quad (2)$$

where M is all the microstates, P_i is the probability of having the system in a state/configuration i.

We are also utilizing the Metropolis algorithm which basically checks if we can get a lower energy for the system if we flip a spin, and if that is the case, it flips the spin.

The pseudocode looks as follows:

```

for Temperature ;

    for MonteCarlo Cycle ;

        -Metropolis algorithm
        -Sum all values

    end for MonteCarlo loop

    -Divide values by MC cycles
    -Output values

```

end **for** Temperature loop

2.4 Analyzing the probability distribution

We will also compute the probability of the energy, $P(E)$ for the system with $L = 20$ with the temperatures $T = 1, 2.4$. This is computed by counting the number of times a given energy appears in our computation. The computation will start at a number of Monte Carlo cycles of which we know that the system is stable. We will also compare the results with the computed variance energy σ_E^2 and discuss the behavior.

3 Results

3.1 2×2 lattice, analytical expressoins

If we scale the value of β from $1/k_B T$ to $1/J$ (Scaling factor $k_B T/J$) in the analytical expression from section 2.2, we will get a good benchmark for computer computations to come. These values are listed in table 2 below. Note that all values are divided by four, since we want the values per bond, and not for the entire lattice.

Mean energy, $\langle E \rangle$:	-1.9960
Mean absolute magnetization, $\langle \mathcal{M} \rangle$:	0.9987
Specific heat capacity, C_V :	0.0321
Susceptibility, χ :	3.9933

Table 2: Benchmark for material characteristics per bond for a 2×2 lattice

3.2 Ising model: simulation over temperature

We ran the program for different amounts of Monte Carlo cycles and plottet the error (analytical - simulated) in figure 1 below. It seems we want to use around 10^7 MC cycles or more to get a good simulation.

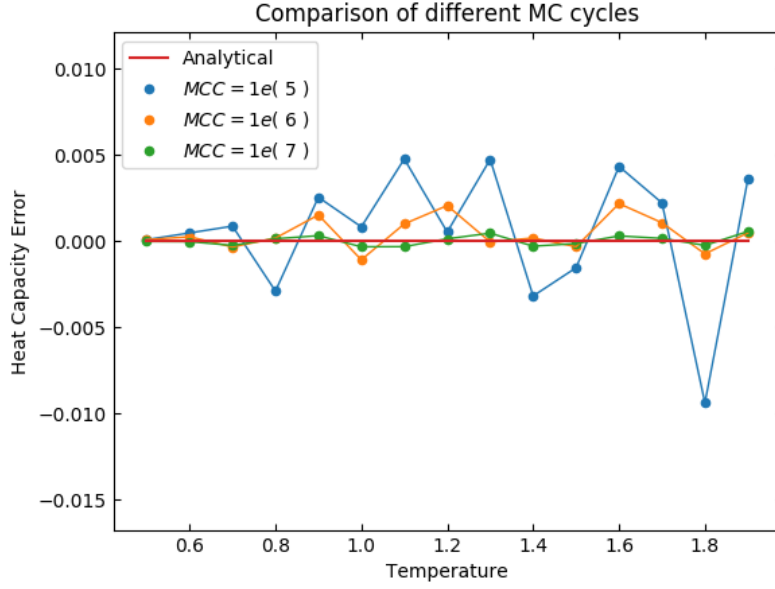


Figure 1: Shows the accuracy of different amount of MC cycles over temperature.

4 Discussion

5 Conclusion

6 Appendix

6.1 GitHub

6.2 Calculations

Energy expectation value, $\langle E \rangle$

$$\begin{aligned}
 \langle E \rangle &= \frac{1}{2e^{-\beta 8J} + 2e^{\beta 8J} + 12} (2 \cdot -8J \cdot e^{\beta 8J} + 2 \cdot 8J \cdot e^{-\beta 8J}) \\
 &= \frac{1}{2e^{-\beta 8J} + 2e^{\beta 8J} + 12} (-16J e^{\beta 8J} + 16J e^{-\beta 8J}) \\
 &= 8J \frac{1}{e^{-\beta 8J} + e^{\beta 8J} + 6} (e^{-\beta 8J} - e^{\beta 8J}) \\
 &= -8J \frac{\sinh(\beta 8J)}{\cosh(\beta 8J) + 3}
 \end{aligned} \tag{3}$$

$$\begin{aligned}
\sigma_E^2 &= \langle E^2 \rangle - \langle E \rangle^2 = \frac{1}{Z} \sum E_i^2 e^{-\beta E_i} - \left(\frac{1}{Z} \sum E_i e^{-\beta E_i} \right)^2 \\
&= \frac{1}{2e^{-\beta 8J} + 2e^{\beta 8J} + 12} \left(2 \cdot (-8J)^2 \cdot e^{\beta 8J} + 2 \cdot (8J)^2 \cdot e^{-\beta 8J} \right) \\
&\quad - \left(-8J \frac{\sinh(\beta 8J)}{\cosh(\beta 8J) + 3} \right)^2 \\
&= 128J^2 \frac{2\cosh(\beta 8J)}{4\cosh(\beta 8J) + 12} - \left(-8J \frac{\sinh(\beta 8J)}{\cosh(\beta 8J) + 3} \right)^2 \\
&= 64J^2 \frac{\cosh(\beta 8J)}{\cosh(\beta 8J) + 3} - \left(-8J \frac{\sinh(\beta 8J)}{\cosh(\beta 8J) + 3} \right)^2 \\
&= 64J^2 \left(\frac{\cosh(\beta 8J)}{\cosh(\beta 8J) + 3} - \left(\frac{\sinh(\beta 8J)}{\cosh(\beta 8J) + 3} \right)^2 \right) \tag{4}
\end{aligned}$$

Magnetization, \mathcal{M}

$$\begin{aligned}
\langle |\mathcal{M}| \rangle &= \frac{1}{4\cosh(\beta 8J) + 12} (4 \cdot e^{\beta 8J} + 4 \cdot 2 \cdot e^0 + 4 \cdot |-2| \cdot e^0 + |-4| \cdot e^{\beta 8J}) \\
&= \frac{1}{\cosh(\beta 8J) + 3} (e^{\beta 8J} + 2 + 2 + e^{\beta 8J}) \\
&= \frac{1}{\cosh(\beta 8J) + 3} (2e^{\beta 8J} + 4) \\
&= \frac{2e^{\beta 8J} + 4}{\cosh(\beta 8J) + 3}
\end{aligned}$$

References

- [1] Morten Hjorth-jensen. *Computational Physics Lectures: Statistical physics and the Ising Model*. 2019.