# 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 $2 \times 2$ 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 $\chi$ 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:

$$E_i = -J \sum_{<kl>}^{N} s_k s_l$$

Where $< kl >$ 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 respecitve $E_i$ 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:

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

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

**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 ($\sigma_E$) 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 expectation value, $\mathcal{M}$**

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 (5)):

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

Since the variance of the mean magnetization ($\sigma_M$) is needed for the susceptibility later, we will calculate this here. For this we will need the mean magnetization square $\langle \mathcal{M}^2 \rangle$, and the mean magnetization $\langle \mathcal{M} \rangle$. $\langle \mathcal{M} \rangle$ is shown to be 0 in the appendix, equation (6), and $\langle \mathcal{M}^2 \rangle = \frac{8e^{\beta 8J}+8}{\cosh(\beta 8J)+3}$ (shown in the appendix, equation (7)). Thus, the variance is:

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

**Specific heat capacity, $C_V$**

The specific heat capacity is defined as

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

Insering the value $\sigma_E^2$ 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,** $\chi$

The susceptibility is defined as

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

Insering the value of $\sigma_{\mathcal{M}}^2$, we get

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

Note that all the four abovementioned characteristics ($\langle E \rangle$, $\langle |\mathcal{M}| \rangle$, $C_V$ and $\chi$) are temperature dependent, through the variable $\beta = \frac{1}{k_B T}$. [1].

## 2.3 Ising model

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

$$E = -J \sum_{<kl>}^{N} s_k s_l \qquad s_k = \pm 1 \tag{1}$$

$N$ 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 $< kl >$ the above equation. For $J > 0$ it is energetically favorable for neighboring spins to align. Leading to, at low temperatures, $T$, spontaneous magnetization. A probability distribution is needed in order to calculate the mean energy $\langle E \rangle$ and magnetization $\langle \mathcal{M} \rangle$ at a given temperature. The distribution is given by:

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

where $M$ is the number of microstates and $P_i$ is the probability of having the system in a state/configuration $i$.
We utilize the Metropolis algorithm, which checks if we get a lower energy for the system by flipping a spin. If that is the case, we flip the spin. This is repeated, in the hopes of it reaching the lowest state in total.
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 $\sigma_E^2$ and discuss the behavior.

## 3 Results

### 3.1 $2 \times 2$ lattice, analytical expressions

If we scale the value of $\beta$ from $1/k_BT$ to $1/J$ (Scaling factor $k_BT/J$) 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, $\langle \mathbf{E} \rangle$** | $-1.9960$ |
| **Mean absolute magnetization, $\langle \lvert\mathcal{M}\rvert \rangle$** | 0.9987 |
| **Specific heat capacity, $\mathbf{C_V}$** | 0.0321 |
| **Susceptibility, $\chi$** | 3.9933 |

Table 2: Benchmark for material characteristics per bond for a $2 \times 2$ lattice

### 3.2 Ising model: simulation over temperature

We ran the program for different amounts of Monte Carlo cycles and plotted the error (analytical – simulated) in figure 1 below. Using $10^7$ Monte Carlo cycles, we seem to be getting pretty accurate results.

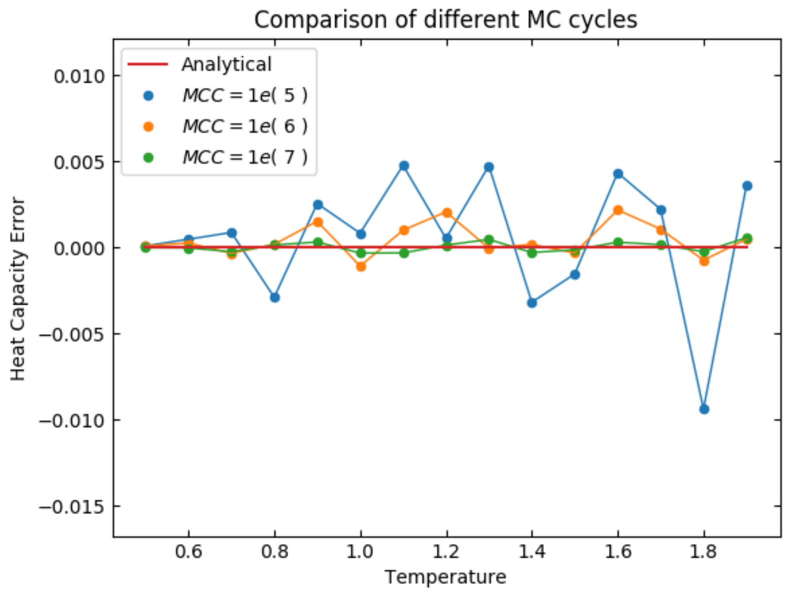


Figure 1: Shows the accuracy of different amount of MC cycles over temperature.

## 3.3 $20 \times 20$ lattice

### Ordered spin orientation

Initializing the spin structure, we first set every spin up for $T < 1.5$ and every spin down for $T \geq 1.5$. In figure 2, the computed values for the mean magnetization and energy are plotted against the number of MC cycles, at $T = 1.0$ and $T = 2.4$:

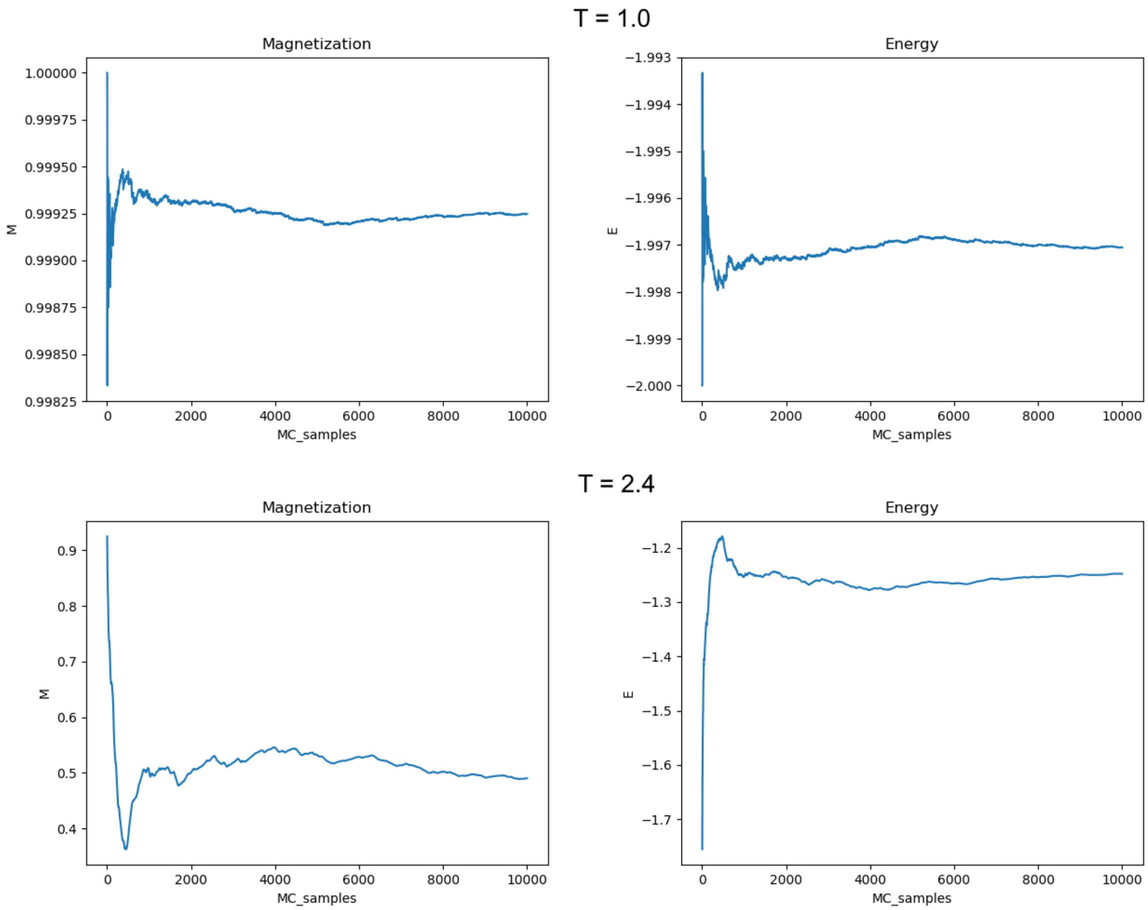


Figure 2: Shows the computed value for the mean magnetization and energy, with ordered initialization, against the number of MC cycles. The scaled temperature is $T = 1.0$ and $T = 2.4$ respectively.

All the plots pretty much stabilize into a value after 8000-1000 MC cycles. For $T = 1.0$, the magnetization stabilizes around the value 0.99950 and the energy around the value $-1.997$. This corresponds pretty good with the analytically calculated values. For $T = 2.4$, the magnetization stabilizes around the value 0.5 and the energy around the value $-1.25$.

### Random spin orientation

Following the ordered initialisation, we also initialized the crystal randomly. In figure 3, the computed values for the mean magnetization and energy are plotted against the number of MC cycles, at $T = 1.0$ and $T = 2.4$:

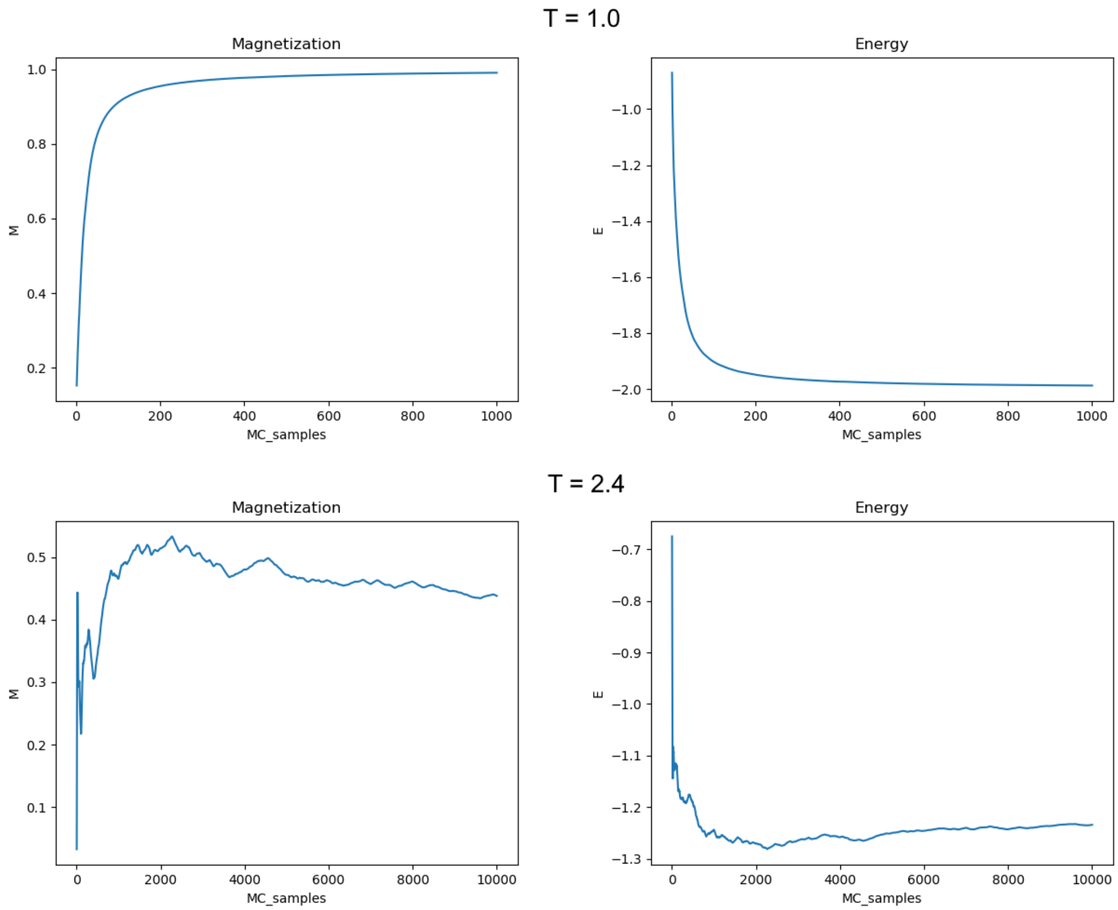


Figure 3: Shows the computed value for the mean magnetization and energy, with random initialization, against the number of MC cycles. The scaled temperature is $T = 1.0$ and $T = 2.4$ respectively.

The plots for $T = 1.0$ follow a clean exponential curve, while the other plots pretty much stabilize after 8000-1000 MC cycles - like the previous ones. For $T = 1.0$, the magnetization ends on the value 1.0 and the energy on the value $-2.0$. This is similar to the analytical values, but does not have the same accuracy. For $T = 2.4$, the magnetization stabilizes around the value 0.45 and the energy around the value $-1.25$.

# 4 Discussion

# 5 Conclusion

# 6 Appendix

## 6.1 GitHub

## 6.2 Calculations

**Energy expectation value, $\langle E \rangle$**

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

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

**Magnetization, $\mathcal{M}$**

$$\begin{aligned}
\langle|\mathcal{M}|\rangle &= \frac{1}{4cosh(\beta 8J)+12}\left(4\cdot e^{\beta 8J}+4\cdot 2\cdot e^{0}+4\cdot|-2|\cdot e^{0}+|-4|\cdot e^{\beta 8J}\right)\\
&= \frac{1}{cosh(\beta 8J)+3}(e^{\beta 8J}+2+2+e^{\beta 8J})\\
&= \frac{1}{cosh(\beta 8J)+3}(2e^{\beta 8J}+4)\\
&= \frac{2e^{\beta 8J}+4}{cosh(\beta 8J)+3}
\end{aligned} \tag{5}$$

$$\begin{aligned}
\langle\mathcal{M}\rangle &= \frac{1}{4\cosh(\beta 8J)+12}\left(4\cdot e^{\beta 8J}+4\cdot 2\cdot e^{0}+4\cdot -2\cdot e^{0}+-4\cdot e^{\beta 8J}\right)\\
&= \frac{1}{\cosh(\beta 8J)+3}\left(4e^{\beta 8J}-4e^{\beta 8J}+8-8\right)\\
&= \frac{1}{\cosh(\beta 8J)+3}(0)\\
\langle\mathcal{M}\rangle &= 0
\end{aligned} \tag{6}$$

$$\begin{aligned}
\langle\mathcal{M}^2\rangle &= \frac{1}{Z}\sum|\mathcal{M}_{\rangle}|^2 e^{-\beta E_i}\\
&= \frac{1}{4\cosh(\beta 8J)+12}\left(4^2\cdot e^{\beta 8J}+4\cdot 2^2\cdot e^{0}+4\cdot|-2|^2\cdot e^{0}+|-4|^2\cdot e^{\beta 8J}\right)\\
&= \frac{1}{4\cosh(\beta 8J)+12}\left(16\cdot e^{\beta 8J}+16\cdot e^{0}+16\cdot e^{0}+16\cdot e^{\beta 8J}\right)\\
&= \frac{4}{\cosh(\beta 8J)+3}\left(2e^{\beta 8J}+2\right)\\
&= \frac{8e^{\beta 8J}+8}{\cosh(\beta 8J)+3}
\end{aligned} \tag{7}$$

# References

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