Project 3

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Abstract

1 Introduction

The Ising model is a statistical model of ferromagnetism. Modelling the atomic spins as discrete values (± 1), the model can identify phase transitions for a periodically repeating crystal of said spins interracting with its neighbours. In this way, the model is also relevant in other studies - modelling the way networks evolve in for example neuroscience and elections.
In this report, we will study the Ising model by applying it to a two-dimensional lattice of spins, with two allowable states. Analytical values are first found for comparison, followed by numerical moddeling utilizing the Metropolis Monte Carlo algorithm.

2 Theory

2.1 The problem

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

Study the magnetisation of a ferromagnetic matrix/crystal with one electronspinn at each lattice site. This is has been modeled as a L$\times$L matrix, where L is the number spinns in one direction. Initilizing both random and not(all spinns the same) to study when the most likely state/equlibrium is reached. Also studied the temperature dependence and have tried to find the critical temperature where ferromagnetism is lost. Methods used are Monte carlo and the Ising model- meaning we could study a 100×100 lattice without it taking too much time.

Using boundary conditions we assume that the last spinn has the same spinn as the one on the opposite side ??? ....

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:

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

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 (5)):

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

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 (6).

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

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 (7)):

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

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 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 (8), and $\langle\mathcal{M}^2\rangle = \frac{8e^{\beta 8J}+8}{\cosh(\beta 8J)+3}$ (shown in the appendix, equation (9)). 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 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

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

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 χ) 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
```

To show that our code has good correspondence to analytical results, we will compare calculations for a 20×20 lattice with the analytical result for the same lattice. This is shown in section 3.2.

2.4 Equlibrium

In order to find the equlibrium of the system, we study a 20×20 lattice. By performing a study of time, corresponding to the number of Monte Carlo cycles, one needs to reach equlibrium

2.5 Analyzing the probability distribution

We will also compute the probability of the energy, $P(E)$ for the system with $L = 20$ with the temperatures $T = 1$ and $T = 2.4$. 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. From the results section 3.3, we see that after the 10000th Monte Carlo cycle we are well beyond the stability limit, so this is what we will be using. We will also compare the width of the gaussian probability distribution (the standard deviation) with the computed variance energy σ_E^2 and discuss the behavior. The standard deviation and the variance should be connected through the fact that standard deviation is the square root of the variance.

2.6 Numerical studies of phase transitions

We wish to study the behavior of the Ising model in two dimensions close to the critical temperature as a function of the lattice size $L \times L$. To do this, we will be calculating the expectation values for energy, $\langle E \rangle$, and absolute magnetisation, $\langle |M| \rangle$, and also the specific heat capacity C_V and the susceptibility χ as a function of the temperature in the interval $T \in [2.0, 2.5]$ with a step of $\Delta T = 0.005$. This will be done for the lattice sizes $L = 20, 40, 60, 80, 100$. From the plots we hope to see an indication of a phase transition.
The code will be paralellized using MPI, and timed using the MPI_Time() function.

2.7 Extracting the critical temperature

We would like to compute the critical temperature T_C in the thermodynamic limit where $L \to \infty$. This will be done using the equation below, together with the exact result of $\nu = 1$.

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu}$$

By using two different lattice sizes, we can calculate the factor a, and then calculate T_C.

$$\begin{aligned} T_C(L_1) - T_C(L = \infty) &= aL_1^{-1/\nu} \\ T_C(L_2) - T_C(L = \infty) &= aL_2^{-1/\nu} \end{aligned}$$

By subtracting the equations we obtain

$$\frac{T_C(L_1) - T_C(L_2)}{L_1^{-1/\nu} - L_2^{-1/\nu}} = a \tag{3}$$

It will now be easy to use the equation below to find the critical temperature for an infinitely large lattice.

$$T_C(L = \infty) = T_C(L) - aL^{-1/\nu} \tag{4}$$

3 Results

3.1 2×2 lattice, analytical expressions

If we scale the value of β 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, 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 plotted the error (analytical – simulated) in figure 1 below. Using 10^7 Monte Carlo cycles, we seem to be getting pretty accurate results.

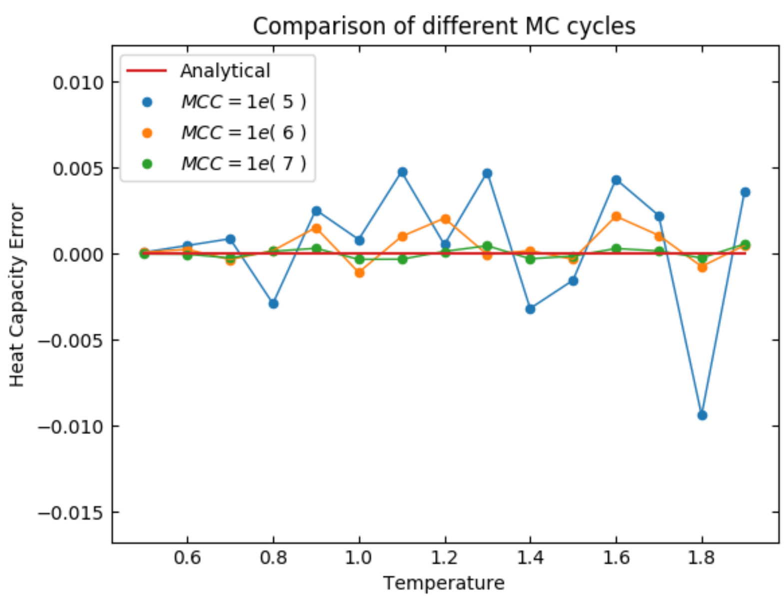

Figure 1: Shows the accuracy of different amount of MC cycles over temperature.

This shows that our computed results are quite close to our analytical results for the 20×20 lattice. This is a good indication of a successfull simulation.

3.3 20×20 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 $T = 2.4$:

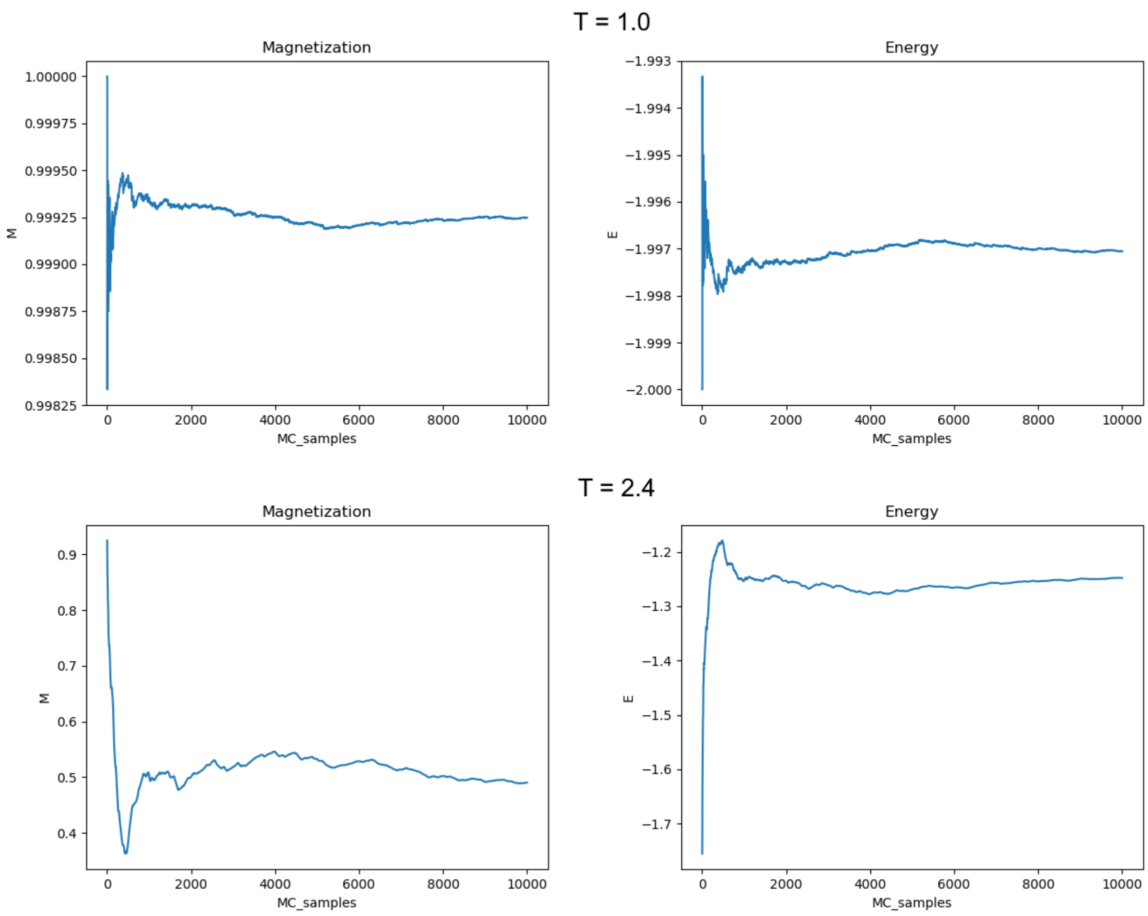

Figure 2: Shows the computed value for the mean magnetization and energy, with ordered initialization, against the number of MC cycles. The scaled temperature is $T = 1.0$ and $T = 2.4$ respectively.

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 $T = 2.4$:

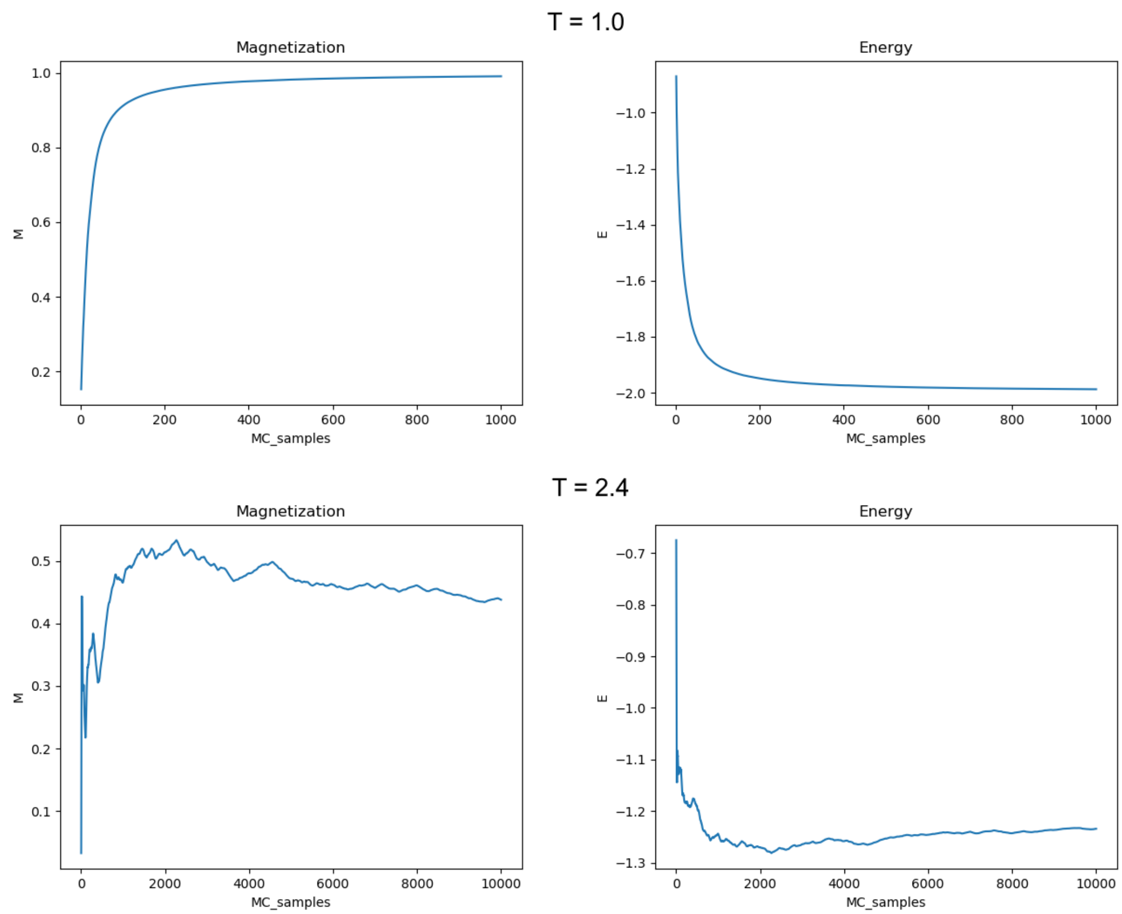

Figure 3: Shows the computed value for the mean magnetization and energy, with random initialization, against the number of MC cycles. The scaled temperature is $T = 1.0$ and $T = 2.4$ respectively.

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.

3.4 Analyzing the probability distribution

In figure 4 you can see the probability distribution for low and high temperature respectively. We can see that for a low temperature, the system tends to settle in the lowest energy state, while for the higher temperature the energies are a bit more spread. In table 3 you will see the computed variance. Note that we calculated standard deviation of the histogram with NUMPY.STD, and took the square root of this to get the variance.

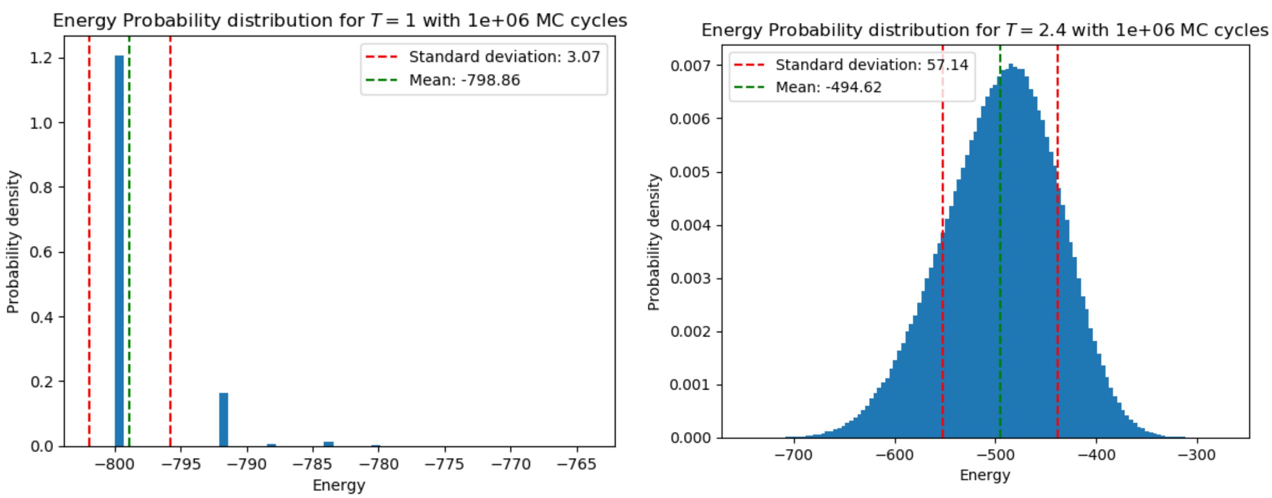

Figure 4: Shows probability distribution for low and high temperature.

Temperature	calculated variance	from histogram	deviation
1	9.375	1.752	81%
2.4	8.053	7.550	6.2%

Table 3: Computed variance

3.5 Numerical studies of phase transitions

After playing around with the domain of the temperature we found that the domain used in figure 5 and 6 nicely presents the phase change of the material. We used 10^6 Monte Carlo Cycles for each temperature step, which had a stepsize of $\Delta T = 0.005$. As shown in the figures we can clearly see that something is happening around $T = 2.3$.

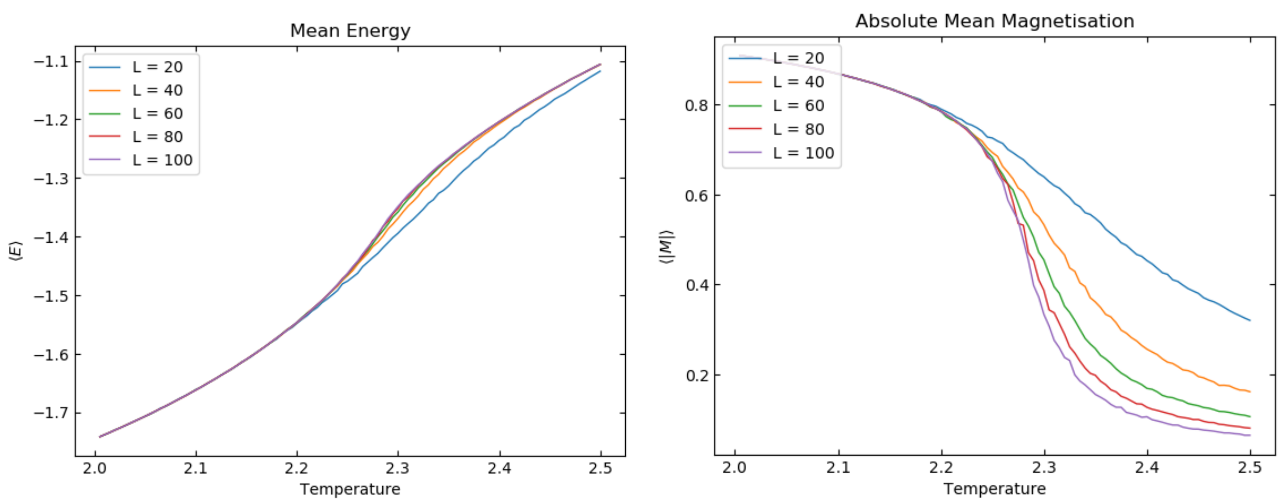

Figure 5: Mean energy and magnetisation over temperature interval $T \in [2.0, 2.5]$ with lattice sizes $L = 20, 40, 60, 80, 100$.

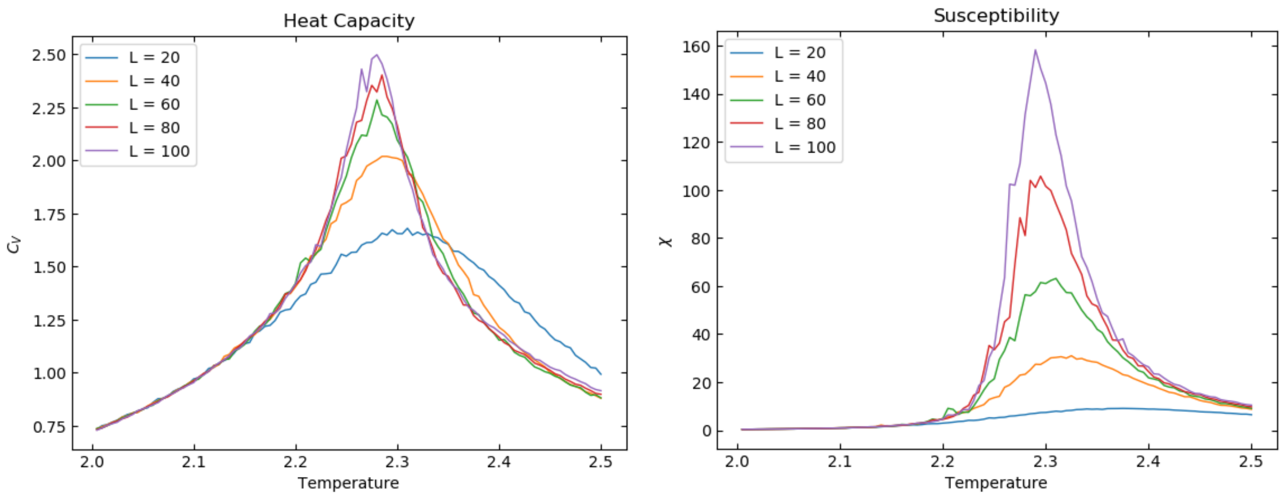

Figure 6: Heat capacity and Susceptibility over temperature interval $T \in [2.0, 2.5]$ with lattice sizes $L = 20, 40, 60, 80, 100$.

The simulations were run on an 16-core AMD Ryzen 1700x with 3.4GHz clock speed. It took approximately 3 hours to complete. To compare parallelized time to using a single core, we ran calculations for the 20x20 lattice with 10^6 Monte Carlo cycles and $T \in [2.0, 2.5]$ with step size $\Delta T = 0.05$. The time is shown in table 4.

Cores	Time spent
1	42s
2	26s

Table 4: Time spent on calculations for different thread-count.

3.6 Extracting the critical temperature

The critical temperatures of the different sized arrays was found by taking the averange of the full width half maximum of the heat capacity and the susceptibility. This resulted in the critical temperatures found in table 5.

Lattice size, L	T_C
40	2.318
60	2.301
80	2.291
100	2.284

Table 5: Critical temperatures of different lattice sizes.

By using equation (3), and (4). we find the constant a, and thereafter the critical temperature for an infinitely large lattice.

Parameter	Value
a	0.000567
T_C	2.2669

Table 6: Numerical values for the parameter a, and the critical temperature.

For reference, the exact result for the criticalt temperature for $L \to \infty$ is $kT/J = 2/ln(1 + \sqrt{2}) \approx 2.269$ after Lars Onsager.[2]

4 Discussion

4.1 Ising model: simulation over temperature

4.2 20×20 lattice

4.3 Analyzing the probability distribution

4.4 Numerical studies of phase transitions

4.5 Extracting the critical temperature

5 Conclusion

6 Appendix

6.1 GitHub

6.2 Calculations

Energy expectation value, $\langle E \rangle$

$$
\begin{aligned}
\langle E \rangle &= \frac{1}{2e^{-\beta 8J} + 2e^{\beta 8J} + 12}\left(2 \cdot -8J \cdot e^{\beta 8J} + 2 \cdot 8J \cdot e^{-\beta 8J}\right) \\
&= \frac{1}{2e^{-\beta 8J} + 2e^{\beta 8J} + 12}\left(-16Je^{\beta 8J} + 16Je^{-\beta 8J}\right) \\
&= 8J\frac{1}{e^{-\beta 8J} + e^{\beta 8J} + 6}\left(e^{-\beta 8J} - e^{\beta 8J}\right) \\
&= -8J\frac{sinh(\beta 8J)}{cosh(\beta 8J) + 3}
\end{aligned} \tag{5}
$$

$$
\begin{aligned}
\sigma_E^2 &= \langle E^2 \rangle - \langle E \rangle^2 = \frac{1}{Z}\sum E_i^2 e^{-\beta E_i} - \left(\frac{1}{Z}\sum E_i e^{-\beta E_i}\right)^2 \\
&= \frac{1}{2e^{-\beta 8J} + 2e^{\beta 8J} + 12}\left(2 \cdot (-8J)^2 \cdot e^{\beta 8J} + 2 \cdot (8J)^2 \cdot e^{-\beta 8J}\right) \\
&\qquad - \left(-8J\frac{sinh(\beta 8J)}{cosh(\beta 8J) + 3}\right)^2 \\
&= 128J^2\frac{2cosh(\beta 8J)}{4cosh(\beta 8J) + 12} - \left(-8J\frac{sinh(\beta 8J)}{cosh(\beta 8J) + 3}\right)^2 \\
&= 64J^2\frac{cosh(\beta 8J)}{cosh(\beta 8J) + 3} - \left(-8J\frac{sinh(\beta 8J)}{cosh(\beta 8J) + 3}\right)^2 \\
&= 64J^2\left(\frac{cosh(\beta 8J)}{cosh(\beta 8J) + 3} - \left(\frac{sinh(\beta 8J)}{cosh(\beta 8J) + 3}\right)^2\right)
\end{aligned} \tag{6}
$$

Magnetization, $\mathcal{M}$

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

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

$$\begin{aligned}
\langle\mathcal{M}^2\rangle &= \frac{1}{Z}\sum|\mathcal{M}_{\rangle}|^2 e^{-\beta E_i}\\
&= \frac{1}{4\cosh(\beta 8J)+12}\left(4^2\cdot e^{\beta 8J}+4\cdot 2^2\cdot e^{0}+4\cdot|-2|^2\cdot e^{0}+|-4|^2\cdot e^{\beta 8J}\right)\\
&= \frac{1}{4\cosh(\beta 8J)+12}\left(16\cdot e^{\beta 8J}+16\cdot e^{0}+16\cdot e^{0}+16\cdot e^{\beta 8J}\right)\\
&= \frac{4}{\cosh(\beta 8J)+3}\left(2e^{\beta 8J}+2\right)\\
&= \frac{8e^{\beta 8J}+8}{\cosh(\beta 8J)+3}
\end{aligned} \tag{9}$$

References

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

[2] Lars Onsager. *Crystal Statistics. I. A Two-Dimensional Model with an Order-Disorder Transition*. 1944. DOI: `https://doi.org/10.1103/PhysRev.65.117`. URL: `https://journals.aps.org/pr/abstract/10.1103/PhysRev.65.117`.