Phase transitions in magnetic systems using the two-dimensional Ising model

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We have studied magnetic system using the two dimensional Ising model. Solved by the Metropolis algorithm. Our system consists of a $L \times L$ quadratic lattice with $N = L^2$ spins. The model exhibits magnetic material properties such as spontaneous magnetization at low temperatures in the absence of external magnetic fields. The theoretical value for critical temperature is $T_C \approx 2.269$. When temperature is varied in the interval $T \in [2.0, 2.3]$, the model undergoes a second order phase transition. Using a 100×100 lattice, we are able to estimate the critical temperature to be $T_C = 2.27$.

I. INTRODUCTION

In this project we have studied phase transitions in magnetic systems using the Ising model in two dimensions. The Ising model is widely popular for simulating phase transitions. In one and two dimensions, the model provides analytical solutions to several expectation values which can serve as benchmark calculations for numerical simulations. The Ising model is an important tool for developing a good qualitatively understanding of phase transitions. Our magnetic system is a two dimensional Ł $\times$ L lattice with N spins.

For a system with a given critical temperature (the Curie temperature), the Ising model exhibits a phase transition from a magnetic phase (where the system has a finite magnetic momentum, or magnetization) to a phase which has zero magnetization. The magnetization of the system is given as the sum over the individual spins that the system consists off.

Assuming that we have a binary system where spin-objects are placed in a lattice. Each object in a lattice site can only take two values for spin (binary), which is either $+1$ or -1 (up or down). In its simplest form, the energy of the Ising model for a specific spin-configuration without any external magnetic field is given as [1]

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

Where $s_k = \pm 1$ is the surrounding spin. N is the total number of spins (or objects), J is a coupling constant which expresses the strength of the interactions between neighbouring spins. The notation $\langle kl \rangle$ indicates that we only sum up the contribution from the nearest neighbors. Using a ferromagnetic ordering, $J > 0$. Ferromagnetic materials lose their spontaneous magnetization at the Curie temperature, meaning that the magnetic dipoles become disordered. This results in a net zero magnetization. The magnetization is given as the sum over all individual spins s_j for a given configuration (microstate)

$$M = \sum_{j=1}^{N} s_j. \tag{2}$$

We will use periodic boundary conditions and the Metropolis algorithm for solving the Ising model, explained further in section (II). Figure (1) shows a sketch of how we model the $L \times L$ spin-lattice. Our goal is to simulate the system as it undergoes a phase transition. By looking at the behaviour of thermodynamic quantities like heat capacity, we will estimate the critical temperature at which phase transitions take place.

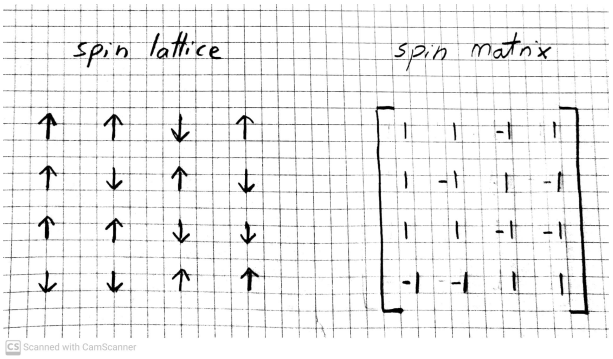

Figure 1. Example of a quadratic spin-lattice and its equivalent interpretation as a spin-matrix in mathematics. Spin up $\uparrow = 1$ and spin down $\downarrow = -1$.

The report is structured into theory, method, results, discussion and conclusion. First an introduction to the theory behind our methods (explaining the Ising model, phase transitions and critical phenomena, and the Metropolis algorithm). In the methods, we look at how we have implemented our model numerically. Results are presented with figures and descriptions, and later discussed critically before arriving at the conclusion of our findings.

II. THEORY

Explaining theoretical models and concepts used for studying magnetic phase transitions.

A. The Ising Model

The Ising model in two dimensions uses a lattice with equally spaced spins as a model of magnetic materials. Equation (1) from the introduction is the energy of the Ising model, without any external magnetic field. By including the magnetic field, B, which is assumed to be uniform, energy is given as [4]

$$E = -J\sum_{\langle kl\rangle}^{N} s_k s_l - B\sum_{k}^{N} s_k, \tag{3}$$

with $s_k = \pm 1$. As mentioned, the sum runs over all N spins, but we only look at the nearest neighbours for each spin. Periodic boundary conditions are applied. This means that the neighbor to a spin on the left end of the lattice is taken to be the spin on the right end of the lattice, and vice versa. Figure (26) shows how periodic boundary conditions are used for the special 2×2 lattice case.

For ferromagnetic materials, the coupling constant $J > 0$. This makes it so that its energetically favorable for neighboring spins to be aligned. At low temperatures, spontaneous magnetization can occur, in the absence of an external magnetic field. The reason for this is because the neighbours interact with each other. These interactions spreads throughout the lattice. Eventually more and more spins are aligned, creating a net magnetization which is favourable (minimized energy). The ground state, which has the lowest energy, is the state where all spins are aligned, pointing either up or down.

We use the **canonical ensemble** with **Boltzmann statistics** to calculate expectation values and thermodynamic quantities, explained further in appendix (A). The partition function Z (A2), which is the sum over all Boltzmann factors, is constant for a given temperature. The expectation value for energy $\langle E\rangle$ (A4) and magnetization $\langle M\rangle$ (A5) can be calculated once we know the partition function for the system. Since the partition function will vary for different temperatures, expectation values will be different for different temperatures. We will use the Metropolis algorithm to solve the Ising model, explained further in subsection (II C). For the 2×2 lattice case, we have obtained analytical expressions for expectation values in appendix (B 1), which will serve as benchmark results. Table (V) shows what we should expect to find as mean values for the low temperature case. We see that $\langle E\rangle \approx -8$, which means that the ground state is most likely. As temperature increase, the partition function reduces because the Boltzmann factors goes to zero, which results in a higher expectation value for energy ($\langle E\rangle \to 0$).

B. Phase Transitions and Critical Phenomena

A phase transition in general is marked by sudden macroscopic changes as external parameters are changed. The point where a phase transition takes place is called a critical point. In magnetic systems, phase transitions can take place when temperature (external parameter) is increased. The critical point is when temperature equals the Curie temperature, T_C. At above this temperature, ferromagnetic materials loose their permanent magnetic properties [5]. Figure (2) shows a sketch of what this will look like in our two dimensional model.

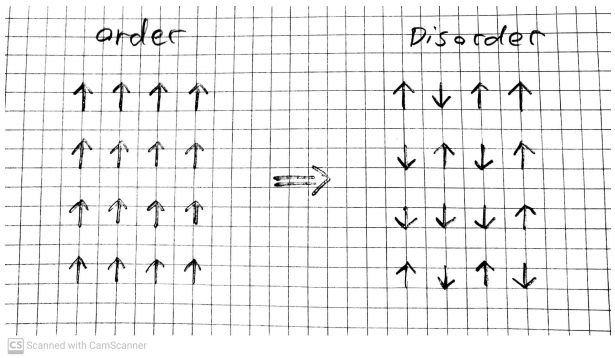

Figure 2. Magnetic phase transition, going from an ordered spin configuration with a net magnetization different from zero, to a disorder spin configuration which has roughly zero magnetization.

Before moving on to explain phase transitions, we have to define some terms. Correlation length, ξ, defines the length scale at which the overall properties of a material start to vary from its bulk properties. Bulk properties are intensive (local) properties of a system that does not depend on the size of the system. For our purposes this could be temperature. Correlation length is therefore a measure of the distance at which fluctuations of the microscopic degrees of freedom are correlated with each other (for example atom positions). It depends on external conditions like pressure and temperature. For the Ising model, the correlation length is related to the spin-correlation function. The spin-correlation function expresses the covariance (joint

variability between variables, degree of correlation) between spins. The spin-correlation function defines the magnetic susceptibility (A9).

There are two types of phase transitions: first-order and second-order (3). First-order phase transitions are discontinuous. They are characterized by two or more states on either side of the critical point that can coexist at the critical point. There is a discontinuous behaviour of thermodynamic functions when passing through the critical point. The continuation of states from below to above the critical point is discontinuous. The continuation is stable so that the system may take some time to readjust (metastable state). Temperature remains constant. The correlation length is usually finite at the critical point.

Second-order phase transitions are continuous, and generally more difficult to understand than first-order phase transitions. At the critical point, the correlation length diverges ($\xi \to \infty$) such that fluctuations are correlated over all distance scales. In a way, all the spins are "seeing each other" and interacting. This forces the system to be in a unique critical phase where two phases on either side of the critical point become identical. A classical example for magnetic systems is the disappearance of spontaneous magnetization. This is the phenomena we are interested in. The Ising model allows us to identify where such phase transitions take place.

We are using Helmholtz free energy (A3) as our thermodynamic potential in the canonical ensemble. A characteristic which is important when using the Ising model is that the first derivative with respect to $\beta = (kT)^{-1}$ of the Helmholtz potential should be continuous at the critical point. The second derivative should diverge at the critical point. Using the relation [5]

$$F = -kTlnZ,$$

with Z being the partition function. We have the following expressions the expectation value for energy

$$\langle E \rangle = -\frac{\partial lnZ}{\partial \beta} = \frac{\partial \beta F}{\partial \beta},$$

and heat capacity

$$C_V = \frac{1}{kT^2}\frac{\partial^2 lnZ}{\partial \beta^2} = -\frac{1}{kT^2}\frac{\partial^2 \beta F}{\partial \beta^2}.$$

This shows that we expect energy $\langle E \rangle$ to be continuous at the critical point because its related to the first derivative of F. Heat capacity should diverge at the critical point because its related to the second derivative of F. In the Ising model however, for a finite sized lattice, heat capacity peeks to the right of the theoretical critical temperature, it does not diverge to infinity. It therefore allows us to identify the critical temperature. We also expect the mean absolute magnetization $\langle |M| \rangle$ to drop off to zero at the critical temperature, because magnetization is lost. Figure (4) shows an expected behaviour of the heat capacity.

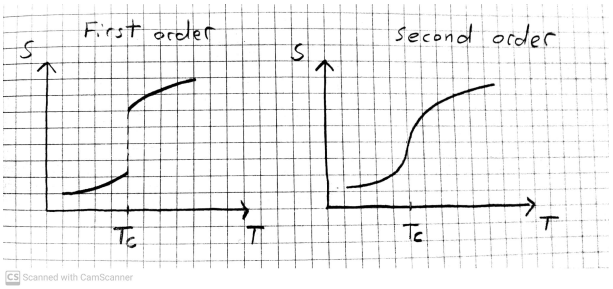

Figure 3. Illustration of what first-order and second-order phase transitions might look like. $S(T)$ is the entropy as a function of temperature T.

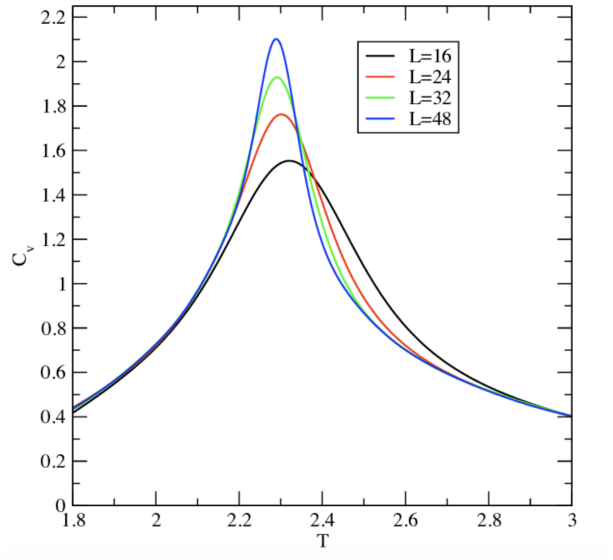

Figure 4. Expected behaviour of the heat capacity during second order phase transitions in the Ising model [7].

When temperature approaches the Curie temperature, $T \to T_C$, we characterize the Ising class of models by a power law behaviour. Mean magnetization is given by

$$\langle M(T) \rangle \sim (T - T_C)^{\beta},$$

where $\beta = 1/8$ is called the critical exponent. Similar relations apply to heat capacity C_V and magnetic susceptibility X

$$C_V \sim |T_C - T|^{-\alpha},$$

and

$$X(T) \sim |T_C - T|^{-\gamma},$$

with $\alpha = 0$ and $\gamma = 7/4$. The correlation length ξ is expected to be of the order of the lattice spacing for $T >> T_C$. When $T \to T_C$, the spins become more and more correlated (increasing covariance), and the correlation length increases. The divergent behaviour of ξ near T_C is

$$\xi(T) \sim |T_C - T|^{-\nu}.$$

During second-order phase transitions the correlation length spans the whole system, $\xi \to \infty$. In reality we are limited to a finite lattice ($L \times L$), therefore ξ will be proportional with the size of the lattice. We use finite size scaling relations to relate the behavior at finite lattices with results from infinitely large lattices. Critical temperature is scaled as

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

with a being constant and ν defined above. Setting $T = T_C$, we obtain mean magnetization, heat capacity and magnetic susceptibility respectively as

$$\langle M(T) \rangle \sim (T - T_C)^{\beta} \to L^{-\beta/\nu},$$

$$C_V \sim |T_C - T|^{-\alpha} \to L^{\alpha/\nu},$$

and

$$X(T) \sim |T_C - T|^{-\gamma} \to L^{\gamma/\nu}.$$

The exact theoretical value for the critical temperature T_C is [1]:

$$\frac{kT_C}{J} = \frac{2}{ln(1 + \sqrt{2})} \approx 2.269, \tag{4}$$

with $\nu = 1$.

C. Metropolis Algorithm

Our magnetic system, a $L \times L$ lattice consisting of $N = L^2$ total spins, has the lowest energy in the ground state. In this case, all spins is pointing in the same direction, either up or down. The Metropolis algorithm should simulate the system as it drives towards equilibrium (minimum energy) at a given temperature. To do this, we change the magnetization in hope of finding a new state which has lower energy than the previous state.

In appendix (A) we have introduced Boltzmann statistics and how to calculate probabilities for specific microstates. In order to make an effective numerical implementation, we don't want to calculate the partition function for finding probabilities during each Monte Carlo cycle. The number of configurations in the two dimensional Ising Model is given by 2^N. Calculating the partition function would therefore require a large number of floating point operations in each cycle. In the Metropolis algorithm, we only consider ratios of probabilities and therefore the partition function cancels out.

Assume that we have defined an initial random magnetization for the lattice. The algorithm then goes as follows [3]:

- Establish an initial energy E_i for the chosen initial configuration.
- Change the initial configuration by flipping one random spin only. Compute the new energy E_j for this configuration.
- Calculate the energy difference $\Delta E = E_j - E_i$.
- If $\Delta E < 0$, accept the new configuration. The next step is to update expectation values and other quantities of interest. Go back to the first step and repeat.
- If $\Delta E > 0$, we calculate the relative Boltzmann factor $w = e^{-\beta \Delta E}$.
- Generate a random number $r \in [0, 1]$. If $r \leq w$, we accept the new configuration. Else, we keep the old configuration.
- The next step is to update expectation values and other quantities of interest. Go back to the first step and repeat.

One Monte Carlo cycle consists of sweeping through the hole lattice (summing over all N spins). We can think of each cycle as a measurement (a sample of data). At the end, we divide the expectation values and other quantities of interest by the number of Monte Carlo

samples (measurements).

Example of implementation shown is in appendix (C). This example show how to calculate the mean energy, which is an expectation value. However, the implementation is not very effective because of the number floating point operations and if-tests during each cycle.

When we only flip one spin at the time, it turns out that there are only **five possible energy difference values** for the two dimensional Ising Model. The reason for this is when one spin is flipped, the energy change within the system only depends on the interactions between the nearest neighbours. This is illustrated in figure (5). These five values are $\Delta E = \{-8J, -4J, 0, 4J, 8J\}$.

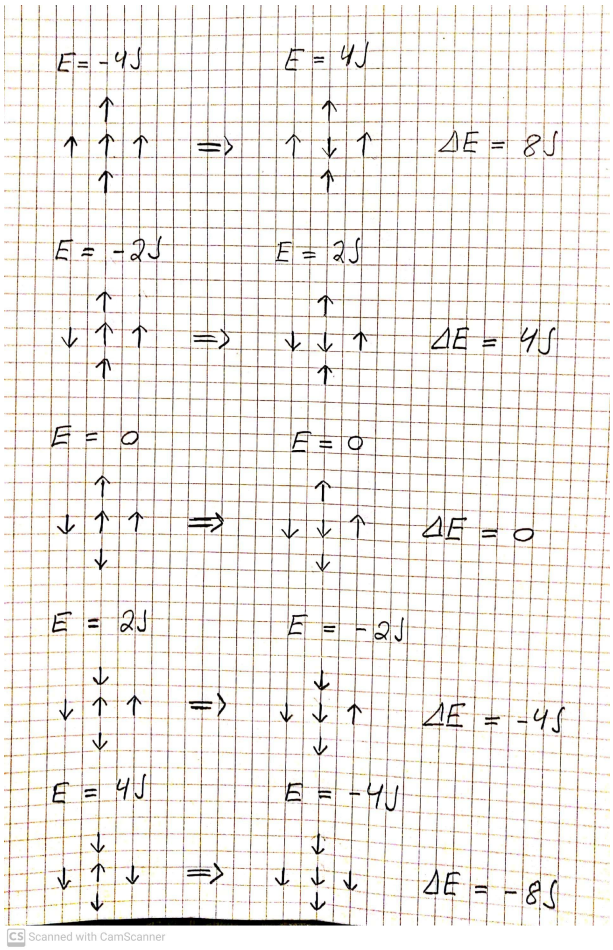

Figure 5. Five possible energy difference values. Two dimensional Ising Model [3].

Without any external magnetic field, energy is given by equation (1). Energy difference between two configurations, state 1 and state 2, are given as

$$\Delta E = E_2 - E_1 = -J \sum_{\langle kl \rangle}^{N} s_k^2 (s_l^2 - s_l^1),$$

where the sum runs only over the nearest neighbors k. The spin s_l^1 is flipped to s_l^2. Since $s_l^1 = \pm 1$ and $s_l^2 = \mp 1$, it is evident that $s_l^2 - s_l^1 = \pm 2$. Energy differences can therefore be coded efficiently as

$$\Delta E = 2J s_l^1 \sum_{\langle k \rangle}^{N} s_k.$$

Similarly, the difference in magnetization between state 1 and state 2 can be simplified. Using equation (2), the change in magnetization is

$$\Delta M = M_2 - M_1 = \sum_{j=1}^{N} (s_j^2 - s_j^1) = s_l^2 - s_l^1 = \pm 2,$$

because only one spin is flipped at the time, $s_j^2 = s_j^1$ expect when $j = l$. The change in magnetization is therefore just $\Delta M = 2s_l^2$, and

$$M_2 = M_1 + 2s_l^2.$$

III. METHOD

Explaining the numerical implementation of the Ising model and Metropolis algorithm. As well as how to improve efficiency in calculations and validation of results through selected runs. The full content is available at GitHub [6].

Since the change in energy can only take on known discrete values we start by pre-calculating all the possible changes in energy for the lattice.

```
    // setup array for possible energy changes
    for( int de =-8; de <= 8; de+=4)
    EnergyDifference(de+8) = exp(-de/Temperature);
```

Then we initialize the lattice with either ordered or unordered spins. This is done in the InitializeLattice function and implemented as follows.

```
void IsingModel::InitializeLattice()
{

  // setup spin matrix and initial magnetization
  if(order=="Ordered"){
    for(int x =0; x < NSpins; x++) {
      for (int y= 0; y < NSpins; y++){
        SpinMatrix(x,y) = 1.0; // all spins up
        MagneticMoment +=  (double) SpinMatrix(x,y);
      }
    }
  }
```

```
  else if(order=="Unordered"){
    for(int x =0; x < NSpins; x++) {
      for (int y= 0; y < NSpins; y++){
        SpinMatrix(x,y) = minus_one_or_one(); // random spin
        MagneticMoment +=  (double) SpinMatrix(x,y);
      }
    }
  }
  else{
    //Prints error message in terminal
    cout << "Wrong Ordered/Unordered" << endl;
    exit(1);
  }
```

When the matrix is initialized we start the Monte Carlo sampling. For each Monte Carlo cycle we sample L^2 times(one for each spin in the lattice). For each sample we pick a random (x, y) index of the spin matrix, flip it, and calculate the change in energy ΔE.

```
    int ix = (int) (RandomNumberGenerator(gen)*(double)NSpins);
    int iy = (int) (RandomNumberGenerator(gen)*(double)NSpins);
    int deltaE =  2*SpinMatrix(ix,iy)*
      (SpinMatrix(ix,PeriodicBoundary(iy,NSpins,-1))+
       SpinMatrix(PeriodicBoundary(ix,NSpins,-1),iy) +
       SpinMatrix(ix,PeriodicBoundary(iy,NSpins,1)) +
       SpinMatrix(PeriodicBoundary(ix,NSpins,1),iy));
```

We pick a random index using a random number generator(RNG) based on the Mersenne algorithm. This RNG has a period of $2^{32} \approx 10^9$. This is more than the maximal number of MC-cycles we will use. This is initialized with the following code.

```
  // Initialize the seed and call the Mersenne algo
  std::random_device rd;
  std::mt19937_64 gen(rd());
  // Set up the uniform distribution for x \in [[0, 1]
  std::uniform_real_distribution<double>
  RandomNumberGenerator(0.0,1.0);
```

And to calculate the ΔE correctly we implement the periodic boundary conditions(PBC) with the inline function PeriodicBoundary as follows.

```
inline int PeriodicBoundary(int i, int limit, int add) {
  return (i+limit+add) % (limit);
}
```

This function returns the index to the last element if you ask for the -1 index and the first if you ask for $L + 1$.

After the ΔE is calculated we pick a random number between zero and one and use the metropolis algorithm to either accept or decline the spin flip.

```
if ( RandomNumberGenerator(gen) <= EnergyDifference(deltaE+8) ) {
     // flip one spin and accept new spin config
     SpinMatrix(ix,iy) *= -1.0;
     MagneticMoment += (double) 2*SpinMatrix(ix,iy);
     Energy += (double) deltaE;
   }
```

For each cycle we can then save the expectation values for E^2, M, M^2 and $|M|$. Or we can save the energy, magnetization and number of metropolis flips as a function of Monte Carlo cycles. This is done in respectively the functions MetropolisSampling and Get_Energy.

To validate our code we will have a look at the 2x2 case, since this has an analytical solution. The results are calculated in appendix B 1 and can be found in table V. We test this for $T = 1.0$ and use one million MC-cycles with our program. These values are shown in table I. We see agreement with the analytical values and proceeds with our code.

Table I. Expactation values for the 2x2 lattice numerically. Using $\beta = 1$, $T = 1$ and $J = 1$. The analytical values can be found in table V.

Quantity	Symbol	Value
Energy expectation	$\langle E \rangle$	-7.98
Energy variance	σ_E^2	0.130
Heat capacity	C_V	0.130
Magnetization expectation	$\langle M \rangle$	0.23
Magnetization absolute value expectation	$\langle \lvert M \rvert \rangle$	3.99
Magnetic susceptibility	X	0.02

We then choose a lattice with $L = 20$ and will look at how many MC-cycles we need to reach a steady state. To do this we will look at the mean magnetization and mean energy plotted against the number of MC-cycles. We will also look at the number of flips from the metropolis algorithm against the number of MC-cycles. To implement this we save the values for each MC-cycle in vectors.

```
MagneticMoment_vector(cycles) = MagneticMoment;
Energy_vector(cycles) = Energy;
number_of_flips_vector(cycles) = number_of_flips;
```

The data is processed and plotted in python using numpy as matplotlib. This is done in the file *Energy_print.py* on the Github [6]. We do this for $T = 1.0$ and $T = 2.4$ for both the ordered and the unordered initial conditions.

For these temperatures we will also look at the probability of finding the system in a spesific energy. We will discard the first 10% of the MC-cycles to allow the system to reach a steady state. We will process this data in the python script *prob_calc.py* on the Github [6]. This will be plotted against a normal distribution, using the variance $\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2$.

To find a phase transition we will look at the heat capacity C_V. This will give us a peak at the critical temperature, where a phase transition occurs. We will use our program to go over an interval of temperatures $T \in [2.0, 2.3]$ with a step length of $dT = 0.01$. We will save and plot the mean energy $\langle E \rangle$, the mean magnetization $\langle |M| \rangle$, the magnetic susceptibility χ and the heat capacity C_V. From the C_V-plot we will extract the critical temperature T_C. This is done in the python program *lattice_reader.py* on Github [6]

Since this will take a lot of computing power we will parallelize our code. We will use the OpenMP library. To use this is as easy as putting an argument around the code you want to parallelize. This is shown in the code below.

```
#include <omp.h>

#pragma omp_parallel for
for(int i=0;i<N;i++){
...
}
```

We have that the time in seconds is the total cpu time over the number of cpu's. We test our parallelization for the 2x2, 5x5, 10x10 and the 20x20 lattice. We can see the results of this in figure 6.

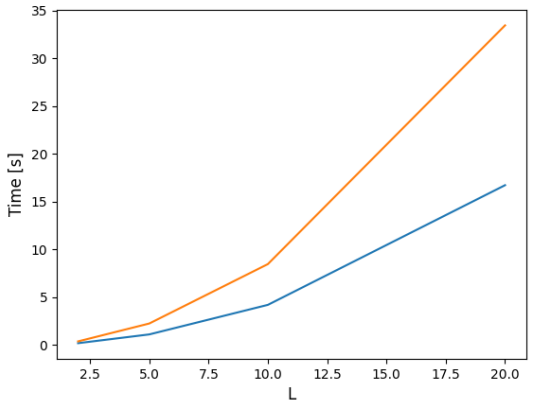

Figure 6. The time spent for parallelized vs. unparallelized code for the 2x2, 5x5, 10x10 and 20x20 lattice. The number of MC-cycles is one million.

IV. RESULTS

Presenting the results obtained from the numerical implementations described in the method section (III).

For the 20×20 lattice, we have studied how many Monte Carlo cycles that are needed in order to reach a the most likely state (equilibrium). Based on these results we can estimate the equilibration time in terms of the number of Monte Carlo cycles used in order to reach equilibrium. One Monte Carlo cycle (or sample) consists off sweeping through the hole lattice. The number of accepted spin-flips have been counted during the calculations in order to create a probability distribution for energy. The behaviour of the system is different depending on the temperature. We have used temperature $T = 1$ and $T = 2.4$ with our scaling of units. The critical temperature is assumed to be somewhere in the range of $T \in [2.0, 2.3]$. The exact result is $T_C \approx 2.269$ (4). For each temperature, we have tested with both ordered and unordered initial spin configurations.

Figure (7) shows how the estimated expectation value for energy per spin varies as a function of Monte Carlo cycles. Starting off in the ground state, which has an ordered spin configuration (all spins up in our case), the energy of the system is already minimized. The most frequent expectation value is $\langle E \rangle = -1.98$. The most likely state is the initial state, therefore the system tends to stay there. This is the low temperature case, with $T = 1$. Figure (8) shows the linear behaviour of the number of accepted spin-flips when solving the Ising model. Figure (9) shows the estimated expectation value for magnetization per spin. The most frequent value is $\langle M \rangle = 1.0$, which is expected as we start off and mostly remain in the ground state.

Figure (10) and (12) shows how the estimated expectation values for energy and magnetization per spin varies as a function of Monte Carlo cycles. Here we start off with an initial random spin-configuration, which has roughly zero internal energy and zero magnetization. Since the temperature is low ($T = 1$), spontaneous magnetization is likely to occur. The system reaches a steady ground state which has $\langle E \rangle \approx -2.0$ and $\langle M \rangle \approx 1.0$, and remains there. The fact that $\langle M \rangle \approx 1.0$ (per spin) reflects that (nearly) all spins are pointing up. Figure (11) shows that there are more accepted spin-flips when the system is going towards equilibrium, than after it has reached equilibrium. This is as expected, since the ground state has minimal energy.

At temperature $T = 2.4$, which is assumed to be higher than the critical temperature (4), we expect that the ferromagnetic material has lost its permanent magnetic properties. Spontaneous magnetization should not occur, and spins will be close to randomly distributed throughout the lattice. Figure (13) and (15) shows the expectation values for energy and magnetization per spin when the initial state is ordered. The system quickly loses its ordered configuration and ends up with a mean net magnetization which fluctuates around zero. We can see that the mean energy is less than in the low temperature case, roughly $\langle E \rangle \approx -1.2$. This indicates that the spin-configuration is not entirely random (it would then be zero). The number of accepted spin-flips behaves linearly as a function of Monte Carlo cycles, shown by figure (14).

Figure (16) and (18) shows the expectation values for energy and magnetization per spin varies as a function of Monte Carlo cycles at $T = 2.4$ with an initial unordered state. The mean magnetization is fluctuating around zero and the mean energy is roughly $\langle E \rangle \approx -1.25$. The number of accepted spin-flips in figure (17) is similar to the previous case. It makes little to no difference starting off with an initial ordered or unordered state when temperature is above the critical value.

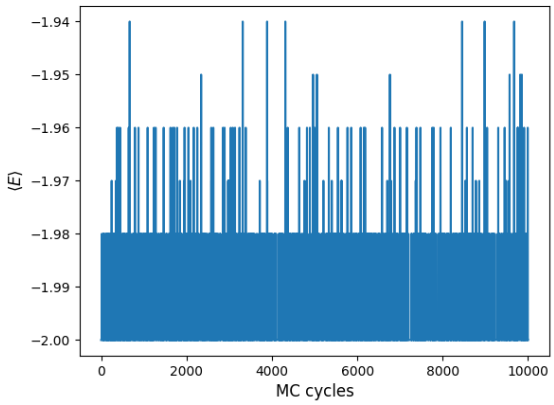

Figure 7. 20×20 lattice. Ordered initial state (ground state). Expectation value $\langle E \rangle$ as a function of Monte Carlo cycles. Temperature $T = 1$.

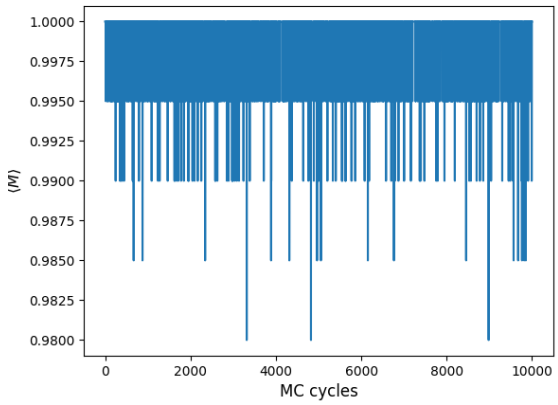

Figure 9. 20×20 lattice. Ordered initial state (ground state). Expectation value $\langle M \rangle$ as a function of Monte Carlo cycles. Temperature $T = 1$.

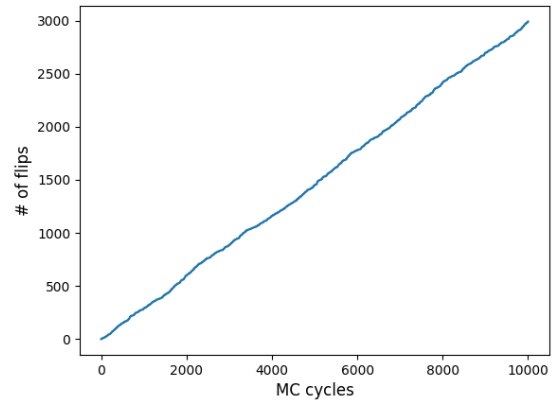

Figure 8. 20×20 lattice. Ordered initial state (ground state). The number of accepted spin-flips as a function of Monte Carlo cycles. Temperature $T = 1$.

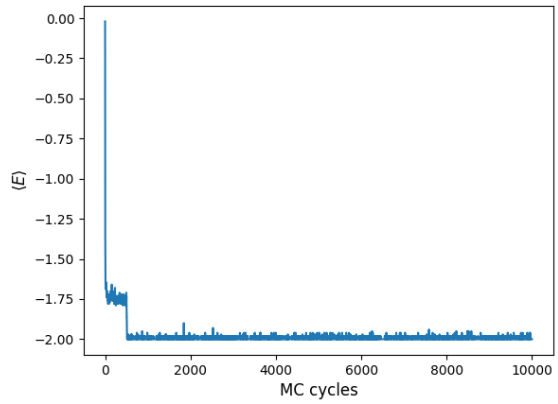

Figure 10. 20×20 lattice. Unordered initial state (random spins). Expectation value $\langle E \rangle$ as a function of Monte Carlo cycles. Temperature $T = 1$.

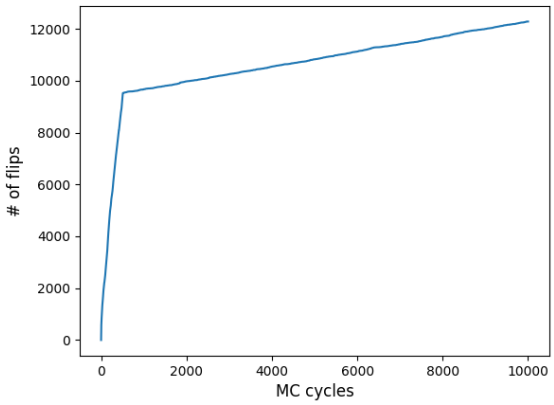

Figure 11. 20×20 lattice. Unordered initial state (random spins). The number of accepted spin-flips as a function of Monte Carlo cycles. Temperature $T = 1$.

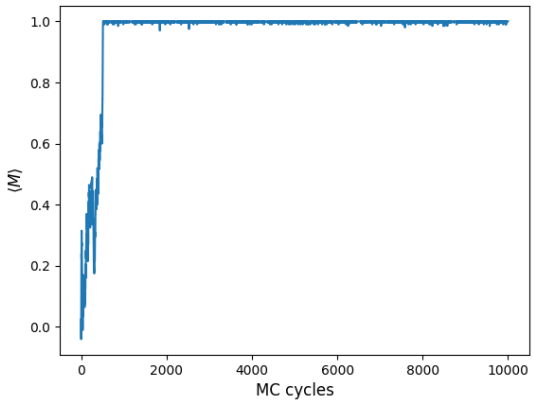

Figure 12. 20×20 lattice. Unordered initial state (random spins). Expectation value $\langle M \rangle$ as a function of Monte Carlo cycles. Temperature $T = 1$

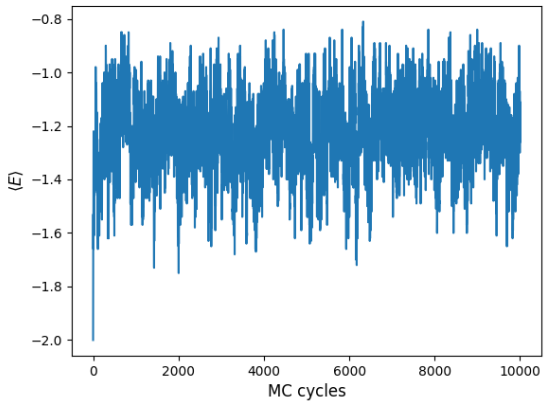

Figure 13. 20×20 lattice. Ordered initial state (ground state). Expectation value $\langle E \rangle$ as a function of Monte Carlo cycles. Temperature $T = 2.4$.

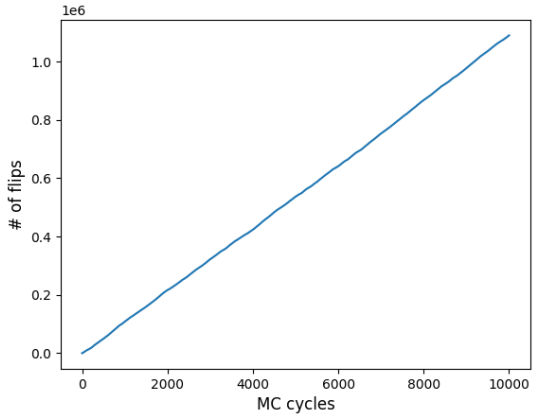

Figure 14. 20×20 lattice. Ordered initial state (ground state). The number of accepted spin-flips as a function of Monte Carlo cycles. Temperature $T = 2.4$.

Once equilibrium is reached, we start the calculations of expectation values. In our case, we have assumed that the first 10% of cycles are used to reach equilibrium, and therefore these data points are considered irrelevant for calculations. Figure (19), (20) and (21) shows the calculated probability distributions for energy at different temperatures, for the 20×20 lattice. In these cases, we are looking at the energy of the system. There are $N = 20 \times 20 = 400$ spins. This is calculated based on how many times a certain energy value appear when solving the Ising model. We have used the Normal distribution with variances obtained from the Metropolis algorithm to compare probabilities. Energy variances as a function of temperature is presented in table (II). Energy variances increase with temperature, showing that it is less likely to find the system in a steady state at higher temperatures.

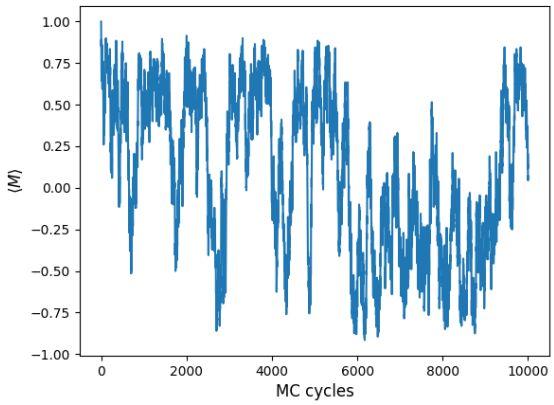

Figure 15. 20×20 lattice. Ordered initial state (ground state). Expectation value $\langle M \rangle$ as a function of Monte Carlo cycles. Temperature $T = 2.4$.

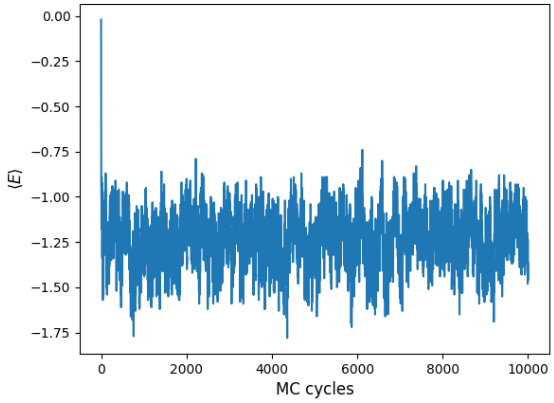

Figure 16. 20×20 lattice. Unordered initial state (random spins). Expectation value $\langle E \rangle$ as a function of Monte Carlo cycles. Temperature $T = 2.4$.

Table II. Energy variance at different temperatures.

Temperature T	Energy variance σ_E^2
1	9.3898
1.5	176.01
2.4	3415.2

At $T = 1$, we expect the system to remain in the ground state. This means that an average value of $E = -800$ is most likely, when looking at the entire system. Figure (19) reflects this, as $P(E)$ peak around $E = -800$. Per spin this corresponds to $\langle E \rangle - 2$ in the 20×20 case, as we have seen in figure (7). As temperature increase, it is more likely to find the system in a state with greater energy. At $T = 1.5$ figure (20) shows a clear shift of the probability distribution to the right

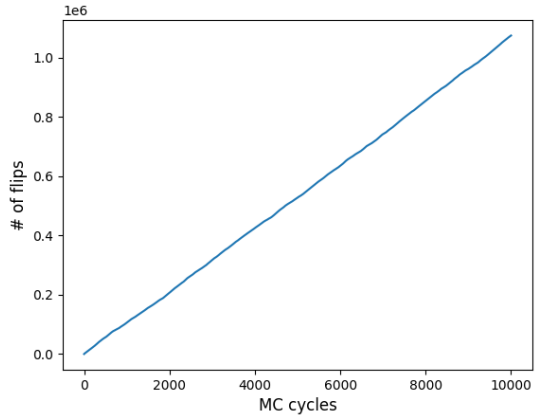

Figure 17. 20×20 lattice. Unordered initial state (random spins). The number of accepted spin-flips as a function of Monte Carlo cycles. Temperature $T = 2.4$.

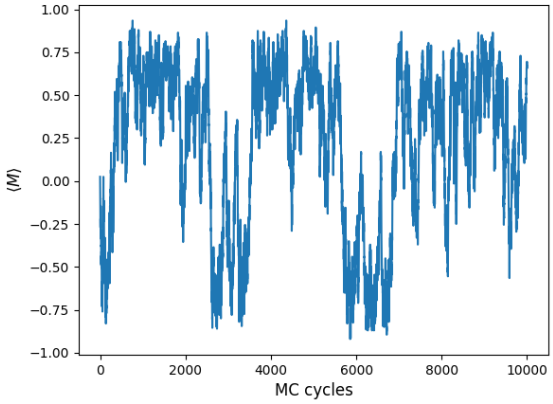

Figure 18. 20×20 lattice. Unordered initial state (random spins). Expectation value $\langle M \rangle$ as a function of Monte Carlo cycles. Temperature $T = 2.4$.

of the energy-spectrum. At $T = 2.4$, we see that the simulated values align well with the Normal distribution. The most likely value for energy is $E = -500$, which corresponds to $\langle E \rangle \approx 1.25$, as we saw in figure (13) and (16).

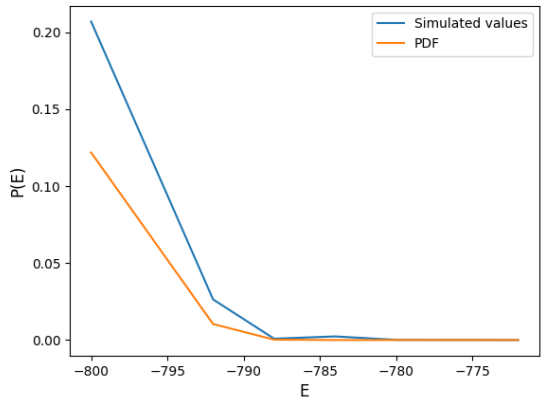

Figure 19. 20×20 lattice. Probability distribution for energy, $P(E)$. Temperature $T = 1$. Compared with the Normal distribution.

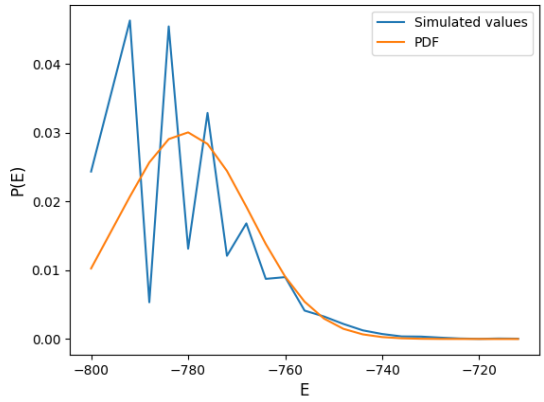

Figure 20. 20×20 lattice. Probability distribution for energy, $P(E)$. Temperature $T = 1.5$. Compared with the Normal distribution.

Figure (22), (24), (23) and (25) shows how different lattice sizes for the Ising model exhibits second order phases transitions around the critical temperature. Energy and magnetization are continuous through the critical point, as expected. The heat capacity peeks consistently to the right of the theoretical value, where it is suppose to diverge in theory. Our model does not diverge, but still allow us to identify approximately where the phase transition takes place. Using the maximum value for heat capacity for each lattice size L, we have obtained the following estimates for the critical temperature in table (III). Our best approximation is $T_C = 2.27$. Temperature steps of $dT = 0.01$ and one million MC-cycles for each temperature.

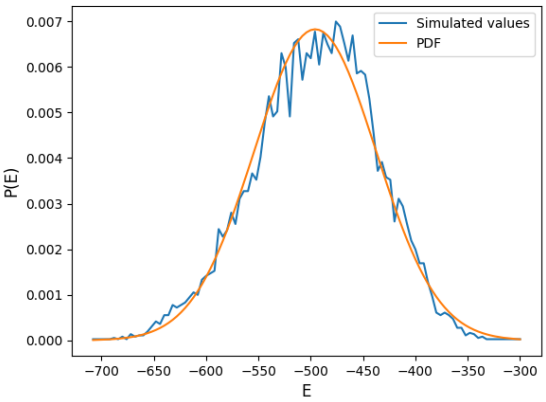

Figure 21. 20×20 lattice. Probability distribution for energy, $P(E)$. Temperature $T = 2.4$. Compared with the Normal distribution.

Table III. Critical temperature T_C estimates for different $L \times L$ lattices.

Lattice size L	Critical Temperature T_C
40	2.29
60	2.27
80	2.28
100	2.27

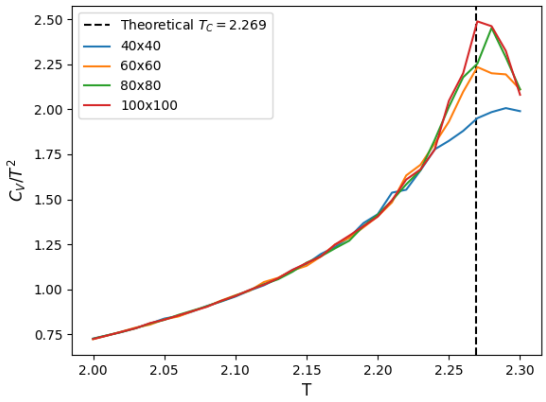

Figure 22. Heat capacity C_V as we pass through the critical point. Second order phase transition.

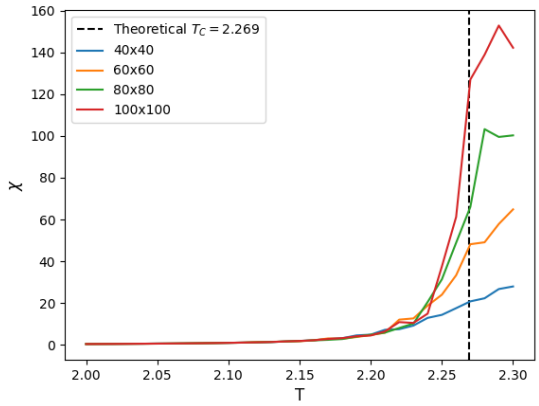

Figure 23. Magnetic susceptibility X as we pass through the critical point. Second order phase transition.

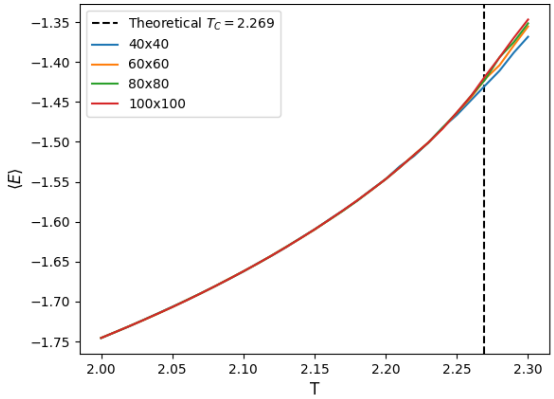

Figure 24. Energy $\langle E \rangle$ as we pass through the critical point. Second order phase transition.

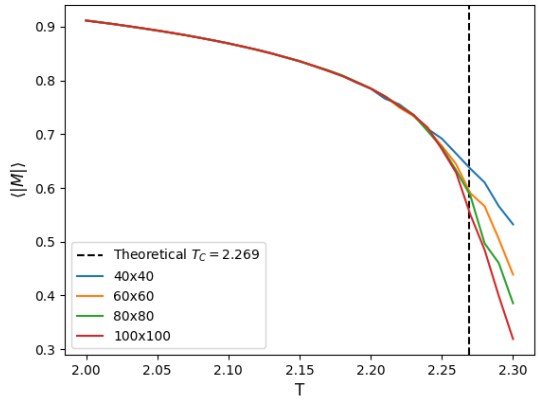

Figure 25. Magnetization $\langle |M| \rangle$ as we pass through the critical point. Second order phase transition.

V. DISCUSSION

Critical discussion of the most important results.

Benchmark results for the 2×2 lattice case are reproduced using our model. Analytical values are presented in table (V). For comparison, our model produces (with one million MC-cycles) table (I). The numbers are roughly equal. This is an important checkpoint for the validity of our results.

When calculating the magnetic susceptibility, we have used the alternative way as presented in appendix (A). The difference is that we are using $\langle M^2 \rangle - \langle |M| \rangle^2$ instead of $\langle M^2 \rangle - \langle M \rangle^2$. The theoretical expectation value for magnetization, $\langle M \rangle$ is zero, because there is an equal probability for the system to have a net magnetization of -1 or $+1$ per spin in the absence of an external magnetic field. In practise, when temperature is low, the system will converge to either -1 or $+1$, such that the mean magnetization differs from zero. Using absolute values instead, it does not matter if all spins are pointing up or down, and the total energy is the same because both states are ground states.

Looking at the low temperature case, $T = 1$. Figure (7) shows mean energy estimates. Fluctuations in energy levels from the ideal ground state value $\langle E \rangle = -2$ from the ground states are small, but also frequent. The reason there are some fluctuations is due to the structure of the Metropolis algorithm and the way we sample using Monte Carlo methods. As explained in the theory (II C), there is a likelihood of accepting a new spin-configuration even though the change in energy is positive. Figure (8) shows how often spin-flips are accepted under these conditions. Most of these accepted flips are due to the random number generated between 0 and 1 being less than or equal to the relative Boltzmann probability factor between two energy states. Figure (9) shows that the mean magnization estimates follows a similar behaviour as the mean energy, a clear tendency to remain in the ground state. When all spins are pointing in the same direction, magnetization per spin $|M| = 1$.

Figure (10) gives an idea of how fast the entire system changes energy when moving towards equilibrium. The macroscopic change is rapid. In general, we see that the system tends to reach equilibrium (energy minimum) fast when the temperature is well below the critical temperature. When we start off with an ordered spin configuration we are already at an energy minimum. All spins aligned is the ground state. Starting off at an unordered configuration, we still reach equilibrium with less

than 1000 Monte Carlo cycles. The equilibration time is short. Figure (11) illustrates this very well. When equilibrium is reached, the number of accepted spin-flips change rate rapidly. Before and after equilibrium, the relationship between accepted spin-flips and MC-cycles is linear, but the slope changes. This is an expected behaviour of the Metropolis algorithm, since spin-flips acceptance rate is associated with the probability of finding a new state with lower energy than the previous. Figure (12) shows how the model exhibits magnetic material properties like spontaneous magnetization. Spins interacting microscopically via their neighbours. As a result, the system changes from having a net magnetization of zero to non-zero (macroscopic change).

The differences between ordered and unordered initial states are less visible at higher temperatures. Shown by figures (13), (15), (16) and (18) for energy and magnetization at temperature $T = 2.4$. This is assumed to be above the critical temperature, which holds a theoretical value of $T_C \approx 2.269$. In both cases, the mean magnetization fluctuates around zero between $(-0.75, 0.75)$ (high variance). The mean energy seems to fluctuate around $\langle E \rangle = 1.25$. If the spins where truly random without any correlation, the energy expectation value is zero, but that would require temperatures $T >> 1$. Still it is clear that the model does not exhibit spontaneous magnetization at temperatures above the critical one, which is important because we have used this model to determine where phase transitions take place in order to estimate the critical temperature. Figure (14) and (17) shows that the acceptance rate of spin-flips remains the same at $T = 2.4$ regardless of initial spin conditions. We could have simulated the system with more MC-cycles, but saw no need as there were no indication of moving towards any steady state (unlike the examples with $T = 1$, where it is quite clear).

Figure (19), (1) and (21) shows the probability distribution $P(E)$ for different energies E. In these calculations, we have wasted 10% of the MC-cycles. Table (II) shows energy variances at different temperatures. Above the critical temperature, energy variance is largely increased. Spins are more randomly distributed. We have compared our probability distributions with the Normal distribution (PDF) f, which is given by

$$f(E) = \frac{1}{\sigma_E \sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{E-\langle E \rangle}{\sigma_E}\right)^2},$$

and assumes real valued random numbers. At $T = 1$ and $T = 1.5$, this comparison shows that the spins are correlated in a large degree since the probability distributions do not align well. At $T = 2.4$, there is a clearly a more random trend between spins, but the system is still biased in favour of having a non-zero, negative energy. We know that spontaneous magnetization does not occur above the critical temperature. Looking at the probability distribution (21) this is evident. The most likely value is roughly $E = -500J$, which correspond to $\langle E \rangle \approx 1.25$ per spin. The probability of finding the system with energy $E = -800$, at which $\langle E \rangle = -2.0$ per spin, is close to zero.

As explained in the theory section (II B), the Ising model exhibits a second order phase transition which we can identify by looking at the behaviour of thermodynamic quantities around the critical temperature. Figure (22), (24), (23) and (25) shows that the Ising model undergoes a phase transition roughly around $T = 2.27$, shown in table (III) to be our best estimate for T_C. The energy is continuous. The mean magnetization drops off towards zero, the heat capacity and magnetic susceptibility peeks around at the critical point. Comparing the heat capacity plot (22) with the expected behaviour from similar research (4). These are all expected behaviours of the Ising model. We see that an increased lattice size approximates the theoretical behaviour of divergence and critical temperature better. Simulating the system for large lattices takes long time to conduct, and therefore we have used a reasonable sized lattice of 100×100, which is enough to clearly see where the phase transitions take place. To make the curve as smooth as possible within reasonable limits, we have used temperature steps of $dT = 0.01$ and one million MC-cycles for each temperature. The relative error between the theoretical value and our best estimate for T_C is

$$\frac{2.27 - 2.269}{2.269} \approx 4.41 \cdot 10^{-4},$$

which is a good indication that the two dimensional Ising model are able to predict critical temperatures and phase transitions with high accuracy in magnetic systems.

VI. CONCLUSION

Using the two dimensional Ising model, we have been successful in modelling magnetic materials as they undergo second order (continuous) phase transitions. We have studied the mean values of energy and magnetization, as well as heat capacity and magnetic susceptibility for a $L \times L$ quadratic lattice system consisting of $N = L^2$ spins. We have studied how these parameters change when the system undergoes a phase transition. Our model can accurately predict the critical temperature value. The theoretical value of the critical temperature is given by (4) as $T_C \approx 2.269$. Our best estimate, using a 100×100 lattice, is $T_C = 2.27$. For these calculations, we have used temperature steps of $dT = 0.01$ over an interval $T \in [2.0, 2.3]$. One million Monte Carlo samples

at each step. The critical temperature is based on the point at which heat capacity is maximum, using figure (22).

When temperature is well below the critical value, the system quickly converges towards equilibrium, and tends to stay there. There are minor fluctuations away from the ground state due to the structure of the Metropolis algorithm. This is illustrated well in figure (12). At temperature above the critical value, the Ising model exhibits loss of spontaneous magnetization, shown in figure (15). The energy distribution at temperature $T = 2.4$ compares well to the Normal distribution, shown by figure (21). Energy variance increases rapidly as $T \to T_C$, shown in table (II). This corresponds well to the fact that heat capacity increases rapidly at the critical temperature.

Possible improvements could be to obtain more precise results. Even though we are able to clearly predict where phase transitions take place and estimate accurately the critical temperature, our model is not without flaws. Simulation of large lattices with adequate number of Monte Carlo samples take long time to conduct. Even with an temperature step of $dT = 0.01$, our plots during the critical phase are choppy. Ideally, we would also like to have more than one million Monte Carlo cycles at each step.

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Appendix A: Canonical Ensemble

Introducing the Boltzmann statistics used for calculating quantities in the canonical ensemble [2]. These are the partition function, expectation (mean, average) values for energy and magnetization, and thermodynamic quantities like heat capacity and magnetic susceptibility.

In the canonical ensemble temperature T is an intensive variable (independent of our systems size). Assuming we have a system in equilibrium with the environment. All microstates of the system are accessible. The system we are looking at can exchange heat with the environment, but not particles. Temperature is determined by the environment. Internal energy may therefore vary, but the number of particles N is held fixed. Volume V is also held fixed. The thermodynamic parameters are: (N, V, T). Internal energy E is an extensive variable which depends on the temperature T, and follows as an expectation value $\langle E \rangle$. Helmholtz free energy, F, functions as our potential. In order to calculate expectation values we use the Boltzmann probability distribution.

The Boltzmann probability distribution is given by

$$P_i(\beta) = \frac{1}{Z} e^{-\beta E_i}, \tag{A1}$$

where $\beta = (kT)^{-1}$ is an inverse function of temperature T and k is the Boltzmann constant. E_i is the internal energy of the system for a given microstate i, and Z is the partition function. The factor

$$e^{-\beta E_i},$$

is called the Boltzmann factor. The partition function Z is given as the sum over all the Boltzmann factors of the system

$$Z = \sum_{i=1}^{m} e^{-\beta E_i}, \tag{A2}$$

where m equals the number of possible microstates. The probabilities given by the Boltzmann distribution (A1) are normalized by the partition function. The Helmholtz free energy potential, F, is then given by

$$F = -kTlnZ = \langle E \rangle - TS, \tag{A3}$$

with k being Boltzmann constant, and S being entropy. Entropy increases as more microstates become accessible (larger degree of disorder), which is maximized in equilibrium. Therefore F is minimized in equilibrium.

When we know the partition function, we can calculate the mean (expectation) values for energy and magnetization (magnetic momentum),

$$\langle E \rangle = \sum_{i=1}^{m} E_i P_i(\beta) = \frac{1}{Z} \sum_{i=1}^{m} E_i e^{-\beta E_i}, \tag{A4}$$

and

$$\langle M \rangle = \sum_{i=1}^{m} M_i P_i(\beta) = \frac{1}{Z} \sum_{i=1}^{m} M_i e^{-\beta E_i}, \tag{A5}$$

where E_i is given by equation (1) and M_i is given by equation (2), explained in the introduction of this report. E_i and M_i are energy and magnetization for a given microstate i.

The variance σ_E^2 corresponding to the mean energy $\langle E \rangle$ is given as

$$\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2, \tag{A6}$$

$$\sigma_E^2 = \frac{1}{Z} \sum_{i=1}^{m} E_i^2 e^{-\beta E_i} - \left(\frac{1}{Z} \sum_{i=1}^{m} E_i e^{-\beta E_i} \right)^2.$$

Similarly, the variance σ_M^2 corresponding to the mean magnetization $\langle M \rangle$ is given by

$$\sigma_M^2 = \langle M^2 \rangle - \langle M \rangle^2, \tag{A7}$$

$$\sigma_M^2 = \frac{1}{Z} \sum_{i=1}^{m} M_i^2 e^{-\beta E_i} - \left(\frac{1}{Z} \sum_{i=1}^{m} M_i e^{-\beta E_i} \right)^2.$$

The variances are used to calculate the thermodynamic quantities like heat capacity C_V and magnetic susceptibility X, through the following relations

$$C_V = \frac{\sigma_E^2}{kT^2}, \tag{A8}$$

and

$$X = \frac{\sigma_M^2}{kT}. \tag{A9}$$

Another useful quantity is the mean absolute value of the magnetization, which is given as

$$\langle |M| \rangle = \sum_{i=1}^{m} |M_i| P_i(\beta) = \frac{1}{Z} \sum_{i=1}^{m} |M_i| e^{-\beta E_i}. \quad \text{(A10)}$$

These equations can be applied to any given two dimensional $L \times L$ lattice using the Ising model for magnetic systems. L defines the number of spins in each dimension.

Appendix B: Benchmark results

Benchmark calculations and analytical results for comparing with numerical results are presented in this appendix.

1. Analytical expressions for the 2×2 lattice.

In the simple 2×2 lattice case, we have $L = 2$ spins in each dimensions and a total number of $N = 4$ spins. If there are only two possibilities for the spin orientation (up or down), there are $2^N = 2^4 = 16$ possible microstates, that is $m = 16$. Applying the equations obtained from appendix (A), we can obtain analytical expressions and use these to validate our numerical implementation.

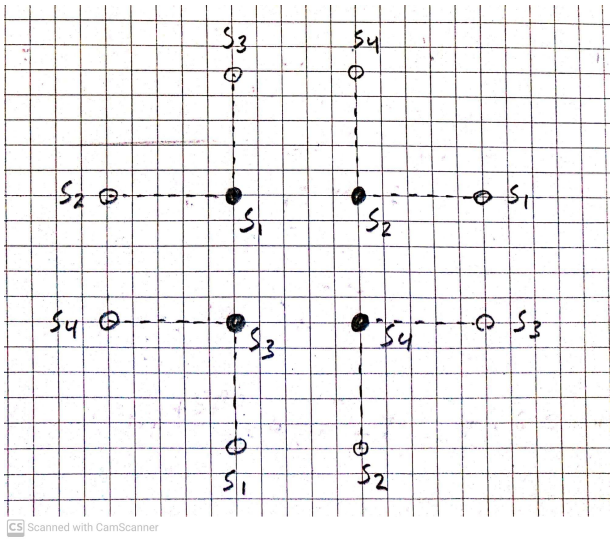

Figure 26. 2×2 lattice, four spins s_1, s_2, s_3, s_4 which in a binary system could be either up or down. Using periodic boundary conditions.

When we calculate energies in any $L \times L$ lattice case, such as this, we will use periodic boundary conditions (PBC). Generally we make an approximation which is that the lattice is infinitely large. When L is large, this approximation is good, but for the 2×2 case we have to make sure we don't double count the energy contributions between each spin when applying periodic boundary conditions. Figure (26) shows how we implement periodic boundary conditions in the 2×2 case. We then apply equation (1) and (2) to calculate energy and magnetization respectively for a given microstate i. Calculating magnetization is straight forward. Energies are calculated by going through the lattice spins and adding up the neighbour-interactions:

$$E_i = -J(s_1 s_2 + s_1 s_3 + s_2 s_1 + s_2 s_4 + s_3 s_4 + s_3 s_1 + s_4 s_3 + s_4 s_2).$$

To avoid double counting interactions, we move to the right in each row and look at the neighbours upwards and leftwards as we move on. The results are shown in table (IV). Each macrostate (spin up) has some multiplicity which correspond to the number of microstates that have this configuration. For example, there is only one macrostate where all the spins are pointing up ($\uparrow\uparrow\uparrow\uparrow$), therefore this macrostate has multiplicity one. This macrostate and the opposite where all spins are pointing down, have energy equal to $-8J$, where $J > 0$ for ferromagnetic materials (J is a constant). Most of the other macrostates have energy equal to zero, expect for those who have the specific ordering $\uparrow\downarrow\downarrow\uparrow$ or $\downarrow\uparrow\uparrow\downarrow$. These macrostates have energy equal to $8J$.

Table IV. Macrostates for the 2×2 lattice.

Spin up $\uparrow$	Multiplicity	E_i	M_i
4	1	$-8J$	4
3	4	0	2
2	4	0	0
2	2	$8J$	0
1	4	0	-2
0	1	$-8J$	-4

The first quantity of interest for this system is the partition function. Using equation (A2), we find

$$Z = \sum_{i=1}^{16} e^{-\beta E_i} = 2e^{-8\beta J} + 2e^{8\beta J} + 12e^0,$$

$$Z = 2e^{-8\beta J} + 2e^{8\beta J} + 12 = 4cosh(8\beta J) + 12.$$

Where we have used that $2cosh(x) = e^x + e^{-x}$. Using equation (A4), we can calculate the mean energy of the 2×2 lattice system

$$\langle E \rangle = \frac{1}{Z} \sum_{i=1}^{16} E_i e^{-\beta E_i},$$

$$\langle E \rangle = \frac{1}{Z}\left(2 \cdot (-8J)e^{8\beta J} + 2 \cdot 8Je^{-8\beta J} + 12 \cdot 0\right),$$

$$\langle E \rangle = \frac{16J}{Z}\left(e^{-8\beta J} - e^{8\beta J}\right) = \frac{32J}{Z} sinh(-8\beta J).$$

Where we have used that $2sinh(-x) = -(e^x - e^{-x})$. We also need the average value of the squared energy to calculate heat capacity, this is

$$\langle E^2 \rangle = \frac{1}{Z}\sum_{i=1}^{16} E_i^2 e^{-\beta E_i},$$

$$\langle E^2 \rangle = \frac{1}{Z}(2 \cdot (-8J)^2 e^{8\beta J} + 2 \cdot (8J)^2 e^{-8\beta J}),$$

$$\langle E^2 \rangle = \frac{128J^2}{Z}(e^{8\beta J} + e^{-8\beta J}) = \frac{256J^2}{Z} cosh(8\beta J).$$

The variance σ_E^2 of the mean value for energy is given by equation (A6) and is used to calculate the heat capacity C_V by equation (A8).

The mean value of magnetization is calculated by equation (A5)

$$\langle M \rangle = \frac{1}{Z}\sum_{i=1}^{16} M_i e^{-\beta E_i},$$

$$\langle M \rangle = \frac{1}{Z}(4e^{8\beta J} + 4 \cdot 2e^0 + 6 \cdot 0 + 4 \cdot (-2)e^0 - 4e^{8\beta J}),$$

$$\langle M \rangle = \frac{1}{Z}(4e^{8\beta J} + 8 - 8 - 4e^{8\beta J}) = 0.$$

The mean magnetization is zero. This is expected for a quadratic lattice where the spins can be ± 1 randomly. Most microstates have a net magnetization of zero, and the other microstates have anti-symmetric magnetization. The mean absolute value for magnetization is calculated by equation (A10)

$$\langle |M| \rangle = \frac{1}{Z}\sum_{i=1}^{16} |M_i| e^{-\beta E_i},$$

$$\langle |M| \rangle = \frac{1}{Z}(2 \cdot 4e^{8\beta J} + 8 \cdot 2e^0 + 6 \cdot 0),$$

$$\langle |M| \rangle = \frac{1}{Z}(8e^{8\beta J} + 16) = \frac{8}{Z}(e^{8\beta J} + 2).$$

We need the average value of the squared magnetization to calculate magnetic susceptibility, this is given by

$$\langle M^2 \rangle = \frac{1}{Z}\sum_{i=1}^{16} M_i^2 e^{-8\beta J},$$

$$\langle M^2 \rangle = \frac{1}{Z}(2 \cdot 4^2 e^{8\beta J} + 8 \cdot 2^2 e^0 + 6 \cdot 0),$$

$$\langle M^2 \rangle = \frac{32}{Z}(e^{8\beta J} + 1).$$

The variance σ_M^2 of the mean value for magnetization is given by equation (A7) and is used to calculate magnetic susceptibility X by equation (A9). Alternatively one could use the absolute value of magnetization to calculate magnetic susceptibility. To distinguish, we use a different notation for this version of magnetic susceptibility: X_{alt}, which is then given by

$$X_{alt} = \frac{1}{kT}(\langle M^2 \rangle - \langle |M| \rangle^2).$$

These formulas are evaluated in the low temperature case $T = 1$ using natural units $k = 1$ in the program example shown below. The results are shown in table (V) and will serve as benchmark results for validation.

```
# Simple program for the 2x2 lattice.
# Calculating expectation values and thermodynamic quantities
# using analytical expressions.

import numpy as np

J = 1             # Magnetic material constant.
k = 1             # Boltzmann constant.
T = 1             # Temperature.
B = 1/(k*T)       # Beta.

# Partition function Z.
Z = 4*np.cosh(8*B*J) + 12

# Mean energy <E>.
E = 32*J/Z * np.sinh(-8*B*J)

# Mean square energy <E^2>.
E2 = 256*J**2/Z * np.cosh(8*B*J)

# Energy variance sigma_E^2.
E_var = E2 - E**2

# Heat capacity Cv.
Cv = E_var/(k*T**2)

# Mean magnetization <M>.
M = 0

# Mean abs magnetization <|M|>.
M_abs = 8/Z * (np.exp(8*B*J) + 2)
```

```
# Mean square magnetization <M^2>.
M2 = 32/Z * (np.exp(8*B*J) + 1)

# Magnetization variance sigma_M^2.
M_var = M2 - M**2

# Magnetic susceptibility X.
X = M_var/(k*T)

# Alternative way, magnetic susceptibility:
M_var_alt = M2 - M_abs*M_abs
X_alt = M_var_alt/(k*T)
```

Table V. Expectation values and thermodynamic quantities for the 2×2 lattice. Using $\beta = 1$ and $J = 1$.

Quantity	**Symbol**	**Value**
Partition function	Z	$5.97 \cdot 10^3$
Energy expectation	$\langle E \rangle$	-7.98
Energy squared expectation	$\langle E^2 \rangle$	63.9
Energy variance	σ_E^2	0.128
Heat capacity	C_V	0.128
Magnetization expectation	$\langle M \rangle$	0
Magnetization squared expectation	$\langle M^2 \rangle$	16
Magnetization absolute value expectation	$\langle \lvert M \rvert \rangle$	3.99
Magnetization variance	σ_M^2	16
Magnetic susceptibility	X	16
Magnetic susceptibility	X_{alt}	0.016

Appendix C: Metropolis Algorithm example

Example of how the Metropolis algorithm can be implemented. In this program, we simulate the system in order to find a steady state (ground state) with minimum energy, calculating the mean energy on the way and returning the final state.

```
# Ising Model for LxL lattice.
# Using periodic boundary conditions.

import numpy as np
import random

L = 4            # Number of spins in each dimension.
J = 1            # Magnetic material constant.
k = 1            # Boltzmann constant.
T = 1            # Temperature.
N = L*L          # Number of spins in LxL lattice.
beta = 1/(k*T)   # Dimension constant for Boltzmann factors.
MCS  = int(1e5)  # Monte Carlo Samples.

# Initial microstate: All spins pointing up, ground state:
lattice_0 = np.ones((L,L))   # LxL lattice with N = LxL spins.

# You can also initiate with random spins:
# lattice_0 = [[-1,1,1,1],[1,-1,-1,1],[-1,1,1,1],[-1,1,-1,-1]]

def PBC(k,limit,add):
    # Periodic boundary conditions.
    return (k + limit + add) % limit     # Indexing.

def energy(lattice):
    # Calculating energy for a given microstate in the lattice.
    energy = 0
    for i in range(L):
        for j in range(L):
            Eij = -J*(lattice[i][j]*(lattice[PBC(i,L,-1)][j] + lattice[i][PBC(j,L,-1)]))
            energy = energy + Eij
    return energy

def metropolis(MCS, lattice):
    # Metropolis algorithm, using Monte Carlo sampling.
    E = energy(lattice)
    for i in range(MCS):      # Monte Carlo cycles.
        for j in range(L):
            for k in range(L):
                r1 = random.uniform(0,1)         # Random float between 0 and 1.
                r2 = random.randint(0,L-1)       # Random integer between 0 and L-1.
                r3 = random.randint(0,L-1)       # Random integer between 0 and L-1.
                Ei = energy(lattice)             # Initial energy.
                lattice[r2][r3] = lattice[r2][r3]*(-1)   # Flip spin, random index.
                Ej = energy(lattice)             # New energy.
                dE = Ej - Ei                     # Energy difference.
                if dE <= 0:
                    E = E + dE            # Accept new configuration.
                else:
                    w = np.exp(-beta*dE)  # Relative probability, Boltzmann factor.
                    if r1 <= w:
                        E = E + dE        # Accept new configuration.
                    else:
                        # Deny new configuration, flip spin back.
                        lattice[r2][r3] = lattice[r2][r3]*(-1)
                        E = E + Ei
    return E, lattice

E, lattice = metropolis(MCS, lattice_0)
E_mean = E/MCS/N
```