Numerical studies of phase transitions in magnetic systems using an Ising model

Astrid Bragstad Gjelsvik and Erlend Andreas Longva*
Department of Physics, University of Oslo, P.O. Box 1048 Blindern, N-0316 Oslo, Norway

In this project we implement Monte Carlo simulations using the Metropolis algorithm to study a 2D Ising model. The project studies the energy probability distributions for $T = 1$ and $T = 2.4$, the behavior of the model around the phase transition, and finds an estimated critical temperature. We derive analytical solutions for a small 2×2 lattice which we use to test the numerical model. For a 20×20 lattice the Monte Carlo cycles needed to reach a steady state is found to be $\approx 10^5$. The simulations of the phase transition clearly reproduces the expected behavior. The value of the critical temperature is found using the obtained data for magnetic susceptibility yielding an estimated $T_C \approx 2.265$.

I. INTRODUCTION

For a long time in human history the phenomenon of magnetism was something inexplicable and magical. The compass is believed to have been discovered by ancient Chinese mystics who observed that their lodestone fortune-telling tables tended to align themselves in the same direction. Developments in statistical mechanics at the end of the 19th century and the birth of quantum mechanics enabled physicists to build more accurate models of magnetic materials. In 1920, Wilhem Lenz invented a model for ferromagnetic materials. The model was then solved by his student Ernst Ising in one dimension in 1924, hence, it is known as the Ising model. In 1944 the model was solved analytically in two dimensions by Lars Onsager[2], who managed to extract an analytical value for the critical temperature where the phase transition occurs. The 3D Ising model is yet to be solved analytically.

The aim of this project is to numerically implement and test the 2D Ising model. We will simulate its behavior using the Metropolis algorithm. The main goal is then to get familiar with Monte Carlo simulations, find an estimate of how many cycles is needed to reach a steady state for the model, and to learn more about parallel programming by implementing it in our method. By doing this we hope to achieve estimates of the behavior of the model around the phase transition. The hope is then to observe the spontaneous magnetisation that Ising developed the model to show. The main result will therefore be our estimate of the critical temperature T_C.

The content that follows is a presentation of the methods and theory we have used in the section "Method", followed by a presentation of our results in "Results". After this we discuss our findings in "Discussion", and finally conclude with a consideration of further prospects.

* astridbg@student.matnat.uio.no
e.a.longva@fys.uio.no

II. METHOD

In this section we begin by introducing the two-dimensional Ising model. We illustrate how the expected energy, the expected magnetisation, the heat capacity and the magnetic susceptibility of the model can be calculated analytically using periodic boundaries, and find these expressions for the case of a 2×2 lattice. Moving on, we present how the Metropolis algorithm can be implemented in order to estimate these properties numerically. We present crucial ways to ensure algorithm efficiency, including both pre-calculation of transition probabilites and implementation of periodic boundary condition. Finally, we present how we can study phase transitions of the model and estimate the critical temperature in the thermodynamic limit.

For all program code, tests runs, output files and plots obtained see our GitHub-repository.

A. Two-Dimensional Ising Model

The two dimensional Ising model in its simplest form models the behavior of binary elements in a regular and periodic two dimensional lattice. In our case the elements are spins having either spin up or down corresponding to $s = \pm 1$. The energy of the Ising model can then be expressed as:

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

where J is the interaction strength between neighboring spins and N is the total number of spins. Writing $\langle kl \rangle$ means that we take the sum over all neighboring lattice sites for each lattice site, in other words we sum over all spins interactions which contribute to the total energy. This means that each interaction, or product $s_k s_l$, should only be counted once.

1. *Analytical* 2×2 *lattice expressions*

We first study the simple case of a 2×2 lattice analytically in order to have exact expressions to compare with our numerical simulations. All the microstates of the system are presented in table II in Appendix A. From these we find the analytical Boltzmann distribution and expectation values for energy $\langle E \rangle$, and absolute value of magnetic moment $\langle |M| \rangle$, as well as heat capacity C_V, and magnetic susceptibility χ.

The Boltzmann distribution $P_i(\beta) = e^{-\beta E_i}/Z$ gives the probability of being in a specific energy state E_i given the $\beta = 1/k_B T$ of the system (k_B being the Boltzmann constant and T being the temperature). The partition function Z is the normalization constant of the distribution, and is defined as

$$Z = \sum_{i=1}^{n} e^{-\beta E_i} \tag{2}$$

where n is the total number of possible microstates (here $n = 2^4 = 16$). We use periodic boundary conditions, meaning that where a spin is situated on the edge of the lattice, we allow an energy contribution from the corresponding spin on the other side of the lattice. From considering the possible energy states for our 2×2 lattice case in table II, we get

$$\begin{aligned} Z &= \sum_{i=1}^{16} e^{-\beta E_i} && (3)\\ &= 2e^{-\beta \cdot 8J} + 12e^{-\beta \cdot 0} + 2e^{-\beta \cdot (-8J)} && (4)\\ &= 12 + 2(e^{8J\beta} + e^{-8J\beta}) && (5)\\ &= 12 + 2(2\cosh(8J\beta)) && (6)\\ &= 12 + 4\cosh(8J\beta) && (7) \end{aligned}$$

We calculate our expectation values, heat capacity and magnetic susceptibility in the following way:

$$\begin{aligned} \langle E \rangle &= \frac{1}{Z} \sum_{i=1}^{n} E_i e^{-\beta E_i} && (8)\\ \langle |M| \rangle &= \frac{1}{Z} \sum_{i=1}^{n} |M_i| e^{-\beta E_i} && (9)\\ C_V &= \frac{\sigma_E^2}{k_B T^2} = \frac{1}{k_b T^2} \left(\langle E^2 \rangle - \langle E \rangle^2 \right) && (10)\\ \chi &= \frac{\sigma_M^2}{k_B T} = \frac{1}{k_b T} \left(\langle M^2 \rangle - \langle |M| \rangle^2 \right) && (11) \end{aligned}$$

When calculating expected energy and heat capacity, we can simply make use of the fact that $\langle E \rangle = -\frac{1}{Z}\frac{\partial Z}{\partial \beta}$ and $\langle E^2 \rangle = \frac{1}{Z}\frac{\partial^2 Z}{\partial \beta^2}$. This gives us

$$\begin{aligned} \langle E \rangle &= -\frac{1}{Z}\frac{\partial}{\partial \beta}(12 + 4\cosh(8J\beta)) && (12)\\ &= -\frac{1}{Z}(32J\sinh(8J\beta)) && (13)\\ \langle E^2 \rangle &= \frac{1}{Z}\frac{\partial^2}{\partial \beta^2}(12 + 4\cosh(8J\beta)) && (14)\\ &= \frac{1}{Z}\left(256J^2\cosh(8J\beta)\right) && (15) \end{aligned}$$

We can then find variance of the energy (for full calculation, see appendix section A 2) as

$$\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2 = \frac{1}{Z^2}\left(1024J^2(1 + \cosh(8J\beta))\right) \tag{16}$$

The full calculations for the expectation value for absolute magnetic moment and corresponding variance can be found in appendix section A 3. This gives us

$$\begin{aligned} \langle |M| \rangle &= \frac{1}{Z}\left(16 + 8e^{8J\beta}\right) && (17)\\ \sigma_M^2 &= \frac{1}{Z^2}\left(64(3 + e^{-8J\beta} + 3e^{8J\beta})\right) && (18) \end{aligned}$$

We can thereby find our calculations of heat capacity and magnetic susceptibility as

$$\begin{aligned} C_V &= \frac{1}{k_B T^2}\frac{1024J^2(1 + \cosh(8J\beta))}{Z^2} && (19)\\ \chi &= \frac{1}{k_B T}\frac{64(3 + e^{-8J\beta} + 3e^{8J\beta})}{Z^2} && (20) \end{aligned}$$

These analytical results will help us test our 2D Ising model implementation. The method we use to test our numerical model is to see if it reproduces the analytical ones for the 2×2 lattice. More specifically we will compare the variance of the mean magnetisation and the variance of the expectation value of energy. We do this by comparing the relative error between the numerical values and the analytical ones derived here.

B. Metropolis algorithm

The Ising model is implemented numerically using a matrix of size $L \times L$ filled with ± 1 corresponding to spins up or spins down. We consider both cases where the spins can be distributed randomly, and initialized in an ordered way (all spins up or all spins down). We use equation (1) with periodic boundary conditions to calculate the energy of the system. Instead of determining the thermodynamical properties using the partition function, we now allow the system to fluctuate in a certain way that allows us to extract the properties we are interested in. This is what we call the Metropolis algorithm. The Metropolis algorithm is a Markov chain Monte Carlo

method. The general idea is that we allow the system to evolve by performing random fluctuations in the energy state that are more or less likely to occur depending on the given temperature.

1. Transition probabilities

When performing the fluctuations, we can consider individual spins in the lattice and find the energy change associated with flipping it. The change in energy for one spin flip will then be equal to

$$\Delta E = 2Js_l^1 \sum_{\langle k \rangle}^{N} s_k \tag{21}$$

where s_l^1 corresponds to the spin of the flipped spin and $\sum_{\langle k \rangle}^{N} s_k$ is the sum over he nearest neighbors of the flipped spin. By the periodic boundary conditions, each spin will effectively have four neighboring spins. This means that we know all the five possible changes in energy we can have if we flip a spin, since there are five possible configurations for the four neighboring spins (all up, one down, two down, three down and all down). This corresponds to the five possible values for energy differences $\Delta E = -4J, -2J, 0, 2J$ and $4J$, using equation (21).

A given energy change should be more or less probable depending on the temperature of the system. For each energy change ΔE we have a transition probability, given by the Boltzmann factor $w = e^{-\beta \Delta E}$. We would like to accept a spin flip if it reduces the energy of the system, $\Delta E < 0$, giving a transition probability $w > 1$. However, in order for the system to end up in the equilibrium state given by the temperature, and not simply the lowest energy state, we would also like to accept some energy changes that could increase the energy. We implement the algorithm so that a positive energy change can occur if a generated random number is lower than the transition probability $w = e^{-\beta \Delta E}$.

Computing the transition probability for each spin is computationally expensive. However, since there are only five possible energy changes in each spin flip, there will be only five possible transition probabilities to be considered. Therefore, we can compute these in advance. We can also make use of the fact that the energy changes are all integer numbers. These can therefore be used as indices in an array containing all transition probabilities.

If the generated random number is lower than the transition probability, we add the energy change to the energy. We also change the absolute magnetisation by adding

$$\Delta |M| = 2s_l^2 \tag{22}$$

where s_l^2 is the spin after the flip. An implementation of this can be found below in section II B 3.

2. Periodic boundary conditions

We want to encode periodic boundary conditions in such a way that if we consider a spin at the edge of the lattice, the neighbouring spin should become the spin at the other side of the lattice. A way to encode this is to index our neighboring spins using a function that returns the remainder of the index with respect to the lattice dimension. This is known as a modulo operation. If the number we try to index our spin with is larger than the lattice dimension, the function returns the integer we get if we divide the number by the lattice size. In other words, we get the index of the spin on the other side of the lattice. The function can be implemented as

```
PB(index, limit, add)
{return (index+limit+add) % (limit);}
```

where the `PB`-function takes as argument the index of the spin we are considering, the lattice size `limit` and the index difference `add` of the neighboring spin we want to consider (± 1). The functions returns the remainder from the modulo operation.

3. Metropolis algorithm implementation

The Metropolis algorithm itself can be implemented as a loop over a certain number of Monte Carlo cycles with a loop over the whole lattice for each Monte Carlo cycle. The following is an example of an implementation:

```
for (cycles=1; cycles<=MCcycles; cycles++):
  for (Spins=0; Spins<AllSpins; Spins++):
    ix = (int) RandomNumber*NSpins;
    iy = (int) RandomNumber*NSpins;
    dE = (int) 2*SpinMatrix(ix,iy)*
        (SpinMatrix(ix,PB(iy,NSpins,-1))+
        SpinMatrix(PB(ix,NSpins,-1),iy) +
        SpinMatrix(ix,PB(iy,NSpins,1)) +
        SpinMatrix(PB(ix,NSpins,1),iy));
    if (RandomNumber <= BoltzmannFactor(dE+8)):
        SpinMatrix(ix,iy) *= -1.0;
        MagneticMoment += 2.0*SpinMatrix(ix,iy);
        Energy += dE;
```

For each lattice "sweep" we consider a random spin situated in the lattice (here represented as `SpinMatrix`) and find the energy change `dE` if we were to flip it. We use the periodic boundary condition function `PB` from section II B 2 to ensure periodic boundary conditions. We have a pre-calculated array `BoltzmannFactor` where the index given by the `dE+8` corresponds to the transition probability. Each `RandomNumber` corresponds to a new generated random number between 0 and 1. We use the Mersenne Twister pseudo-random generator in our program. If a transition is accepted, the total `MagneticMoment` and `Energy` of the model is updated according to equations (22) and (21) respectively. This code implementation is built on the work of Morten Hjort-Jensen [1].

4. Extracting thermodynamical properties

To simulate our Ising model we use the Metropolis algorithm, and run it for a number of Monte Carlo cycles. After a certain number of Monte Carlo cycles, the system reaches an approximate thermal equilibrium where the microstates have the same expectation values. We therefore want to run a certain number of "burn-in" cycles, and start extracting thermodynamical properties *after* we have reached steady state. In order to find the required number of cycles we should run before we start extracting properties, we first find how the expectation values evolve as a function of Monte Carlo cycles. After finding this value, we run consequently run this number of cycles before we start extracting other thermodynamical properties.

C. Phase transitions

The Ising model undergoes a phase transition at the critical temperature T_C. Physically this means that the system we study rapidly changes its observable quantities around this temperature. In our case, this represents the spontaneous magnetisation of a ferromagnetic material. For the two dimensional Ising model we have the following relations:

$$\langle M(T)\rangle \sim (T - T_C)^{\beta} \tag{23}$$

$$C_V(T) \sim |T_C - T|^{-\alpha} \tag{24}$$

$$\chi(T) \sim |T_C - T|^{-\gamma} \tag{25}$$

where $\langle M\rangle$ is the mean magnetisation, $C_V(T)$ is the specific heat capacity at constant volume and $\chi(T)$ is the magnetic susceptibility. The exponents β, α and γ are the critical exponents. In our case the values of these are: $\beta = 1/8$, $\alpha = 0$ and $\gamma = 7/4$. Additionally we have the relation:

$$\xi(T) \sim |T_C - T|^{-\nu} \tag{26}$$

describing the correlation length ξ which is a measure of how correlated the spins in our system are. This quantity measures the areas of spins having the same orientation, in terms of the maximum length of such areas. When $T \gg T_C$, ξ is expected to be of the order of the lattice spacing, since mostly all spins will be uniformly and randomly oriented. However, when $T \to T_C$ we expect ξ to go towards the length of the entire lattice because of the spontaneous magnetisation.

The phase transitions we study are second-order phase transitions. The analytical result for the critical temperature T_C derived by Lars Onsager [2] for an infinite lattice is $k_B T_C/J = 2/\ln 1 + \sqrt{2} \simeq 2.269$ with $\nu = 1$. Since we are restricted to finite-size lattices we need to relate our results to the infinite lattice to be able to compare our results with Onsager's analytical result. This can be done using a finite-size scaling relation for the critical temperature:

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu} \tag{27}$$

where a is a constant, L is the dimension of our lattice, and ν is the critical exponent of the correlation length ξ, found in equation (26). Using this we may rewrite all relations to approximate the infinite lattice.

$$\langle M(T)\rangle \sim (T - T_C)^{\beta} \to L^{-\beta/\nu} \tag{28}$$

$$C_V(T) \sim |T_C - T|^{-\alpha} \to L^{\alpha/\nu} \tag{29}$$

$$\chi(T) \sim |T_C - T|^{-\gamma} \to L^{\gamma/\nu} \tag{30}$$

We simulate the phase transitions simply by running our numerical models for temperatures in the expected phase transition temperature region. This region is about $T = 2.269 \pm 2$. We expect to get the best results by running simulations for bigger lattice sizes and so the sizes $L = 40, 60, 80, 100$, where L is the lattice dimension, will be used. Using this method we simulate the expectation value of energy, mean magnetisation, heat capacity and magnetic susceptibility as functions of temperature. The simulations were produced by parallel computing using the `MPI` library for `C++`. Additional optimisation was obtained by using the `-O3` flag. To check the speed up we get from parallelisation we time some selected runs using 1, 2, and 4 processor cores.

After having found these functions we will then use the results for the magnetic susceptibility to carve out our numerical estimate of the critical temperature T_C. We expect it to be sharply peaked at the point of the cirtical temperature. To do this the susceptibility data for the different lattice sizes is interpolated around the peak, using the function `CubicSpline` from the `SciPy` package, and the maxima of each lattice size is extracted. The temperatures at each of these maxima is then used in a linear fit. Here, we have using the `polyfit` from the `NumPy` package. Using the infinite lattice approximation (27) we then find the critical temperature estimate from the constant term in the linear fit.

III. RESULTS

In this section we present our main findings. We begin by comparing how our model performs compared to analytical expressions. We move on to presenting how our model reaches equilibrium, and our estimates for the time (expressed by Monte Carlo cycles) this process takes for different temperatures and initial states. Thereafter we present the probability distributions of the energy of the Ising model for two different temperatures, with corresponding variances. Moreover we present our studies of phase transitions, and finally our estimates for the critical temperature in the thermodynamic limit.

A. Comparing numerical and analytical results

We have tested our Ising model implementation by comparing the numerical results for a 2×2 lattice with the analytical results derived in II A. The initial state of the system was ordered with every spin oriented in the same direction. We compared the numerical and analytical variance σ^2 for the energy E and absolute magnetisation $|M|$ and computed the relative error. We found that the relative error approaches 0 at approximately 10^4 Monte Carlo cycles. Here the system was not prepared with any burn in cycles.

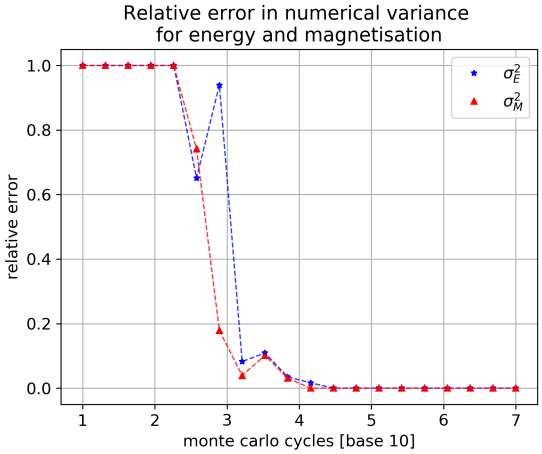

Figure 1. Relative error between the analytical and numerical variance for energy and magnetisation for increasing number of Monte Carlo cycles. Here we have used $T = 1$, $J = 1$, $k_b = 1$. The dimensions of the lattice are 2×2.

B. Estimate of burn-in cycles

We calculated the expectation values of energy and magnetisation as a function of Monte Carlo cycles for a 20×20 lattice. The simulation was done for $T = 1$ and $T = 2.4$ and for both temperatures ordered and random generated spin orientations were used. The steady state where the system approaches thermal equilibrium was observed to occur at approximately 10^4 cycles for energy and approximately 10^5 for magnetisation. However, fluctuations are still present. We therefore take the estimate of Monte Carlo cycles needed for the burn in to be approximately 10^5.

The simulation of the expectation value of energy is presented in figure 2, additionally the expectation value of magnetisation is presented in figure 14, in the appendix.

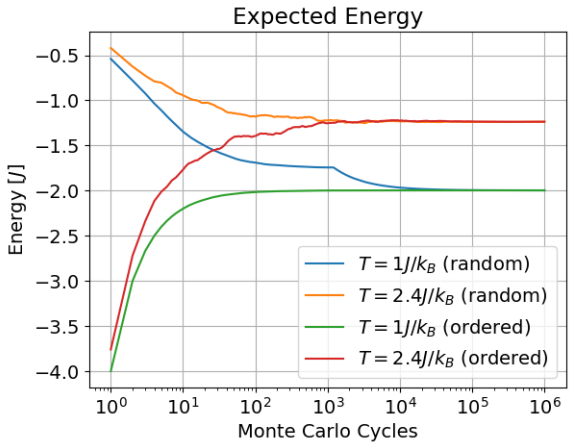

Figure 2. This plot illustrates the Monte Carlo cycles needed for a 20×20 lattice to approximately reach thermal equilibrium. It shows the energy expectation value as a function of Monte Carlo cycles. Here, random means that the system was initialized with random spin orientations, and ordered means that the spins were initialized with all spins up. Energy is in units of J, which here corresponds to the coupling constant. We set $J = 1$ and $k_B = 1$ in this simulation.

Furthermore, a plot showing the accepted states, or spin flips, generated by the metropolis algorithm for T =1, 1.5, 2.0 and 2.5 is presented in figure 3. The same lattice size and constant convention was used for this plot. The resulting plot shows the same inclination for higher temperatures, but an increasing constant term.

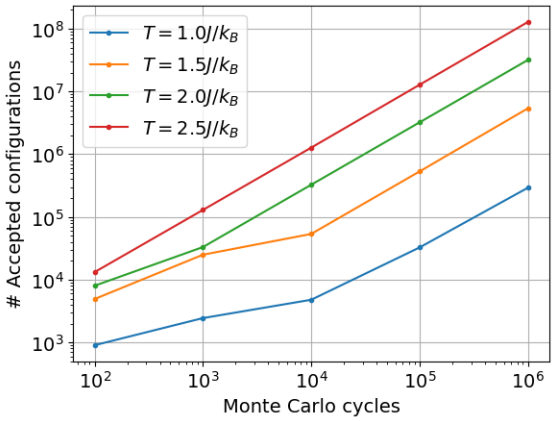

Figure 3. Accepted configurations as a function of Monte Carlo cycles for varying temperatures. The logarithmic plot yields a linear dependence on Monte Carlo cycles.

C. Probability distributions

Here we have found the energy probability distributions for a 20×20 lattice for $T = 1.0$ and $T = 2.4$. The resulting distribution for $T = 1.0$ is observed to be sharply peaked around $E = -2$ J and is presented in figure 4. The variance in the distribution is found to

be $\sigma_E^2 \approx 5.82 \times 10^{-5}$ J^2. For $T = 2.4$ the distribution peaks around $E = -1.2$ J but is more spread out. The histogram is presented in figure 5. The variance in the distribution is found to be $\sigma_E^2 \approx 2.03 \times 10^{-2}$ J^2, which is three orders of magnitude higher than for $T = 1.0$.

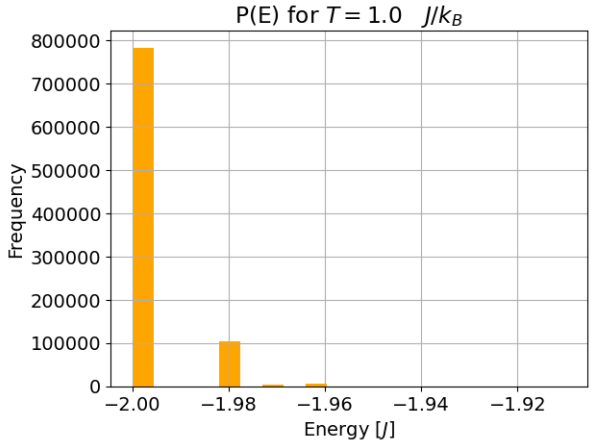

Figure 4. Energy probability distribution for a 20×20 lattice with a temperature $T = 1$. Coupling constant $J = 1$ and in units of the Boltzmann constant $k_B = 1$.

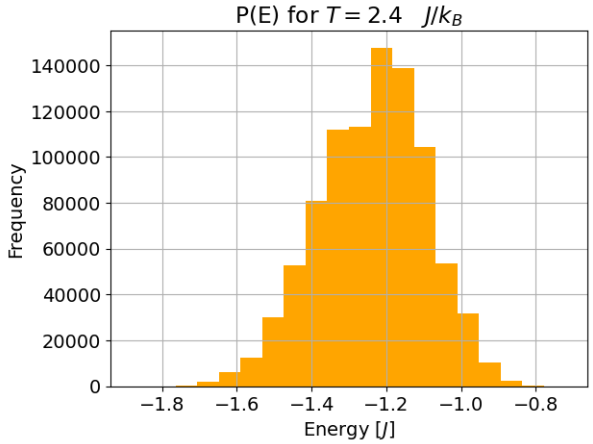

Figure 5. Energy probability distribution for a 20×20 lattice with a temperature $T = 2.4$. Coupling constant $J = 1$ and in units of the Boltzmann constant $k_B = 1$.

D. Studies of phase transitions

The behaviour of the 2D Ising model around the critical temperature T_C was studied by calculating the expectation values of energy $\langle E \rangle$ and mean magnetisation $\langle |M| \rangle$, heat capacity C_V and magnetic susceptibility χ in the temperature range $T \in [2.0, 2.4]$. The resulting plots are presented in figure 6, 7, 8 and 9. The behaviour was studied for increasing lattice sizes $L \times L$ for $L \in [20, 40, 60, 80, 100]$. The greater lattice sizes were found to produce more defined phase transitions. A more narrow temperature region and smaller temperature steps ΔT was used for the computationally heavy lattice sizes.

For some selected runs the phase transition was timed simulating using 1 to 4 CPU cores. The results are presented in the appendix A 4.

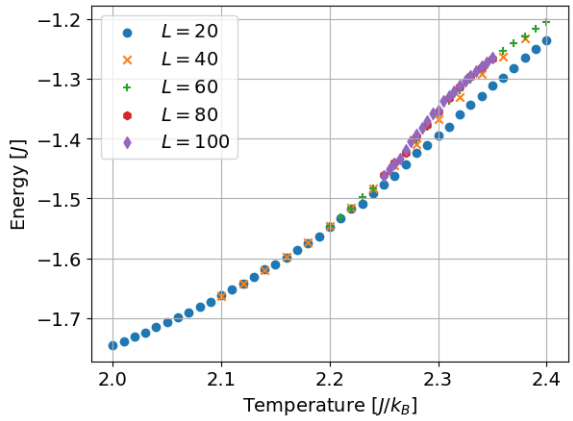

Figure 6. Expectation value of energy $\langle E \rangle$ as a function of temperature T for varying lattice size L.

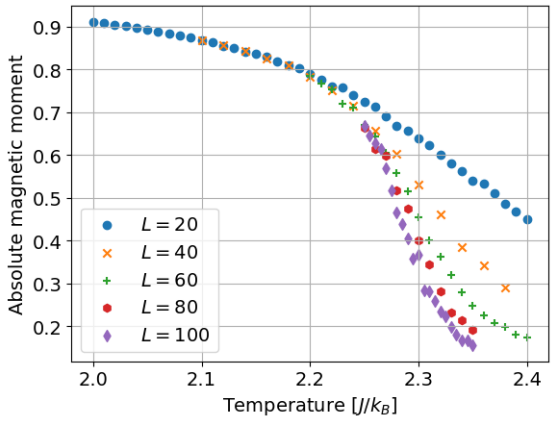

Figure 7. Mean magnetisation $\langle |M| \rangle$ as a function of temperature T for varying lattice size L.

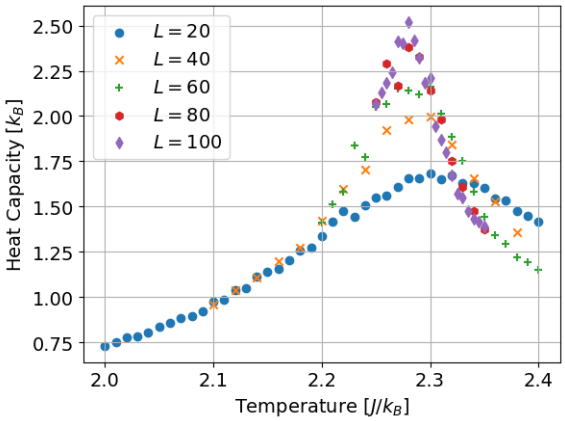

Figure 8. Heat capacity C_V as a function of temperature T for varying lattice size L.

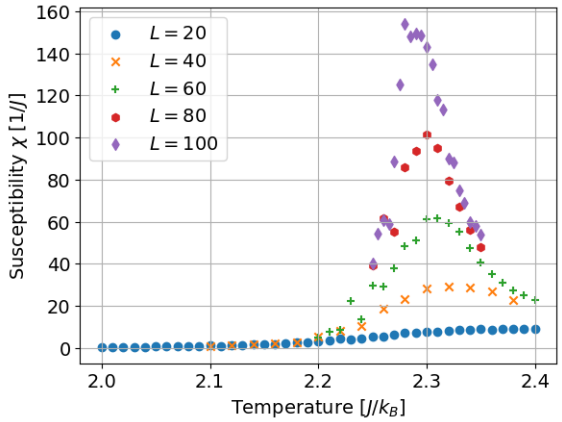

Figure 9. Magnetic susceptibility χ as a function of temperature T for varying lattice size L.

E. Critical temperature

The maxima of the magnetic susceptibility was found for the lattices of size $L \in [40, 60, 80, 100]$ where the temperature of the maxima corresponds to that of the estimated critical temperature T_C. We interpolated the values of the magnetic susceptibility and marked the maxima, the resulting plot is presented in figure 10. Using these results the critical temperature was estimated by a linear fit to the temperatures of the magnetic susceptibility maxima. This was done to approximate the analytical results of the infinite lattice size discussed in section II C. The obtained value for the critical temperature is $T_C \approx 2.65$. The plot of this linear fit is presented in figure 11.

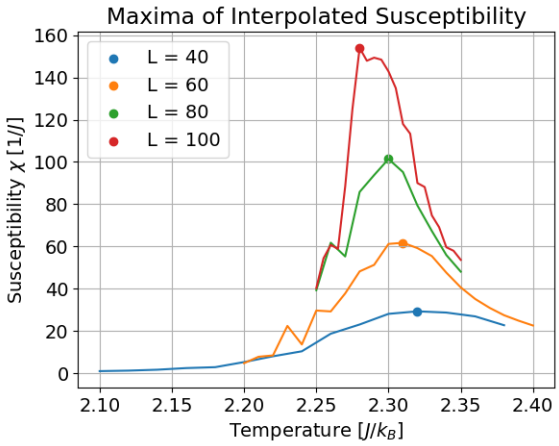

Figure 10. Magnetic susceptibility as a function of temperature for increasing lattice size. The values are interpolated to approximate smooth functions. The maximum value of susceptibility for each lattice size is marked by a dot.

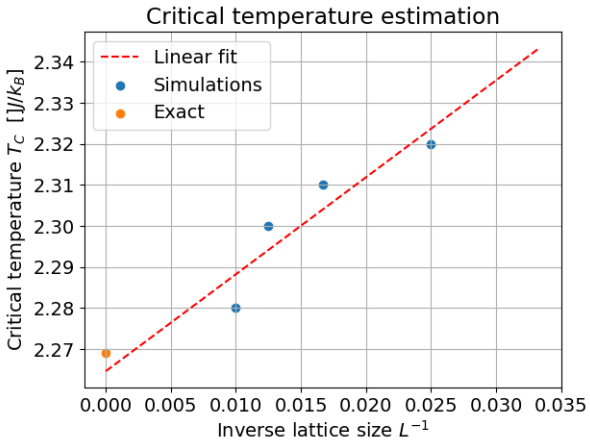

Figure 11. Estimate of the analytical infinite lattice critical temperature. The constant term of the linear fit, dashed red line, corresponds to the estimated critical temperature. The orange dot marks the analytical solution while the blue dots are the four temperatures at the simulated susceptibility maximum values.

IV. DISCUSSION

The results obtained for the phase transition of the 2D Ising model and the critical temperature, as well as the test simulation of the simple 2×2 lattice shows that our numerical implementation works as intended. We were able to optimize the numerical method by calculating the energy change probabilities prior to running the Monte Carlo cycles as explained in II B 1. The modulo method did also prove to be a good method of implementing periodic boundary conditions. Running the phase transition simulations in parallel yielded the expected speedup having each added CPU core doubling the amount of com-

puted Monte Carlo cycles while keeping the time consumption mostly equal.

We found that using 10^5 burn in cycles was sufficient for the accuracy and precision in this project. As expected we observed that for $T = 2.4$ the system fluctuated more and required more cycles than the system at $T = 1$. We also showed that increasing the temperature lead to more states, or "spin flips", being accepted in the Metropolis algorithm. This is as expected since higher temperature systems have a greater amount of available micro states to choose from. With Monte Carlo types of simulations it is far from surprising that more cycles yields better results. As with all numerical projects, a sober assessment of the time consumption versus the accuracy and precision is required. Hence, our choice of burn in cycles should be sufficient for the scope of this project.

We found probability distributions for the 20×20 lattice at $T = 1$ and $T = 2.4$. These are both in good agreement with what we would expect, which is that at lower temperature the less energetic micro states dominate. At higher temperatures more energetic states are available so we get a a more spread out distribution around more energetic states. This is evident from how the energy variance σ_E^2 for lower temperatures was significantly lower than for higher temperatures.

The results we obtained for the different properties of our model around the phase transition seems to be in good agreement with what to expect. We observe that as the lattice size increases the effects of the phase transition becomes much more clear. The most interesting result here is perhaps the spontaneous magnetisation. In figure 7 the model exhibits two distinct behaviours around some temperature $T \sim T_C$ where the magnetisation rapidly increases. This result is what Ising and Lenz was looking for when developing the model and was vital in explaining the spontaneous magnetisation of ferromagnets. The model is of course a major simplification of nature since it only accounts for the interactions between neighboring spins.

Lastly, we estimated the critical temperature where the phase transition occurs. The result we got $T_C \approx 2.265$ is quite close to the analytical result derived by Onsager, and misses the mark by ~ 0.004. For a more detailed analysis of this we would have to improve the number of Monte Carlo cycles used, and likely higher dimension lattices would yield much more accurate results. However, the method used to obtain this, which was the focus of this project, works well, and increasing the amount of cycles and dimension of the lattices is a simple task of increasing some numbers and decreasing the amount of time your computer gets to play its favourite video game.

V. CONCLUSION

In conclusion this project has been fairly successful, and the Metropolis algorithm proves to be quite robust. The model was tested and found to replicate the analytical results well within a decent amount of Monte Carlo cycles. We estimated that about 10^5 Monte Carlo cycles would provide results within the scope of this project. This estimate proved to be good since it was clearly shown that at about $T \simeq 2.265$ the 2D Ising model has a phase transition. To expand upon our work it could have been interesting to also model the behavior with varying coupling constant J or for external magnetic fields, having for example, some periodic pulse and see what this would do to our simulations. Another natural way of expanding our model would be to add a third dimension. Our model clearly showed the spontaneous magnetisation that we expect from real life ferromagnetic materials. Implementing the 2D Ising model was by no means a trivial task and served as a good introduction to Monte Carlo simulations and to parallel programming. Additionally, it provided us with a lot of useful physical understanding.

[1] Morten Hjort-Jensen. Computational physics: Lecture notes fall 2015. 2015.

[2] Sterling Chemistry Laboratory, Yale University, New Haven, Connecticut Lars Onsager. Crystal Statistics. I. A Two-Dimensional Model with an Order-Disorder Transition, 1943. Hyperlink.

Appendix A: Calculations

1. Possible microstates for 2×2 lattice using periodic boundary conditions

Table I. Microstates for a 2×2 Ising model lattice using periodic boundary conditions

N. o. spins up	N.o. microstates	Energy	Magnetisation
4	1	-8J	4
3	4	0	2
2	4	0	0
2	2	8J	0
1	4	0	-2
0	1	-8J	-4

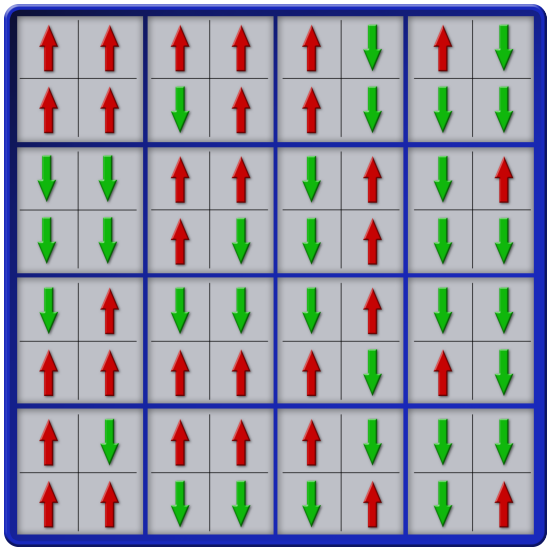

Figure 12. Table of every micro state for the 2×2 lattice.

2. Calculation of energy variance

$$\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2 \tag{A1}$$

$$= \frac{256J^2 \cosh(8J\beta)}{Z} - \frac{1024J^2 \sinh^2(8J\beta)}{Z^2} \tag{A2}$$

$$= \frac{256J^2 \cosh(8J\beta)(12 + 4\cosh(8J\beta)) - 1024^2 J^2 \sinh^2(8J\beta)}{Z^2} \tag{A3}$$

$$= \frac{3072J^2 \cosh(8J\beta) + 1024J^2 \cosh^2(8J\beta) - 1024^2 J^2 \sinh^2(8J\beta)}{Z^2} \tag{A4}$$

$$= \frac{3072J^2 \cosh(8J\beta) + 1024J^2(\cosh^2(8J\beta) - \sinh^2(8J\beta))}{Z^2} \tag{A5}$$

$$= \frac{3072J^2 \cosh(8J\beta) + 1024J^2}{Z^2} \tag{A6}$$

$$= \frac{1024J^2(1 + \cosh(8J\beta))}{Z^2} \tag{A7}$$

3. Calculation of expectation value for absolute magnetic moment and magnetisation variance

$$\langle |M| \rangle = \frac{1}{Z} \sum_{i=1}^{n} |M_i| e^{-\beta E_i} \tag{A8}$$

$$= \frac{1}{Z} \left(2 \cdot 4 \cdot e^{-\beta(-8J)} + 8 \cdot 2 \cdot e^{-\beta \cdot 0} + 4 \cdot 0 \cdot e^{-\beta \cdot 0} + 2 \cdot 0 \cdot e^{-\beta 8J} \right) \tag{A9}$$

$$= \frac{1}{Z} \left(16 + 8e^{8J\beta} \right) \tag{A10}$$

$$\langle M^2 \rangle = \frac{1}{Z} \sum_{i=1}^{n} M_i^2 e^{-\beta E_i} \tag{A11}$$

$$= \frac{1}{Z} \left(2 \cdot 4^2 \cdot e^{-\beta(-8J)} + 8 \cdot 2^2 \cdot e^{-\beta \cdot 0} + 4 \cdot 0 \cdot e^{-\beta \cdot 0} + 2 \cdot 0 \cdot e^{-\beta 8J} \right) \tag{A12}$$

$$= \frac{1}{Z} \left(32 + 32e^{8J\beta} \right) \tag{A13}$$

$$\sigma_M^2 = \langle M^2 \rangle - \langle |M| \rangle^2 \tag{A14}$$

$$= \frac{32 + 32e^{8J\beta}}{Z} - \frac{(16 + 8e^{8J\beta})^2}{Z^2} = \frac{(32 + 32e^{8J\beta})Z - (16 + 8e^{8J\beta})^2}{Z^2} \tag{A15}$$

$$= \frac{(32 + 32e^{8J\beta})(12 + 2(e^{8J\beta} + e^{-8J\beta})) - (16 + 8e^{8J\beta})^2}{Z^2} \tag{A16}$$

$$= \frac{(384 + 64e^{8J\beta} + 64e^{-8J\beta} + 384e^{8J\beta} + 64e^{16J\beta} + 64) - (256 + 256e^{8J\beta} + 64e^{16J\beta})}{Z^2} \tag{A17}$$

$$= \frac{192 + 64(e^{8J\beta} + e^{-8J\beta}) + 128e^{8J\beta}}{Z^2} \tag{A18}$$

$$= \frac{64 \left(3 + e^{-8J\beta} + 3e^{8J\beta} \right)}{Z^2} \tag{A19}$$

4. Processor core timing benchmarks

Table II. A selected run of the phase transition simulations for a 20×20 lattice with 10^5 burn in cycles. From $T = 2$ to $T = 2.4$ with a temperature step of $dT = 0.05$. Showing the time usage and total number of Monte Carlo cycles.

Processes	Monte Carlo cycles	total time (seconds)
1	10^5	0.169762
2	2×10^5	0.166754
3	3×10^5	0.147631
4	4×10^5	0.155447

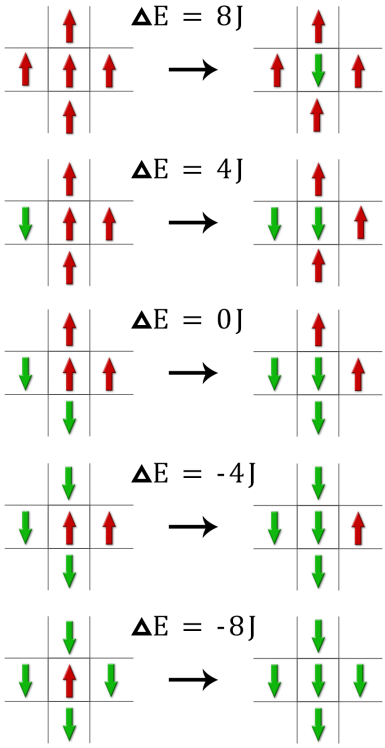

Figure 13. Table of all possible energy differences when a spin is flipped during the Metropolis algorithm.

Appendix B: Figures

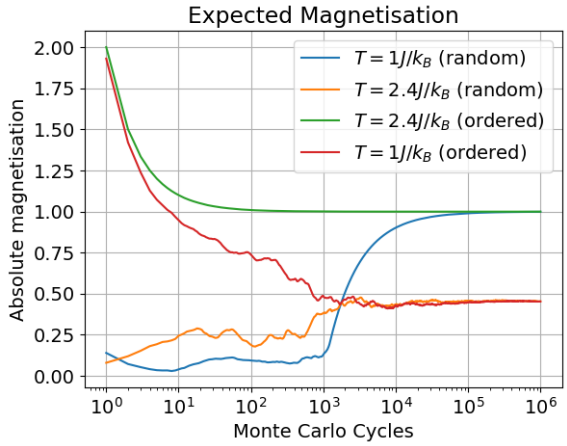

Figure 14. Expectation value of magnetisation as a function of Monte Carlo cycles.