A numerical study of phase transitions in ferromagnetic substances using the Ising model and Metropolis algorithm

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In the heating of substances, it is well known that physical properties change at certain critical temperatures. These phase transitions, which can completely transform the traits of a substance, are vital aspects in our understanding of the physical world. This paper seeks to take a deep dive into the aspects of magnetism and the critical temperature at which ferromagnetic substances lose their magnetic properties, through the fairly simple yet realistic Ising model. In order to calculate values using this model we will also apply the Metropolis algorithm, and explain the mathematics behind the two, while also considering numerical challenges associated with numerical algorithms. We were able to calculate the critical temperature in dimensionless units with a relative error of 0.00837, but with many hours of computation time. In general we were able to calculate properties such as susceptibility or expected energy to four of five digit accuracy, but this required tens of millions of Monte Carlo cycles.

I. INTRODUCTION

To better our understanding of the behaviour of atoms, molecules and materials it is of prime importance to understand phase transitions. When a material is heated to a certain degree, the physical properties can change dramatically. The most common everyday examples is the forming and melting of ice, for example on the windshield of your car the night before you have to be at work early. But another transition of perhaps less day to day relevance, but important none the less is that of magnetism in materials.

When it comes to studying these transitions, there is one model which despite its simplicity manages to encompass many of the central properties we wish to look at in phase transitions in magnetic materials. The so called Ising model, which we study in this paper, is a two dimensional binary system, which consists of atoms in a lattice which represents our material. The spin states of the atoms in this lattice is what defines the energy of the system, and is what we will study in this paper. We will start off by creating a benchmark based on the 2×2 lattice, before we move over to the 20×20 lattice and observe when it reaches its equilibrium state. In the end we will look at the critical temperature, where the phase transition happens, for larger systems.

II. THEORY

The Ising model is a binary model, where the particles at each lattice site can take only one out of two values (in our case ± 1). These values represent spin up (+1) or spin down (-1), and are usually arranged as a lattice, allowing each spin to interact with its neighbours. We will examine a two dimensional lattice since these have a known analytical values.

One important thing to note is our use of periodic boundary conditions. This means that the particles (A.K.A. spin states) at the edges of the lattice, which normally have no neighbour next to them, instead loop around and interact with the particle on the opposite side of the lattice (shown below).

$$\begin{array}{ccccccc} & & \uparrow & & \downarrow & & \\ & & \vdots & & \vdots & & \\ \uparrow & \dots & \downarrow & \uparrow & \dots & \downarrow & \\ \downarrow & \dots & \uparrow & \downarrow & \dots & \uparrow & \\ & & \vdots & & \vdots & & \\ & & \downarrow & & \uparrow & & \end{array}$$

Here, the four arrows in the centre is the lattice in question. Each arrow loops around and connects to the one on the opposite side, symbolised by the arrows separated with dots. The reason for using periodic boundary conditions is to better simulate an extremely large system with fewer simulated particles.

The energy in our Ising model, without an external magnetic field applied, is given as the sum of the product of the nearest neighbours.

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

where $s_k = \pm 1$ represents the orientation of the spin, N is the total number of spins and J is a coupling constant which expresses the strength of the interaction between neighbouring spins. Note that one cannot sum over all possible combinations of neighbours for each spin, since we then end up counting some states twice. If one spin has been multiplied and summed up with another, as well as the one which loops around to the other side, any other combination of these two specific spins should not be counted.

A. Phase Transition

For $J > 0$ the energy is the lowest when s_k and s_l are aligned. This leads to a phenomenon called spontaneous magnetization. Meaning since the system wishes to achieve the lowest possible energy, the spins must align. Since all atoms now point in the same direction, the magnetic fields generated by each atom add to the total magnetization of the lattice. This leads to the substance having a strong magnetic field on a macroscopic level.

When the temperature of the system is increased, the configuration which produces the lowest energy is no longer necessarily the one in which all spins point in the same direction. This is due to the fact that the system wishes to have the highest possible entropy, whilst at the same time achieving the lowest possible energy. This means in practice that the total magnetization of the substance decreases as temperature increases until a critical point is reached. This critical point is characterized by the fact that the given substance looses its total magnetic field on a macro scale. All atoms still project its own magnetic field, but since there is no uniformity in the arrangement of the spin states, most of these simply cancel each other out. The actual temperature of this point is an easily measurable physical phase transition, and is to a large degree replicable through the Ising model.

Another physical phase transition that occurs through heating of our non descript substance is that of correlation length. Correlation length is a measure of to what degree a given atom is affected by another atom at a distance away. At low temperatures, the changing of one spin state only affects the most immediate neighbours, meaning the correlation length is very low. As the temperature nears the critical point, this correlation length goes to infinity, meaning in theory that all particles are affected by each and every other particle in the substance, leading to large macroscopic effects. This discontinuous behavior of the correlation ξ near the critical temperature T_C is

$$\xi(T) \sim |T_C - T|^{-\nu}. \tag{2}$$

In the calculations of a two dimensional Ising model, we are limited to a finite lattice size. This causes the correlation length to be proportional with the lattice size at the critical point. Through finite size scaling relations, the behavior at finite lattices can be related to the results of infinite large lattices. The critical temperature scales then as

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu}, \tag{3}$$

with a a constant and ν is defined in equation 2 with the exact result $\nu = 1$. The constant a can be determined from equation 3 by defining two different lattice sizes, then subtracting the two resulting equations which can be rewritten as follows

$$a(L_1^{-1/\nu} - L_2^{-1/\nu}) = (T_C(L_1) - T_C(L_1 = \infty).)$$

Here L_1 and L_2 are two different lattice sizes used in equation 3. We assume $T_C(L_1 = \infty) = T_C(L_2 = \infty)$ and get the following expression for a

$$a = \frac{T_C(L_1) - T_C(L_2)}{L_1^{-1/\nu} - L_2^{-1/\nu}}. \tag{4}$$

The exact result for the critical temperature (after Lars Onsager) is $kT_C/J = 2/\ln(1+\sqrt{2}) \approx 2.269$ with $\nu = 1$.

B. The 2×2 lattice

In looking at our specific model it should be noted that the two dimensional case is very important. This is because a three dimensional case has no analytical solution. We therefore use a very simple case of a 2×2 lattice, in order to benchmark our code. We essentially use this as a way of unit testing our code. Below is an example of a configuration of spin states in our two by two lattice.

$$\begin{bmatrix} \uparrow & \uparrow \\ \uparrow & \uparrow \end{bmatrix}$$

In this case, all spins are up $(+1)$, meaning the total energy as given equation 1 is $-J(1 \cdot 1 + 1 \cdot 1 + 1 \cdot 1 + 1 \cdot 1 + 1 \cdot 1 + 1 \cdot 1 + 1 \cdot 1 + 1 \cdot 1) = -8J$.
In a different configuration, where one row of spins are similar, and opposite to the other row of spins, the total energy is zero.

$$\begin{bmatrix} \downarrow & \uparrow \\ \downarrow & \uparrow \end{bmatrix}$$

$< E >= -J((-1) \cdot (-1) + 1 \cdot (-1) + (-1) \cdot (-1) + (-1) \cdot 1 + (-1) \cdot 1 + 1 \cdot 1 + 1 \cdot 1 + 1 \cdot (-1)) = 0$
In general, each micro state for a given macro state has the same energy level. Only the configurations of all up or all down gives an energy of $-8J$

Table I. Degeneracy, energy and magnetization for the two-dimensional Ising model with $N = 2 \times 2$ spins and periodic boundary conditions.

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

C. Canonical Ensemble

We will be working with the canonical ensemble, with energy as an extensive variable following an expectation value. To calculate expectation values at a given temperature, we need a probability distribution. This is given by the Boltzmann distribution

$$P_i(\beta) = \frac{e^{-\beta E_i}}{Z}, \tag{5}$$

where $\beta = 1/k_b T$ is the inverse temperature, k_b is the Boltzmann constant, E_i is the energy of a microstate i and Z is the partition function for the canonical ensemble. Z is defined as

$$Z = \sum_{i=1}^{M} e^{-\beta E_i}, \tag{6}$$

where M is the number of microstates. We can then calculate the expected energy value from the probability distribution with

$$\langle E \rangle = \frac{1}{Z} \sum_{i=1}^{M} E_i e^{-\beta E_i}. \tag{7}$$

In the same manner, we find the expectation value of the magnetization as follows

$$\langle M \rangle = \frac{1}{Z} \sum_{i=1}^{M} M_i e^{-\beta E_i}. \tag{8}$$

These quantities can be used to calculate the specific heat Cv and the susceptibility χ

$$Cv = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_B T^2} \tag{9}$$

$$\chi = \frac{\langle M^2 \rangle - \langle M \rangle^2}{k_B T} \tag{10}$$

D. Analytical Solution

By using Table I, we can calculate the analytical expression for the partition function and the corresponding expectation values for the energy E, the mean absolute value of the magnetic moment $|M|$, the specific heat Cv and the susceptibility χ as functions of T using periodic boundary conditions for a 2×2 lattice. The 2×2 lattice gives $2^4 = 16$ configurations. The partition function is then given by

$$\begin{aligned} Z &= \sum_{i=1}^{16} e^{-\beta E_i} \\ &= 2e^{-8J\beta} + 2e^{8J\beta} + 12 \\ &= 4\left(\frac{e^{8J\beta} + e^{-8J\beta}}{2}\right) + 12 \\ &= 4\cosh(8J\beta) + 12 \end{aligned} \tag{11}$$

We then calculate the expected energy value using equation 6

$$\begin{aligned} \langle E \rangle &= \frac{1}{Z}\left(2 \cdot (-8J) e^{8\beta J} + 2 \cdot (8J) e^{-8J\beta}\right) \\ &= -\frac{J}{Z}\left(32 \sinh(8J\beta)\right) \\ &= -\frac{8\cosh(8J\beta)}{\cosh(8J\beta) + 3} \end{aligned} \tag{12}$$

Continuing in the same manner gives the following results

$$\langle M \rangle = 0 \tag{13}$$

$$\langle |M| \rangle = \frac{2e^{8J\beta} + 4}{\cosh(8J\beta) + 3} \tag{14}$$

$$\langle E^2 \rangle = \frac{64\cosh(8J\beta)}{\cosh(8J\beta) + 3} \tag{15}$$

$$\langle M^2 \rangle = \frac{8e^{8J\beta} + 8}{\cosh(8J\beta + 3} \tag{16}$$

These quantities can then be used in the expression for the specific heat and the susceptibility. The analytical expressions are then given by

$$Cv = \frac{1}{k_B T^2}\left(\frac{64\cosh(8J\beta)}{\cosh 8J\beta + 3} - \left(\frac{8\cosh(8J\beta)}{\cosh(8J\beta) + 3}\right)^2\right) \tag{17}$$

$$\chi = \frac{1}{k_b T}\left(\frac{8e^{8J\beta} + 8}{\cosh(8J\beta + 3}\right) \tag{18}$$

III. METHOD

With the theoretical groundwork out of the way, we can focus on the actual implementation of the algorithm.

Without going into too much detail, what the algorithm does is implement the lattice with a spin state in each point. A random point is then picked, and the change in energy is calculated if this spin state was to be reversed. Whether the new state is accepted is decided by the Metropolis algorithm.
A general pseudo code showcasing the algorithm is shown below.

A. Metropolis Algorithm

The Metropolis algorithm is implemented as a nested list, where the outer sums over the number of Monte Carlo cycles, and the inner sums over the number of spins in the lattice.

Algorithm 1 Metropolis Algorithm

```
Initialize variables, define Monte Carlo cycles
for i = 1 : Monte Carlo cycles do
    for i = 1 : number of spins do
        Suggest new state
        Calculate ΔE
        Pick a random number r ∈ [0, 1] with uniform PDF
        if r ≤ e^{−βΔE} then
            Accept suggested move
        end if
    end for
    Update expectation values
end for
Normalize expectation values
```

The actual code used in this project can be found in the Appendix.

One important thing to note is our handling of the data in these algorithms. Since a Monte Carlo method is stochastic, the result gets better for a higher number of Monte Carlo cycles. This means that when calculating the mean and expected values of energy and magnetization we exclude the first few data points, seeing as how these are so inaccurate for reasons just stated. Looking at figure 1 and 2 one can see that the expected energy oscillates massively in the first few numbers of Monte Carlo cycles, but then settles to oscillate around the correct values. If we then exclude the first 7000 data points in these data sets, we will get a lot more accurate values.

B. Random Number Generator

In this algorithm, as with all Monte Carlo algorithms, the use of random numbers plays a central role. It is therefore important to ensure a high quality of randomness in our code. For example, calculating with a lattice of size $20x20$ and $1,000,000$ Monte Carlo cycles, $1,200,000,000$ random numbers are called.
To ensure a high quality of randomness we use Mersenne Twister, which has a period of 2^{19937} [1].

IV. RESULT

A. The 2×2 lattice

To test our method, we compare our results for a 2×2 lattice with the analytical values calculated in section II D for increasing number of Monte Carlo cycles.

Table II. The expected energy and magnetization for the two-dimensional Ising model with temperature $T = 1.0$ and periodic boundary conditions for $L = 2$. The expected energy reaches two leading digits after 1e4 Monte Carlo cycles and five leading digits after 1e8 cycles. For the magnetization, we reach three leading digits after 1e4 Monte Carlo cycles. The specific heat converges to two leading digits for $n = 1e7$ and the susceptibility converges to three leading digits for $N = 1e7$

N	1e4	1e5	1e6	1e7	1e8	Analytic
$\langle E \rangle$	-1.9966	-1.99654	-1.99608	-1.9961	-1.99598	-1.99598
$\langle \lvert M \rvert \rangle$	0.9985	0.99885	0.99871	0.998704	0.998659	0.99866
C_v	0.0399154	0.0379909	0.0343265	0.032918	0.0322562	0.032075
χ	3.96168	3.83193	3.99277	3.99324	3.99326	3.993303

B. Time required to reach equilibrium state

Moving on to a 20×20 lattice, we investigate how many Monte Carlo cycles is needed before the system reaches an equilibrium state. We look at the difference of starting from a random spin orientation compared to an ordered spin orientation. This is done fore temperatures at both $T = 1$ and $T = 2.4$.

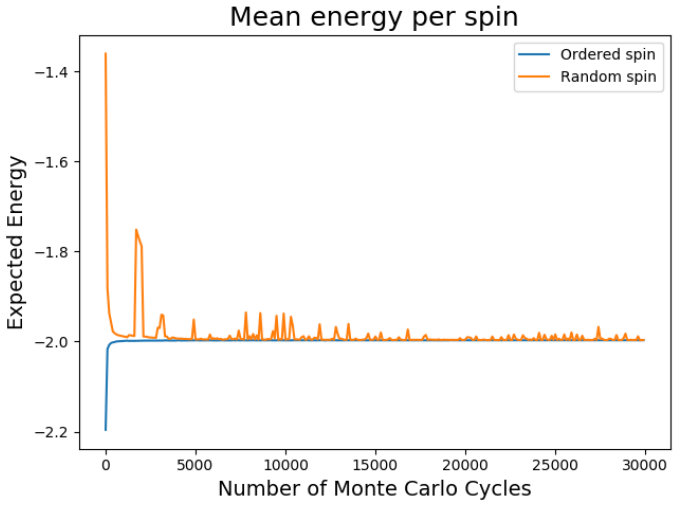

Figure 1. The mean energy per spin with ordered and random spin orientation as a function of time, here represented as Monte Carlo cycles, for a 20×20 lattice and $T = 1$. We need about 5000 Monte Carlo cycles to reach an equilibrium situation.

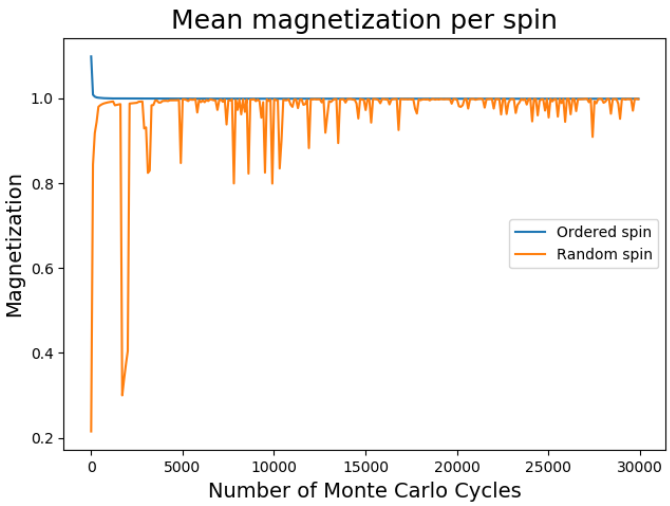

Figure 2. The mean magnetization per spin with ordered and random spin orientation as a function of time, here represented as Monte Carlo cycles, for at 20×20 lattice and $T = 1$. We need about 5000 Monte Carlo cycles to reach an equilibrium situation.

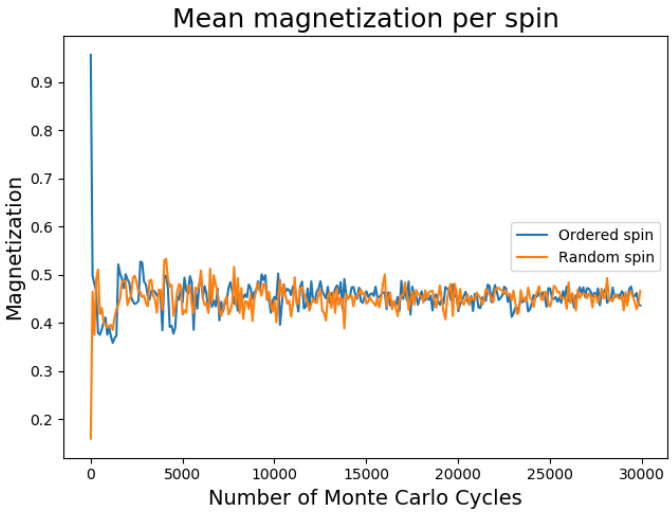

Figure 4. The mean magnetization per spin with ordered and random spin orientation as a function of time, here represented as Monte Carlo cycles, for at 20×20 lattice and $T = 24$. We need about 7000 Monte Carlo cycles to reach an equilibrium situation.

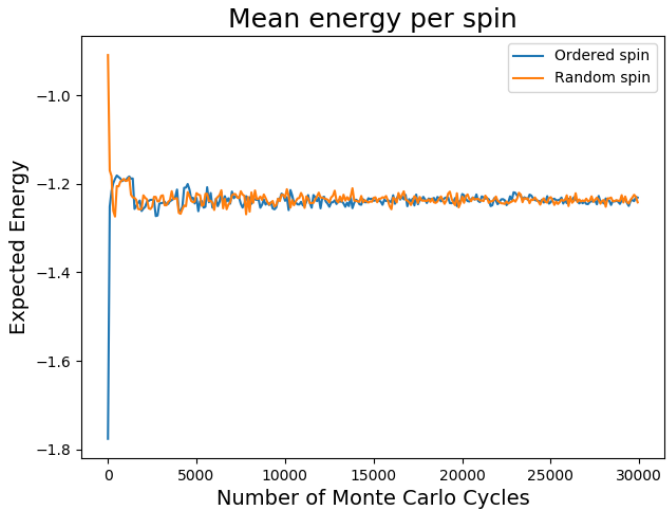

Figure 3. The mean energy per spin with ordered and random spin orientation as a function of time, here represented as Monte Carlo cycles, for a 20×20 lattice and $T = 2.4$. We need about 7000 Monte Carlo cycles to reach an equilibrium situation.

Finally, we plot the total number of accepted flips as function of time.

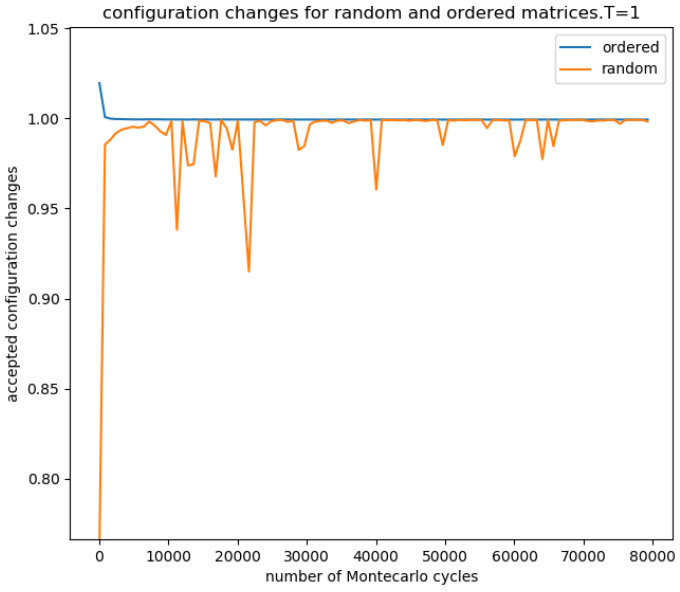

Figure 5. The total number of accepted state changes per spin in the Metropolis algorithm for a total number of spins for both ordered and random initial state with $T = 1.0$ and the lattice size $L = 20$ An ordered initial state means that all the spins in the lattice point the same direction from the start, and a random initial state means that each point in the lattice has been assigned a state randomly.

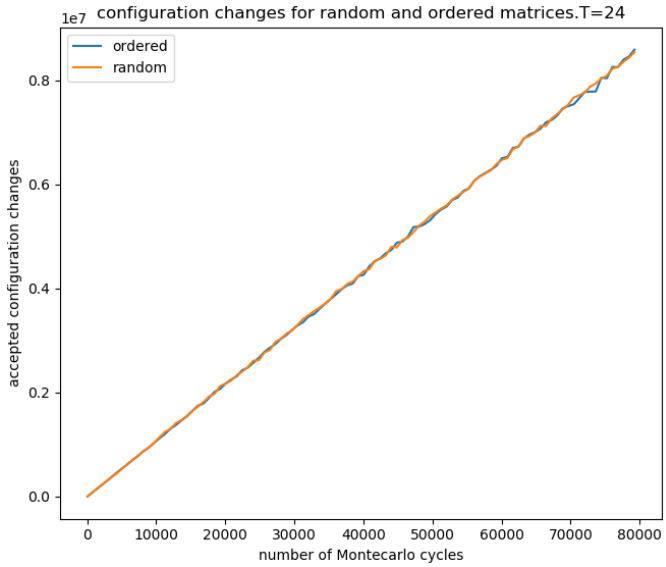

Figure 6. The total number of accepted state changes per spin in the Metropolis algorithm for a total number of spins for both ordered and random initial state with $T = 2.4$ and the lattice size $L = 20$ An ordered initial state means that all the spins in the lattice point the same direction from the start, and a random initial state means that each point in the lattice has been assigned a state randomly.

C. Analyzing the probability distribution

Here we compute the probability of a certain energy occurring after the equilibrium state for $T = 1$ and $T = 2.4$ respectively.

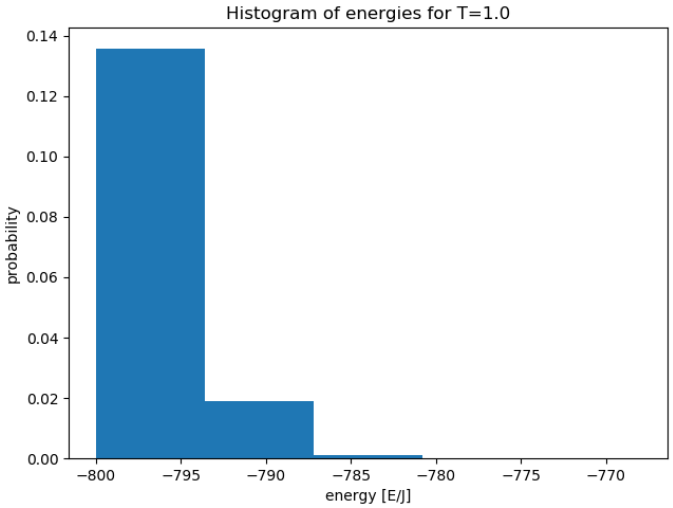

Figure 7. A histogram of the different energy levels for a temperature of $T = 1$. The standard deviation for this sample is $\sigma = 6.64$ and the mean value is -798.55. Here a lattice size of $L = 20$ and $30,000$ Monte Carlo cycles was used

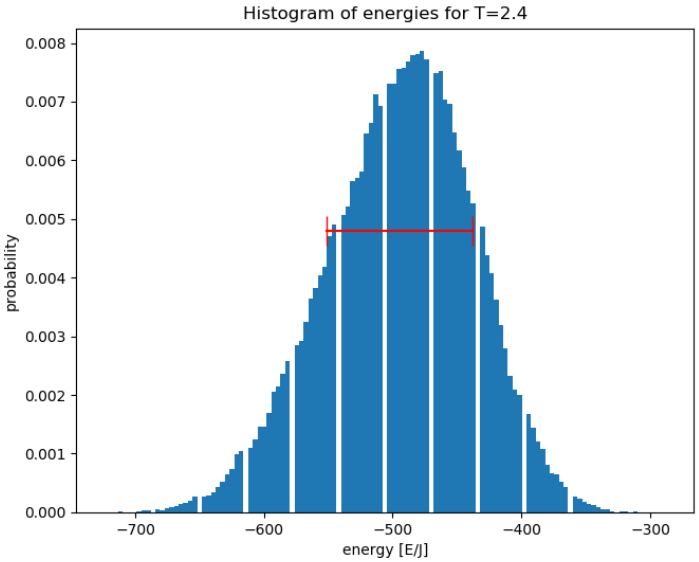

Figure 8. A histogram of the different energy levels for a temperature of $T = 2.4$. The standard deviation for this sample is $\sigma = 56.65$ and the mean value is -494.58. Here a lattice size of $L = 20$ and $30,000$ Monte Carlo cycles was used.

D. Numerical Studies of Phase Transition

For the lattices $L = 40, 60, 80, 100$ we plot the expected energy, magnetization, heat capacity and susceptibility for 60 temperatures in the range $T = 2.1, 2.4$. They are all run with 50000 Monte Carlo cycles, with the 7000 first cycles excluded.

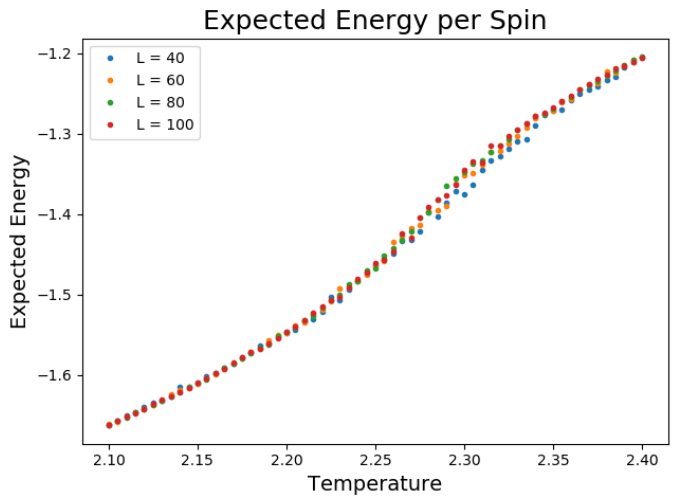

Figure 9. The expected energy $[E/J]$ per spin for temperatures $[k_B T]$ near the critical temperature with step 0.005, simulated with 50 000 Monte Carlo cycles with the 7000 first cycles excluded.

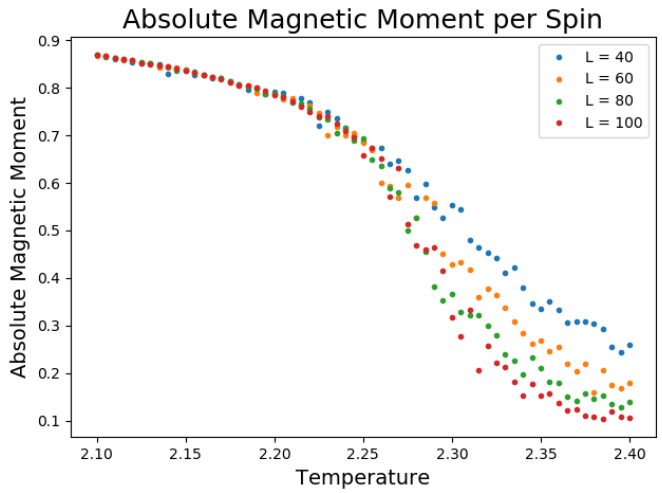

Figure 10. The absolute magnetic moment per spin for temperatures in units $[k_B T]$ near the critical temperature with step 0.005, simulated with 50 000 Monte Carlo cycles with the 7000 first cycles excluded.

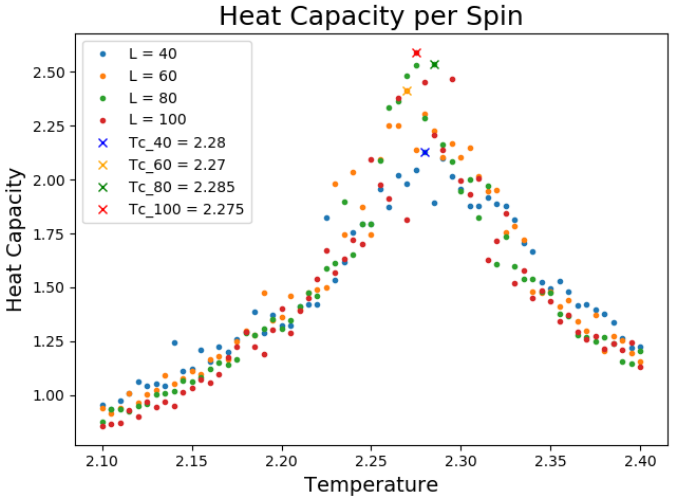

Figure 11. The heat capacity in units $[Jk_B]$ per spin for temperatures near the critical temperature in units $[k_B T]$, with step 0.005, simulated with 50 000 Monte Carlo cycles with the 7000 first cycles excluded.

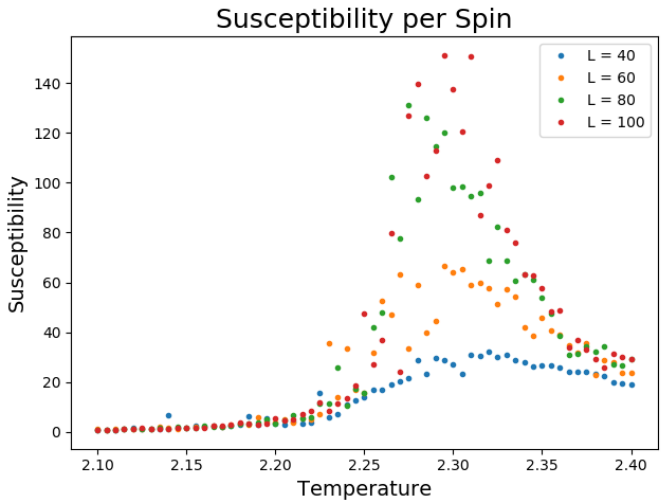

Figure 12. The susceptibility per spin in units $[k_B]$ for temperatures in units $[k_B T]$ near the critical temperature with step 0.005, simulated with 50 000 Monte Carlo cycles with the 7000 first cycles excluded.

Based on our results of the critical temperature for the different lattice sizes, marked as crosses in Figure 11, we extracted the following estimate of the critical temperature T_C in the thermodynamic limit $L \to \infty$.

Table III. The estimated critical temperature using equation 4 for different lattice sizes using the critical temperature found in Figure 11. The exact result for the critical temperature (after Lars Onsager) is $kT_C/J = 2/\ln(1+\sqrt{2}) \approx 2.269$.

L_1	L_2	Estimated T_C	Relative Error
60	40	2.250	0.00837
80	60	2.33	0.0269
100	80	2.235	0.0150

E. Parallelization

Table IV. The CPU time when running a for loop with four temperature values with 50 000 Monte Carlo cycles for a given lattice size L. Parallelized with OpenMP compiled with optimization flag -O3. For a $L = 20$ the run time is reduced by 1/4 and for $L = 40$ the run time is reduced with 1/2.

Lattice size	Without OpenMP [s]	With OpenMP [s]
20	37.41	8.78
40	197.18	77.45

V. DISCUSSION

A. The 2×2 lattice

Table II gives an explicit comparison of the numerical and analytical values for the 2×2 lattice. As expected the values converge towards the analytical solution for

higher number of Monte Carlo cycles, and we assume the simulations will converge for larger lattices as well.

B. The Equilibrium State and the Probability Distribution

In figure 5 the total number of accepted changes in the Metropolis algorithm for a certain number of Monte Carlo cycles is plotted for both ordered and random initial matrix. An ordered initial matrix means that all the spins states in the given lattice have the same state or orientation from the start. As can be seen in the plot, the ordered one starts out a lot closer to the final state, indicated by the fact that no new states is accepted, and from there on oscillates a lot less. The matrix with random initial states oscillate a lot more, even for very high numbers of Monte Carlo cycles. This is due to the fact that a new random initial matrix is picked each time a new number of Monte Carlo cycles is calculated.

As we know from the 2×2 lattice example, the lowest energy state for that system at low temperatures was all particles with the same orientation. This can be used to explain why the ordered matrix reaches the final state so quickly, since the lowest energy state most likely is most or all spins in the same direction. A certain random configuration of spins might be very far away from this configuration, and hence needs a lot of Monte Carlo cycles to reach the final state.

For $T = 2.4$ in 6 we see that the number of accepted configuration changes climbs linearly with the number of Monte Carlo cycles. This is due to the fact that the number of states the system can inhabit is larger. If we look at the histograms for the energy levels of the system, the lower temperature 7 has only three or so states which the system inhabits, while the higher temperature 8 has a much larger amount. This means that the number of different states the system can inhabit is a lot larger, and hence, a change in the state of the system will be accepted a lot more often. One could extrapolate from this that this must mean the system never reaches a equilibrium, but looking at fig 1 we see that the system oscillates around the final value, and hence, a lot of changes in state is accepted.

C. The Phase Transition

Figure 9, 10, 11 and 12 show the behaviour of the Ising model in two dimensions close to the critical temperature as a function of the lattice size $L \times L$ and the temperature T. When evaluating the susceptibility χ, we used the absolute value $\langle |M| \rangle$, instead of $\langle M \rangle$ as in equation 10. The reason for this is that the magnetic moment $\langle M \rangle$ tend to oscillate for small systems, and we have to run very many Monte Carlo cycles before it converges towards zero. When applying the absolute magnetization instead, we remove this error, and get better results for the susceptibility.

Looking at figure 9 we see that the expected energy per spin increases fairly linearly with temperature. This is as expected, and follows with the observations made in the histogram 8 and 7. For the histogram with $T = 1$ (7) we see that the energies of the systems are all more or less in the -800 to -790 range, where as for the histogram for $T = 2.4$ (8) the energies vary a lot more, but all for higher energy values. From a purely intuitive standpoint, it also makes sense that as the temperature increases, the expected energy of a particle increases as well.

Figure 10 shows the magnetic moment per spin, which behaves as expected. We expected from the theory that as the temperature came closer to the critical point, the magnetic moment in the system would reach zero. As can be seen in the plot, the larger lattice sizes converge to zero at at faster and faster rate. This can seem to indicate that as the lattice size increases the approximation yields better results.

Looking at figure 11 we see that the peak is made higher and higher for each lattice larger than the previous one. A similar behaviour is seen in fig 12 where the susceptibility is shown for a range of temperatures. The peak value of the heat capacity 11 is considered to be the critical temperature of the given lattice size. Since this changes for a larger lattice, we can deduct that this converges on the actual critical temperature as the size of the lattice goes to infinity.

It is clear from Table III that we get the best estimate of the critical temperature by applying $L_1 = 40$ and $L_2 = 60$ in equation 4, and use the result in equation 3. We expected the estimate to become better with greater lattice size, since the specific heat develops a sharper peak around the critical temperature when the lattice size increases. The results might had become better if we had simulated with a smaller step size, but we did not have the time due to time constraints. Another consideration that could better our results is the use of a spline, or a polynomial fit to get an approximation of the peak with the given data points.

D. Parallelization

In Table IV we compare the run time when parallelizing with OpenMP using four cores and no parallelization. For a 20×20 lattice we got a speed up of $1/4$ using OpenMP and a speed up of $1/2$ for the 40×40 lattice. This shows that even a simple parallelization of a for loop with OpenMP can make huge improvements on the run time of a program.

VI. CONCLUSION

The Ising model with use of the canonical ensemble and Metropolis algorithm replicates the theory in a very close fashion. All phase transitions, changes in physical properties and the temperature at which these occur follow the theoretical values at which we expected they would. The critical temperature in dimensionless units was found within a relative error of 0.00837. The number of Monte Carlo sweeps, and the size of the lattice necessary in order to achieve a very high accuracy however can be a challenge when time and hardware is limited. In order to achieve around four digit accuracy we needed 10^8 Monte Carlo cycles (see II). This, for a 20×20 lattice took a few minutes on our admittedly limited hardware. In addition to this, it is necessary to run this calculation for many different values of temperature. In order to obtain the data set we used in calculating the critical temperature we had to run a computer for about 25 hours straight, only to gain three digit accuracy. Parallelizing did significantly decrease the time the calculations took, but despite this we found it to be the main limiter, and can see that this could be used as criticism against the Metropolis or even the Ising model itself.

There is also an inherent weakness in the Metropolis algorithm, as it is not very effective for temperatures near the critical temperature T_c. Other algorithms, such as the Swendsen-Wang, Wolff or clustering algorithm [3] are more efficient in simulating the behaviour around these critical temperatures if one wishes to find the critical temperature. If a spline or similar polynomial fit is used to interpolate the data points it might be possible to get a better approximation of the critical temperature.

As a method of achieving greater understanding and insight into the behaviour of materials, we found that the Ising model, along with the statistical physics elements in the Metropolis algorithm proved itself capable of doing this. The Ising model and Metropolis algorithm prove simple to understand, relatively easy to implement numerically, and able to reliably produce results that correspond to theory. There were however several limitations in computing time, and the number of Monte Carlo cycles needed to achieve a greater accuracy.

In future work, we would recommend looking at ways to make the general algorithm more effective, such that the use of large computers are not necessary in calculating the physical properties of substances to a high degree of accuracy.

APPENDIX

See https://github.com/elinfi/FYS3150/tree/master/Project4 for code. There is two versions of the code, which handles different parts of the project. Mainly the code in FYS3150/Project4/main-program handles the most of it, but the plotting of the histogram and accepted spin changes in the Metropolis algorithm is done in FYS3150/Project4/main-program/project4 .

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