Computational Physics (FYS4150) Project 4

The Ising model and the Metropolis algorithm

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https://github.com/bjorngli/fys4150/tree/master/Project4

Disclaimer

This project was done through a collaborative process working with Bjørn Gilje Lillegraven and Lasse Kvasnes. The project report is self written but the code was worked on as a group and therefor any plots and values obtained are most likely to be similar or the same.

Abstract

In this project I used the two dimensional Ising model, solved through the Metropolis algorithm, to study phase transitions and estimating the critical temperature T_c as proved analytically by Lars Onsager to be $T_c = 2.269$. I also verified that the code implementation worked by comparing it to analytic expressions for the 2×2 lattice, as well as finding 200 MC cycles be enough for the system to reach equilibrium if the initial state is chosen wisely. The fraction of accepted MC cycles was found to be greatly dependent on the temperature of the system..

Contents

1 Introduction

In this paper we use Monte Carlo methods and the Metropolis algorithm to solve the popular Ising model with a ferromagnetic ordering and no external magnetic field. Monte Carlo methods are used in cases where the actual characteristics are difficult to program and uses instead random sampling to solve the model. Firstly look at solving the 2×2 Ising model and compare the results up against analytic solutions to verify that the model works as intended. We will then move on to the 20×20 lattice to study equilibrum time and temperature dependence. Lastly we will look at phase transitions in the Ising model an how we can estimate the critical temperature at where the phase transition happens.

2 Theory

2.1 The Ising model

A simple binary system consisting of spins configured in a N $\times$ N lattice is the basis for what is called the Ising model. As the term binary implies each spin can only have be in one of two directions, in this case up, which we give a value of +1, and down, which we give a value of -1.

The energy for a spin configuration i in the Ising model is expressed by the Hamilton function and can be written as:

$$E_i = -J \sum_{\langle kl \rangle}^{N} s_k s_l - \mathcal{B} \sum_{\langle k \rangle}^{N} s_k \tag{1}$$

where J is a coupling constant expressing the strength of the interaction between neighboring spins, $s_k = \pm 1$ denotes spin up or spin down, $\mathcal{B}$ represents an external magnetic field interacting with the magnetic moment set up by the spins. The notation <kl> indicates that a spin will only be affected by its nearest neighbours and we will therefore only sum over the nearest neighbours.

In our model we will be excluding any impact from an external magnetic field which reduces our equation to a fairly simple one:

$$E_i = -J \sum_{\langle kl \rangle}^{N} s_k s_l \tag{2}$$

For this project we will be applying periodic boundaries, meaning that if there is no neighbouring spin for a specific spin we will assume the neighbouring spin to equal the spin at the opposite side of the lattice. This will be better visualized when finding analytic expressions for the 2 $\times$ 2 Ising model.

We will also assume there is a ferromagnetic ordering, i.e. $J > 0$.

It is worth mentioning that from equation 1 we see that spin configurations where neighbouring spins have the same spin direction will be having the lowest possible energy and it is therefore energetically favourable for spins to be aligned. This could at low temperatures lead to spontaneous magnetization. For further explanation of the phenomenon see chapter 13.3 in [1].

The magnetization for a spin configuration is defined as:

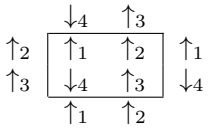
$$\mathcal{M}_i = \sum_{j=1}^{N} s_j \tag{3}$$

2.2 Analytic expressions for the 2 × 2 lattice

Something of great interest would be to find closed-form solutions for some of the variables in the Ising model. Therefore we will in this section look for analytic solutions for the expected value of the energy $\langle E \rangle$, the mean absolute value of the magnetic moment, $\langle |M| \rangle$, the specific heat C_v and the susceptibility χ.

These solutions will serve as important benchmarks for testing the validity of the coded model.

As mentioned in the previous section we will now look at the 2×2 Ising model with periodic boundaries. For this version of the Ising model we have 2^4 possible configurations. An example spin configuration is shown in the figure below which has 4 spins in total, in which 3 are up and 1 down. The way in which the periodic boundaries behave is also visualized in the figure where the non-existent spin to the left of spin s_1 takes the value of s_2.



The energy of this example configuration is:

$$\begin{aligned} E_i &= -J \sum_{\langle kl \rangle}^{4} s_k s_l \\ &= -J(s_1 s_2 + s_1 s_3 + s_2 s_1 + s_{2s4} + s_3 s_1 + s_3 s_4 + s_4 s_3 + s_4 s_2) \\ &= -J(1 + 1 + 1 - 1 + 1 - 1 - 1 - 1) = 0 \end{aligned}$$

And we calculate the magnetization to be:

$$\begin{aligned} \mathcal{M}_i &= \sum_{j=1}^{4} s_j \\ &= (s_1 + s_1 + s_3 + s_4) \\ &= (1 + 1 + 1 - 1) = 2 \end{aligned}$$

The energy and magnetization for all 16 spin configurations can be found in Table 1 just below. Spin configurations with similar characteristics have been grouped.

Spins up	Multiplicity	Energy [J]	Magnetization
4	1	$-8J$	4
3	4	0	2
2	4	0	0
2	2	8	0
1	4	0	-2
0	1	$-8J$	-4

Table 1: Possible spin configurations, their degeneracies, energies and magnetizations.

For calculating the expected value of different variables we use the statistical formula for a random variable X:

$$\langle X \rangle = \sum_{i=1}^{M} X P_i(\beta) \tag{4}$$

where $P_i(\beta)$ is a probability distribution.

For our model we use the probability distribution for the canonical ensemble which is given by the Boltzmann distribution:

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

where $\beta = \frac{1}{kT}$, k is the Boltzmann constant and Z is the partition function defined as:

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

Calculating Z we get:

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

Then the expected energy is calculated as:

$$\begin{aligned}\langle E\rangle &= \sum_{i=1}^{M} E_i P_i(\beta) = \frac{1}{Z}\sum_{i=1}^{M} E_i e^{-\beta E_i} \\ &= \frac{1}{Z}\sum_{i=1}^{M=16} E_i e^{-\beta E_i} \\ &= \frac{1}{Z}(-8Je^{\beta 8J} + 2*8Je^{-\beta 8J} - 8Je^{\beta 8J}) \\ &= \frac{4*-8J}{Z}(\frac{1}{2}e^{\beta 8J} - \frac{1}{2}e^{-\beta 8J} \\ &= \frac{4*-8J}{4cosh(8\beta J)+12}sinh(8\beta J) \\ &= -8J\frac{sinh(8\beta J)}{cosh(8\beta J)+3} \end{aligned} \tag{8}$$

For the expected value of the absolute magnetic moment we use the same expected value equation:

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

The specific heat in the canonical ensemble is defined as:

$$\langle C_v\rangle = \frac{\sigma_E^2}{k_b T^2} = \frac{\langle E^2\rangle - \langle E\rangle^2}{k_b T^2} \tag{10}$$

First we calculate $\langle E^2\rangle$:

$$\begin{aligned}\langle E^2\rangle &= \frac{1}{Z}\sum_{i=1}^{M} E_i^2 e^{-\beta E_i} \\ &= \frac{1}{Z}(2*64J^2e^{-\beta(-8J} + 2*64J^2e^{-\beta(8J}) \\ &= \frac{1}{Z}254J^2cosh(\beta 8J) \end{aligned}$$

Inserting $\langle E^2\rangle$ and the expected energy $\langle E\rangle$ into equation 10 we get:

$$\begin{aligned}\langle C_v\rangle &= \frac{1}{k_b T^2}(\frac{1}{Z}254J^2cosh(\beta 8J) - (-\frac{1}{Z}32Jsinh(8\beta J))^2) \\ &= \frac{1}{k_b T^2 Z}(254J^2cosh(\beta 8J) - \frac{1}{Z}1024J^2sinh(8\beta J)^2) \end{aligned} \tag{11}$$

And lastly the susceptibility χ is defined as:

$$\chi = \frac{\sigma_{\mathcal{M}}^2}{k_b T} = \frac{1}{k_b T}(\langle \mathcal{M}^2 \rangle - \langle \mathcal{M} \rangle^2) \tag{12}$$

$$\begin{aligned}
\langle \mathcal{M}^2 \rangle &= \frac{1}{Z} \sum_{i=1}^{M=16} \mathcal{M}_i^2 e^{-\beta E_i} \\
&= \frac{1}{Z}(16e^{\beta 8J} + 16e^{\beta 8J} + 16e^0 + 16e^0) \\
&= \frac{32}{Z}(e^{\beta 8J} + 1)
\end{aligned}$$

$$\begin{aligned}
\langle \mathcal{M} \rangle &= \frac{1}{Z} \sum_{i=1}^{M=16} \mathcal{M}_i e^{-\beta E_i} \\
&= \frac{1}{Z}(4e^{\beta 8J} - 4e^{\beta 8J} + 8e^0 - 8e^0) \\
&= 0
\end{aligned}$$

Inserting into equation 12 we get:

$$\chi = \frac{32}{k_b T Z}(e^{\beta 8J} + 1) \tag{13}$$

2.3 The Metropolis algorithm

Now we want to look at how our system develops over time. A way to do this is to use the method of Markov chain Monte Carlo simulations which has the advantage that it can be used for systems where behaviours are difficult to predict. Markov chains has the feature that any future events are only dependent on the last event that lead to the current state of the system as well as that the system will tend towards an equilibrium after a specific number of Markov processes. But it also has two conditions that must be met, ergodicity and detailed balance which puts limitations on the acceptance of new states. For further explanation see chapter 12.5 [1].

In our model the system is given an initial spin configuration and then an algorithm is used to see how the spin configuration changes over time. The system isn't actually solved over time but rather over Monte Carlo cycles which we will use The Monte Carlo simulations will be implemented through the Metropolis algorithm which takes into account the any system will tend to a state where the energy is as low as possible. When the system tends towards this lowest possible energy we will say that the system tends towards its equilibrium state. The main steps in the algorithm goes as follows:

1. Start with an initial configuration of the lattice with energy $E_{initial}$.
2. Flip a spin and recalculate the energy $E_{current}$.

3. If the change in energy is negative, i.e. $\Delta E = E_{current} - E_{initial} < 0$, we accept the flip as a valid change as it lowers the energy of our system.

4. If the change in energy is positive, i.e. $\Delta E = E_{current} - E_{initial} > 0$, calculate $w = e^{(-\beta \Delta E)}$ and draw a random number $r/U(0,1)$ from a non-uniform/uniform random number generator.

5. If $r \leq w$ we accept the new configuration, else we keep our old configuration.

   Then we repeat the above steps and let the system go towards an equilibrium state.

This allows us to retain the ergodicity of the system meaning that even tho the systems energy is expected to tend to a lower energy we still need to allow the possibility of moving from one state to any other state.

It is also worth noting that whether or not we accept a flip is dependent on the temperature of the system as β is temperature dependent.

In the calculation of the energy difference from one spin configuration to the other, we will limit the change to the flipping of one spin only. For the Ising model in two dimensions it means that there will only be a limited set of values for E. Actually, there are only five possible values for ΔE, $\pm 8J, \pm 4J$ and 0. Precalculating these and reading them from a matrix instead of calculating them for each iterations will make the code more efficient.

2.4 Phase transitions

In the Ising model we have a 2nd order phase transition. The phase transition happens at a critical temperature T_c below which we will experience the phenomenon of spontaneous magnetization with $\langle M \rangle \neq 0$. Above we have no spontaneous magnetization, i.e. $\langle M \rangle = 0$. The disappearance of a the mean magnetization above the critical temperature is what's referred to as a critical phenomenon.

It can be shown that the mean magnetization below the T_c can be written as:

$$\langle M(T) \rangle \sim (T - T_c)^{\beta} \tag{14}$$

where $\beta = 1/8$ is a critical exponent.

We have similar expressions for the specific heat C_v:

$$C_v(T) \sim |T - T_c|^{-\alpha} \tag{15}$$

and susceptibility χ:

$$\chi(T) \sim |T - T_c|^{-\gamma} \tag{16}$$

where $\alpha = 0$ and $\gamma = -\frac{7}{4}$ are the critical exponents.

These are the expressions for a infinite lattice. In our model we can obviously not work with an infinitely large lattice since a computer can only handle finite numbers, and is limited by memory. So we will instead use the correlation

length, which is proportional to the lattice size at the critical point, to establish and approximation of the above equations for a finite lattice.

The critical temperature scales as:

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu} \tag{17}$$

where a is a constant and v is defined by the correlation length for a finite lattice size:

$$\xi(T) \propto L \sim |T_c - T|^{-\nu} \tag{18}$$

Then the approximations are as follows:
Magnetization:

$$\langle M(T) \rangle \sim (T - T_c)^{\beta} \propto L^{-\frac{\beta}{\nu}} \tag{19}$$

Specific heat C_v:

$$C_v(T) \sim |T - T_c|^{-\alpha} \propto L^{\frac{\alpha}{\nu}} \tag{20}$$

And susceptibility χ:

$$\chi(T) \sim |T - T_c|^{-\gamma} \propto L^{\frac{\gamma}{\nu}} \tag{21}$$

The exact result for the critical temperature was found by Lars Onsager[2] to be: $kT_C/J = 2/\ln(1 + \sqrt{2}) \approx 2.269$, with $\nu = 1$.

2.5 Probability distribution

After the system has reached equilibrium one can look at finding the underlying probability distribution of the system by counting how many times a specific energy appears, plotting it on a histogram and then see the probability of a specific energy.

3 Implementation

Code provided by Morten Hjorth-Jensen was used as a basis for solving different tasks related to the Ising model. The code contains a main program ising2dim as well as several subroutines. The subroutines are:

- **ReadInput** which reads in the parameters for the system as f.ex. the number of Monte Carlo trials, lattice size and temperature.
- **Initialize** which sets up the systems initial energy and magnetization.
- **Metropolis** which performs the metropolis algorithm
- **WritetoFile** which divides all expectation values from the metropolis algorithm before writing to file.

In the main program, MPI is used to parallelize the code to improve the run time. The program also sets up the initial spin configuration and calls the subroutines for in the end finding the expectation values.

4 Results and discussion

4.1 Model verification

Looking back at the analytic solutions we now want to compare them up against the values obtained form the model. We see from table 2 that the expected values of energy and magnetization are fairly close to the analytic solution even for a low number of Monte Carlo cycles. But for the specific heat and susceptibility we see a need for about around 1000000 Monte Carlo cycles, or more depending on how accurate one wants the numerical solution to be.

MC	$\langle E \rangle$	C_v	$\langle \lvert M \rvert \rangle$	χ
100	-2	0	1	4
1000	-1.98800	0.09542	0.99650	3.02229
10000	-1.99510	0.03910	0.99840	3.47795
100000	-1.99644	0.02843	0.99880	3.85162
1000000	-1.99601	0.03318	0.99867	3.99284
10000000	-1.99598	0.03206	0.99866	3.99329
Analytical	-1.99598	0.03208	0.99866	3.99330

Table 2: Possible spin configurations, their degeneracies, energies and magnetizations.

4.2 MC cycles and temperature dependency

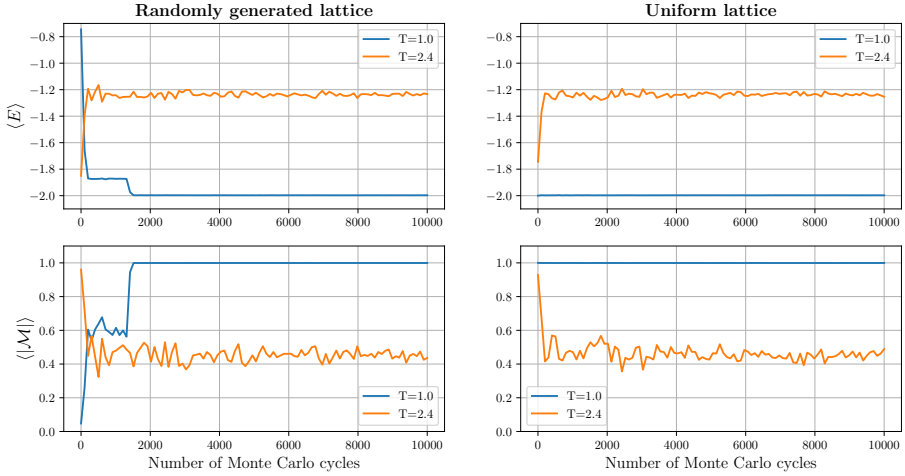


Figure 1: Expected values of energy and magnetization vs number of MC cycles for a: random spin configuration (left), uniform spin configuration (right) for a 20×20 lattice.

From figure 1 we see that after about 2000 MC cycles the system seem to be at an equilibrium state.

From figure 1 for the Uniform lattice we see that for a temperature $T = 1.0$ that we are already at an equilibrium state, i.e. that the expected energy and

magnetism are constant(usually with some noise term caused by using a random number generator). This is however not true for $T = 2.4$ which instead moves to an equilibrium state within well under 500 MC cycles.

On the left side of the figure we have a randomly generated lattice and we are not anymore at an energetically favourably configuration. For $T = 1.0$ the expected energy and absolute magnetization still approaches the same equilibrium state as for the Uniform lattice but the system needs to run for just below 2000 MC cycles. For $T = 2.4$ we have similar graphs for both random and uniform lattices.

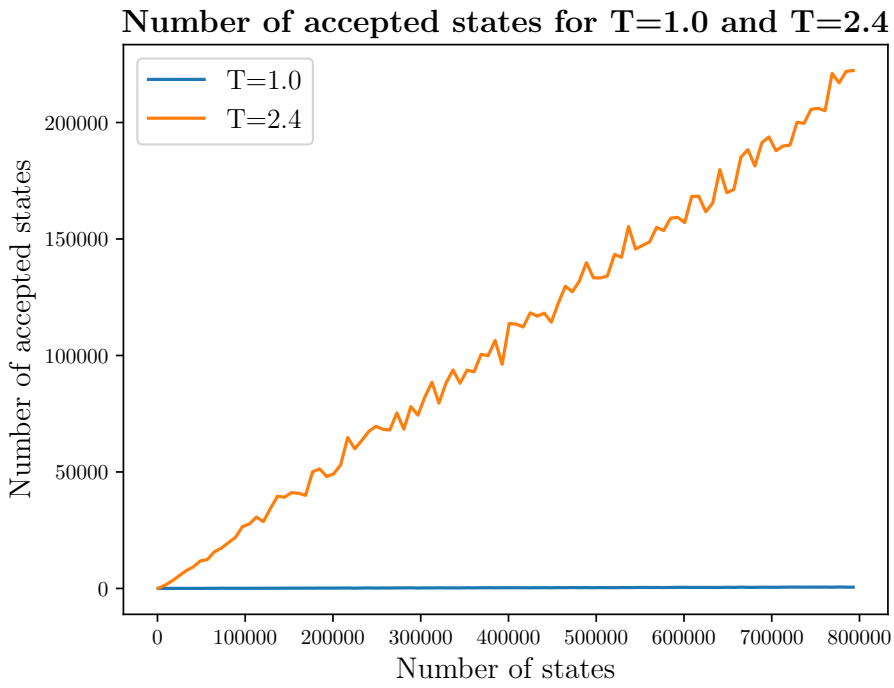


Figure 2: Number of accepted configurations as a function of the number of MC cycles for a 20×20 lattice.

For a system with a given temperature the number of accepted is solely dependent on the acceptance "ratio", determined by the the exponential term in the Metropolis algorithm, and the number of MC cycles one performs. This can be see from figure 2 which shows the number of accepted configurations as a function of the total number of MC cycles for a 20×20 lattice for temperatures $T = 1.0$ and $T = 2.4$. For the temperature $T = 2.4$ we see a linear relationship between accepted configurations and the number of MC cycles. For $T = 1.0$ the graph seems flat but if zoomed in on one still finds a linear relation, just lower compared to the case for $T = 2.4$.

Another figure which shows this trait of increased acceptance ratio is figure 3 were we see a clear increase in the acceptance ratio as the temperature rises. A dotted line is plotted to show the Onsager limit $T_c = 2.269$ and we see the position coincides well with where the graph changes from concave up to

concave down.

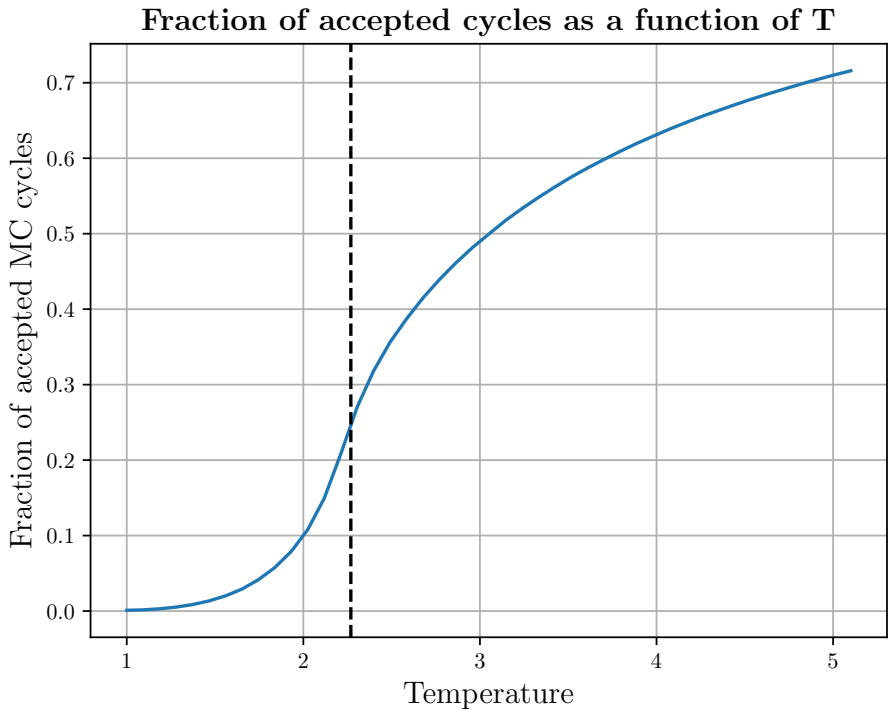


Figure 3: Fraction of accepted configurations as a function of temperature

4.3 Probability distribution

The goal was to make a probability distribution plot but I was not successful in creating it. What I expect would have happened was in the case of $T = 1.0$ for the energies to be mostly located at the same energy since the system should be quite stable. As for $T = 2.4$ I would expect there to be more fluctuations in the energies.

4.4 Studies of phase transition

In this section we are to look at how the Ising model behaves around the critical temperature. In figure 4 one can see how the expected absolute magnetization goes towards zero when we are above the critical temperature, as mentioned briefly earlier.

The critical temperature, where we have the phase transition, is expected to be where the specific heat and susceptibility diverges. For the specific heat C_v and susceptibility χ in figure 4 we see clear peaks of graphs close to the dotted critical temperature line, especially for larger lattice sizes. Estimating the critical temperature for a system of a specific lattice size can then be done by taking the maximum value of the graphs for C_v and χ. These estimates can be found in table 3. If we had not known the exact critical temperature one

could use equation 17 with $\nu = 1$ for two different lattice sizes to estimate the constant a, then estimate $T_C(L = \infty)$, something we will attempt in the last section. This is because we can not model an infinitely large lattice for which we would expect to be able to read out the critical temperature directly.

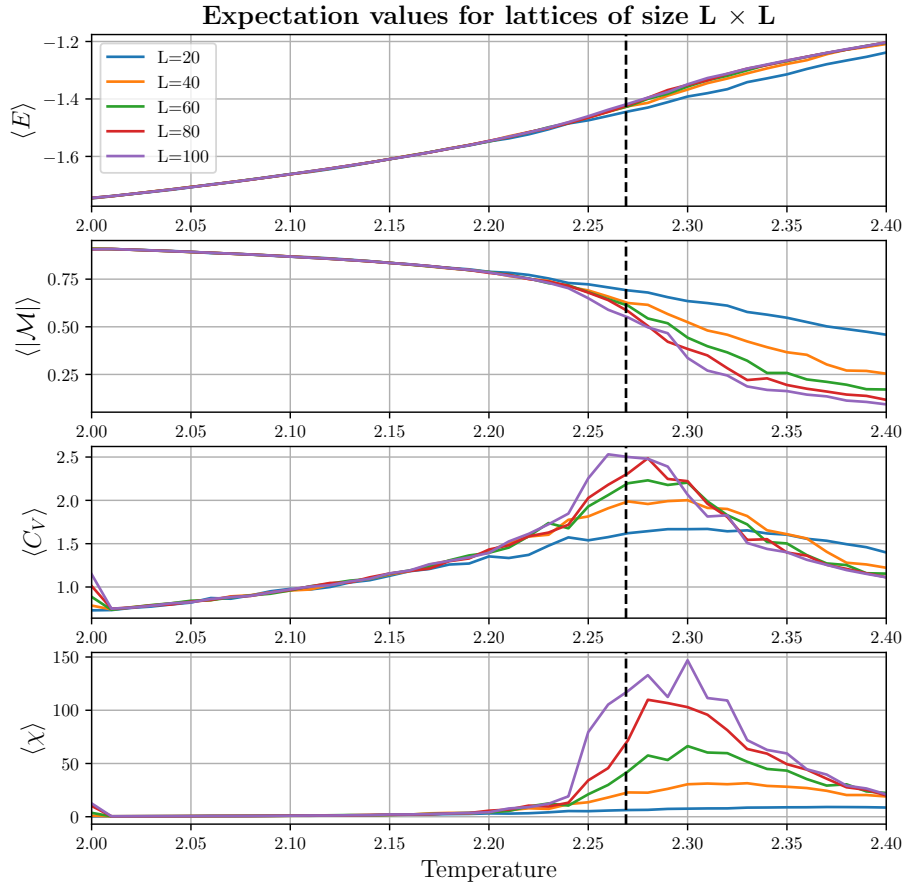


Figure 4: Expectation values for lattices of different length for the temperatures T $\in [2.0, 2.4]$.

L	$T_c(C_v)$	$T_c(\chi)$
20	2.31	2.37
40	2.3	2.33
60	2.28	2.3
80	2.28	2.28
100	2.26	2.3

Table 3: The critical temperature T_c extracted from the graphs of C_v and χ for different lattice sizes.

4.5 Estimating the critical temperature

Lastly we look at how the critical temperature estimated from the Ising model compares up against Lars Onsager exact result. By using equation 17 solved for $T_c(L = \infty)$ one can set up the relation:

$$\begin{aligned} T_c(L_1) - aL_1^{-1} &= T_c(L_2) - aL_2^{-1} \\ \rightarrow a &= \frac{T_c(L_1) - T_c(L_2)}{L_1^{-1} - L_2^{-1}} \end{aligned} \tag{22}$$

When calculating the constant a we will omit $L = 20$ and only compute a for different combinations of $L = 40, 60, 80, 100$. This because in the case of $L = 20$ we are barely able read out the critical temperature from the figure 3 which indicates that its such a bad approximation for the infinite lattice that it would skew our results for the estimated critical temperature.

Taking the mean of all the computed a's gives us:

$$a_{mean}(C_v) = 2.944 \tag{23}$$

and

$$a_{mean}(\chi) = 1.067 \tag{24}$$

Inserting these a_{mean} values into 17 as well as the mean of $T_c(L = 40, 60, 80, 100)$ and of L_{mean}, and then solving for $T_c(L = \infty)$ we get

$$T_c(L = \infty)(C_v) = T_c(C_v)_{mean} - a_{mean}L_{mean} = 2.238 \tag{25}$$

and

$$T_c(L = \infty)(\chi) = T_c(C_v)_{mean} - a_{mean}L_{mean} = 2.287 \tag{26}$$

These estimated critical values are close to Lars Onsager's exact result of $T_C = 2.269$ but as close as expected leading me to believe I've made a mistake in my method for calculating a_{mean} or $T_c(L = \infty)$. But still, by looking at figure 3 it does seem like the graph peaks moves closer to the exact result as the lattice size L grows larger so maybe, as the tendency table 3 shows, a larger lattice would increase the accuracy of the estimated critical temperature.

5 Conclusion

For this project we simulated phase transitions by using the Ising model in two dimensions. We checked the stability of the model by comparing it up against the analytic solution for a 2×2 lattice in which it turned out to work as intended.

For the 20×20 lattice we studied how many MC cycles was needed to reach equilibrium for two types of initial lattices, as well as studying how the temperature of the system affects the number of accepted MC cycles in the Metropolis algorithm. The equilibrium time was found to be below 2000 MC cycles for

the randomly generated lattice and below 500 MC cycles for the uniform lattice implying that the a well chosen initial state lowers the equilibrium time. The fraction of accepted MC cycles turned out to increase with increased temperature.

Our main objective was to find the critical temperature at where the phase transition happens. We studied how the specific heat and susceptibility behaved in the range where we expected the critical temperature to lie. The peaks of the specific heat and susceptibility was found for lattices of different sizes and then used in in the equation for a finite lattice in an attempt to estimate the critical temperature for the infinite lattice. From the specific heat we found the critical temperature to be $T_c(L = \infty)(C_v) = 2.238$ and for the susceptibility we found it to be $T_c(L = \infty)(\chi) = 2.287$. The difference between these values and Lars Onsager's $T_c = 2.269$ were not significantly large and are expected to move closer to $T_c = 2.269$ for larger lattice sizes.

References

[1] Hjorth-Jensen, M. (2015). *Computational Physics - Lecture Notes 2015*. University of Oslo.

[2] Lars Onsager. Crystal statistics. i. a two-dimensional model with an order-disorder transition. *Phys. Rev.,* 65:117-149, Feb 1944.