Numerical study of phase transitions with the Ising model

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(Dated: November 19, 2019)

In this article we go through a numerical study on phase transitions using the Ising model in 2 dimensions with periodic boundary conditions. As benchmarks for our calculations we analytically solve the case with a 2 x 2 lattice. Afterwards we numerically compute the Ising model for a 20 x 20 lattice and use this to determine how many Monte Carlo cycles are needed before equilibrium is reached. By using the Monte Carlo method with the Metropolis algorithm as a sampling rule we get values for the mean energy, the absolute value of the magnetization, the heat capacity and the susceptibility of the spin system. Therefore the use of the numerical Ising model gives a good model for phase transitions in magnetic systems. The crux of this numerical study will be performing Monte Carlo sweeps over larger lattices with a temperature step $\Delta T = 0.01$ from $T = 2.0$ to $T = 2.35$ with 10^7 Monte Carlo cycles for each temperature. We then used this data for different system sizes to calculate the critical temperature for a $\infty \times \infty$ lattice and got $T_C(L = \infty) = 2.270 \pm 0.004$, which is within 0.2σ of the analytical value. We also parallelize our code, and achieve a near optimal speed up, apart from when using all 4 cores available in the system.

INTRODUCTION

In science it is important to study the world of the microscopic which makes up the actual macroscopic world that we live in. However, things get messy quickly as the microscopic world is comprised of an uncountable number of microstates making calculations by hand impossible. This is where numerical methods comes to our rescue. In this article we will be looking at numerical solutions of "The Ising model" in 2D to simulate phase transitions. The model gives us the energy of particles in a 2D lattice, which is based on the "spin" values which can either be "up" (+1) or down"(-1). This system has an analytical solution, first found by Lars Onsager [1]. In this article we will also try to reproduce some of these results numerically.

First we analytically solve the case for a 2 x 2 lattice, which will serve as a benchmark for our numerical calculations. Afterwards we numerically implement the Ising model for a lattice of size 20 x 20. Monte Carlo cycles over the lattice will serve as our time step in predicting how the spin-systems behave. We will find how many Monte Carlo cycles that are needed before the system reaches equilibrium starting from an ordered and a random lattice spin-configuration. Quantities of interest will be the mean energy $\langle E \rangle$,mean absolute magnetization $\langle |M| \rangle$, heat capacity C_v and magnetic susceptibility χ. Furthermore, we will statistically analyze the probability of an energy by counting the number energy occurrences during a Monte Carlo sweep of the system. Lastly, we will study phase transitions by simulating larger lattices, up to 100 x 100, near the critical temperature.

For reproducibility the numerical code used for the results and plots in this article can be found on the website [2].

METHOD

The Ising Model

To simulate phase transitions we will be using the Ising model in two dimensions. The energy of this model without an external magnetic field is given as equation (1), where the sum is taken over $\langle kl \rangle$ the nearest particle neighbours only, up to all N (or n x n) particles/spins. For instance if we look at spin s_k, then s_l is the spin of each neighbouring particle which can either be "up" or "down" $s = \pm 1$. J is an energy constant for the strength of the magnetic interaction between the neighbouring spins. We will be assuming periodic boundary conditions, meaning that the particles on the edges of the lattice will behave as if they have four neighbours. These imaginary neighbours correspond to the particle at the opposite side of the lattice, and we have to make sure that the interactions between two particles are not counted more than once.

$$E = -J \sum_{\langle kl \rangle}^{N} s_k s_l [3] \tag{1}$$

From the analytical solution from Lars Onsager this model exhibit a phase transition near a critical temperature T_C, which for an infinite lattice (when all interaction energies are equal) will be given by [1]

$$\sinh\left(\frac{2J}{kT_c}\right)\sinh\left(\frac{2J}{kT_c}\right) = 1,$$

which we can rewrite as

$$T_C = \frac{2J}{k \ln\left(1 + \sqrt{2}\right)}. \tag{2}$$

It can then be shown that this critical temperature scales with system size as

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

where L is the size of one dimension of the system, so the total number of spins equal $L \times L$

Analytical Solutions for a 2 x 2 Lattice

By using the Ising model for the energy given by equation (1) and assuming periodic boundary conditions we get the results

seen in Table I. Using the table we can do some statistics and calculate the partition function $Z(\beta)$, mean energy $\langle E\rangle$, mean magnetization $\langle|M|\rangle$, heat capacity c_v and magnetic susceptibility χ of the 2 x 2 lattice system.

Table I. Table containing values of all microstates of a 2 x 2 particle lattice with 2 spin states.

E	M	S_{up}	Multiplicity
- 8 J	4	4	1
0	2	3	4
0	0	2	4
+ 8 J	0	2	2
0	- 2	1	4
- 8 J	- 4	0	1

Due to the nature of the problem we will make extensive use of some hyperbolic functions such as

$$\cosh(x) = \frac{e^x + e^{-x}}{2}, \quad \sinh(x) = \frac{e^x - e^{-x}}{2},$$

and

$$\cosh^2 x - \sinh^2 x = 1$$

$$Z = \sum_i e^{-\beta E_i} \tag{4}$$

First we calculate the partition function given as equation (4). This can be used as a normalization constant and a way of finding average values directly. Using the values in Table I we get that the partition function for our system is

$$Z(\beta) = 12 + 4\cosh(8\beta J).$$

Now we can calculate the average energy by using the partition function in the formula,

$$\langle E\rangle = \frac{1}{Z}\sum_i E_i e^{\beta E_i} = -\frac{1}{Z}\frac{\partial Z(\beta)}{\partial\beta} = -\frac{8J\sinh 8\beta J}{3+\cosh 8\beta J}. \tag{5}$$

We can also find the average value of the absolute magnetization using the partition function,

$$\langle|M|\rangle = \frac{1}{Z}\sum_i |M_i| e^{-\beta E_i} = \frac{2(2+e^{8\beta J})}{3+\cosh 8\beta J}. \tag{6}$$

To find the heat capacity we need the mean squared energy

$$\langle E^2\rangle = \frac{1}{Z}\sum_i E_i^2 e^{-\beta E_i} = \frac{1}{Z}\frac{\partial^2 Z(\beta)}{\partial\beta^2} = \frac{64J^2\cosh 8\beta J}{3+\cosh 8\beta J}$$

which gives us the variance:

$$\sigma_E^2 = \langle E^2\rangle - \langle E\rangle^2 \implies$$

$$\sigma_E^2 = \frac{64J^2\cosh 8\beta J}{3+\cosh 8\beta J} - (-\frac{8J\sinh 8\beta J}{3+\cosh 8\beta J})^2 = \frac{64J^2(1+3\cosh 8\beta J)}{(3+\cosh 8\beta J)^2}$$

This variance is then used to find the analytical value of the heat capacity, which is given as the variance divided by Boltzmann's constant and temperature squared,

$$c_v = \frac{\sigma_E^2}{k_B T^2} \tag{7}$$

Similarly, we can find the magnetic susceptibility, first by finding the mean square magnetization

$$\langle|M|^2\rangle = \sum_i |M|^2 e^{-\beta E_i} = \frac{8(1+e^{8\beta J})}{3+\cosh 8\beta J},$$

and then using this to find the variance of the absolute magnetization

$$\sigma_{|M|}^2 = \langle|M|^2\rangle - \langle|M|\rangle^2 =$$

$$\frac{8(1+e^{8\beta J})}{3+\cosh 8\beta J} - (\frac{2(2+e^{8\beta J})}{3+\cosh 8\beta J})^2 = \frac{4(3+2e^{8\beta J}+2\cosh 8\beta J)}{(3+\cosh 8\beta J)^2},$$

thereby leading us to an expression for the magnetic susceptibility,

$$\chi = \frac{\sigma_{|M|}^2}{k_B T} = \sigma_{|M|}^2\beta. \tag{8}$$

Solving the Ising model numerically

To solve the Ising model numerically we initialize our system by creating a matrix which will serve as our lattice. We can choose whether we want our spins to be ordered or to assign each of the spins a value based on a random number generator. An ordered lattice is the representation of a magnetic system in its ground state. In order to get a system that is not in the ground state we want the spins to be up and down randomly. To generate this random spin configuration we use a random number generator to get a number between 0 and 1, if this number is larger than 0.5 we assign spin up, with value +1, otherwise we assign it as down, -1.

In a loop over Monte Carlo cycles we will then evaluate this lattice. An ordering of the spins in the matrix will then be proposed, this will be inserted into the metropolis algorithm, this algorithm is the numerical function that we utilize in order to decide if a spin should be flipped or not. This algorithm decides if the spin should be flipped by the use of a random number, this is in attempt to closely simulate randomness. After the spins have been flipped the energy and magnetisation are updated. These steps are done for all the Monte Carlo cycles.

This process will be repeated for all temperatures we want to consider. For each temperature the values for the energy and magnetisation are then used to find the average energy and the absolute value of the average magnetisation.

The numerical implementation for the Ising model that we have used for the calculations in this article contains relatively large calculations. This is largely because of the use of the Monte Carlo method and Metropolis algorithm, as these contain multiple large loops. Due to this the program is slow in its calculations if we want a high precision. A method of reducing the run time on these operations is to parallelize. We have therefore for the larger matrices parllelized the code using MPI (Message Passing Interface). In addition the program is compiled using optimization flags to reduce the total runtime as much as possible. To test this parallelization, we ran simulations with system sizes $L = 40$ and $L = 100$, and temperatures $T = 1.5$ and $T = 2.3$ and took the average time of 100 runs. We then did this for all four configurations of the values for L and T mentioned. These simulations was done on a computer with an Intel i5-4670K processor with four cores, and with 8 GB of RAM. We timed the simulations using a single to all four cores of the CPU.

When looking at larger lattice sizes (from 40×40 to 100×100) we narrowed the temperature range from 2.00 to 2.35, and used a temperature step of 0.01. For each simulation we then used 10^7 Monte Carlo cycles to calculate the mean energy, heat capacity, mean absolute magnetization and magnetic susceptibility. We did this for the lattice sizes of 40×40. 60×60, 80×80 and 100×100. We then used the temperature where the magnetic susceptibility and heat capacity was highest to approximate the critical temperature. To get a better estimate of this temperature, we used the cubic spline function in `interp1d` from `scipy.interpolate`, and used the maximum temperature from this cubic spline as our estimate for the critical temperature. We then used a linear fit of $1/L$ vs the critical temperature to find a line $T_C(L) = a(1/L) + b$ (from equation (3)), so that when $L = \infty$ $T_C = b$, which we used as our estimate for $T_C(L = \infty)$. To find this line, we used the `polyfit` function from numpy, from this function we also get the covariance matrix. From this we get the variance of b as the bottom right element, we then used the square root of this as the standard deviation for $T_C(L = \infty)$. We looked at heat capacity and susceptibility separately, and then compared the results from the two measurements.

RESULTS

Analytical solutions

The analytical results are very useful for comparison to the values we get from the numerical method. Through setting the constants $k_B = 1$ and $J = 1$ we can calculate the analytical values for the mean temperature, mean magnetization, heat capacity and the susceptibility of the system at differed temperatures. We do this by inserting the temperature we want to look at in the equations for these values given in the methods section, 5, 6, 7 and 8. We use the temperature T=1 to get analytical values, this gives us the following results seen in table II.

Table II. Table showing analytical values per particle ($N = n^2$) for 2 x 2 lattice at a temperature T = 1, with J = k_B = 1.

E	$\mid M \mid$	c_v	χ
-1.99598	0.998661	0.0320823	0.00401074

Time Needed to Reach Equilibrium

We use the numerical implementation of the Ising model with two spins to check if the numerical model corresponds to the analytical value that we have calculated. Table III shows the numerical values for the different properties given a ordered 2x2 lattice. This table shows the values for a different numbers of Monte Carlo cycles. We see in this table that when we have more cycles we will get a values that are closer to the analytical ones.

Table III. Values for energy, mean magnetization, heat capacity and susceptibility given by the number of Monte Carlo cycles. For T=1.

Monte Carlo Cycles	E	$\mid M \mid$	C_v	χ
1000	-1.99400	0.998000	0.047856	0.00598400
10^6	-1.99591	0.998620	0.032653	0.00418238
10^8	-1.99597	0.998656	0.032195	0.00402421

In order to see how many Monte Carlo cycles we need for the values to become stable we have plotted the average energy and the average magnetization as a function of Monte Carlo cycles. The number of Monte Carlo cycles can be seen as the time it takes for the values to become steady. To see how long it takes for the energy and absolute magnetization to stabilise we look at different temperatures and starting configurations of a 20 x 20 lattice. In figure 1 we see the energy and magnetization as a function of time for an ordered lattice at temperature $T = 1$, meaning that all the spins start either up or down. Here we see a stabilization to an even, small oscillation after about 2000-3000 Monte Carlo cycles.

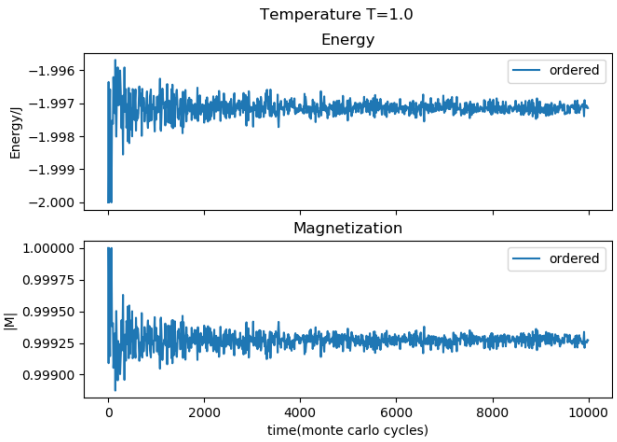

Figure 1. Mean energy and mean magnetization as a function of Monte Carlo cycles for temperature T = 1.0. Starting state is ordered.

In figure 2 we see the same situation as the previous figure except for the fact that these graphs represent a 20x20 lattice that has a randomly configured starting point. We see in this figure that the oscillations in the beginning are larger than for the ordered ones, but it converges to the same values for the mean energy and mean magnetisation. This random system stabilized after more time than the ordered system for the same temperature. In addition this system has larger oscillations around the exact value.

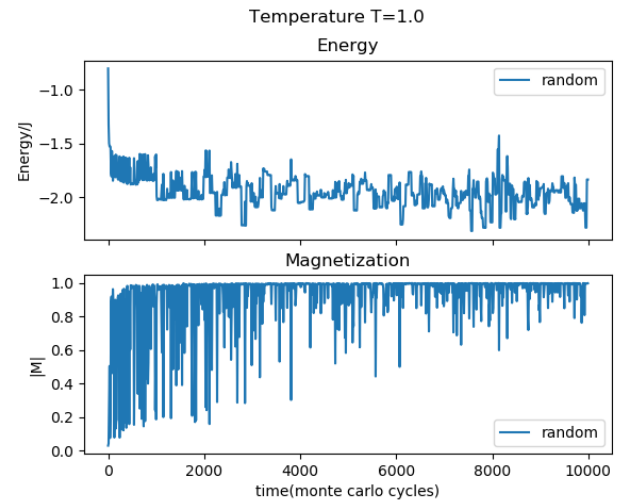

Figure 2. Mean energy and mean magnetization as a function of Monte Carlo cycles for temperature $T = 1.0$. Random initial state.

Figure 3 is similar to the earlier ones, it shows the amount of time needed for the system to reach the steady state with a ordered starting configuration and a temperature of 2.4 k_B/J.

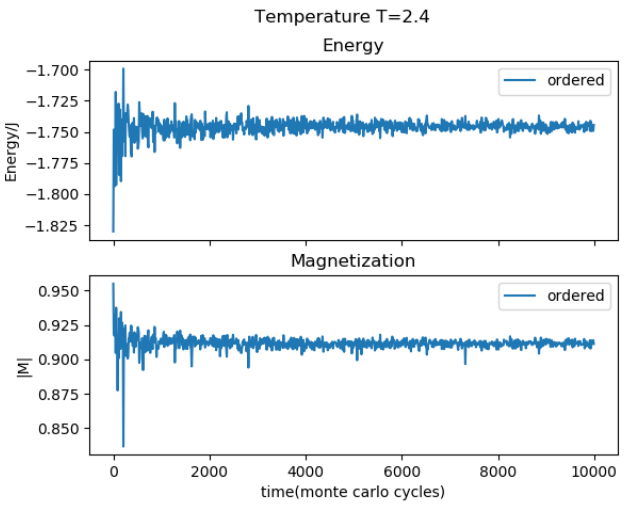

Figure 3. Mean energy and mean magnetization as a function of Monte Carlo cycles. Temperature 2.4 Ordered.

Figure 4 is a plot over the mean magnetization and mean energy for as a function of Monte Carlo cycles. This is a random starting configuration lattice of temperature $T = 2.4$. We can see from this, and the previous figure, that the random configuration has uses a longer time to stabilize and has lager oscillations, but does ultimately converge to the same values.

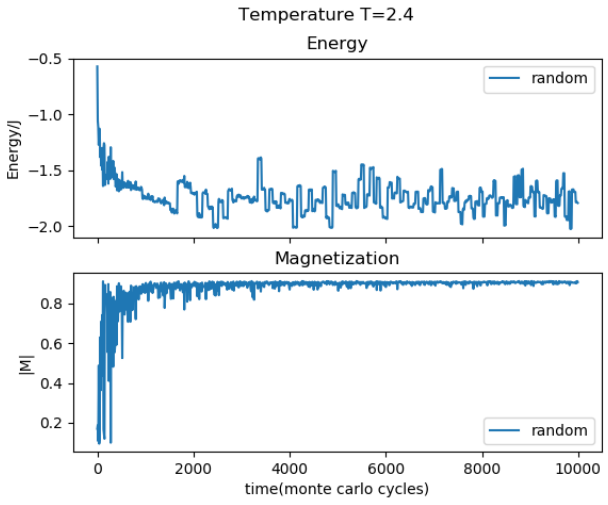

Figure 4. Mean energy and mean magnetization as a function of Monte Carlo cycles, temperature 2.4. Random initial configuration.

We also have plotted the number of accepted configurations (moves) taken due to the metropolis algorithm. See figure 5 for T = 1 and figure 6 for T = 2.4.

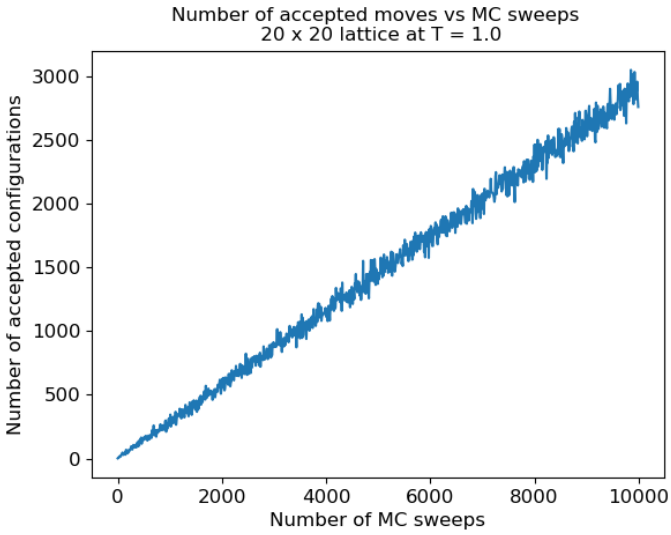

Figure 5. Number of configurations that are accepted by the metropolis algorithm for a 20 x 20 lattice, T = 1

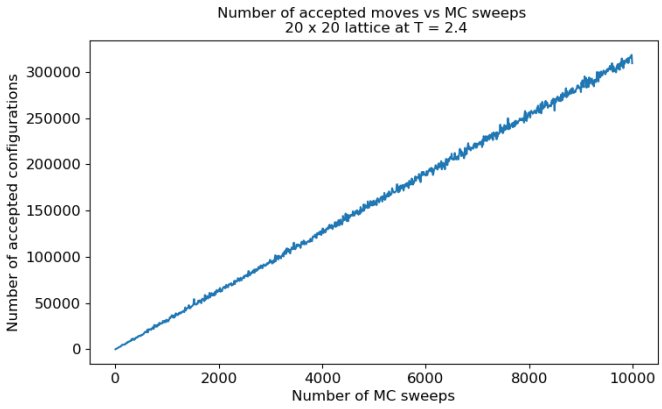

Figure 6. Number of configurations that are accepted by the metropolis algorithm for a 20 x 20 lattice, T = 2.4

Analyzing the Energy Probability

In conjunction with the previous results of a 20 x 20 lattice we have counted the number of occurrences of energies and made a probability histogram $P(E)$ for 10^7 MC cycles, see figure 7, showing results for T = 1 and figure 8 for $T = 2.4$. The histograms are normalized, so that each bin's height represents the probability of an energy and they all sum up to 1.

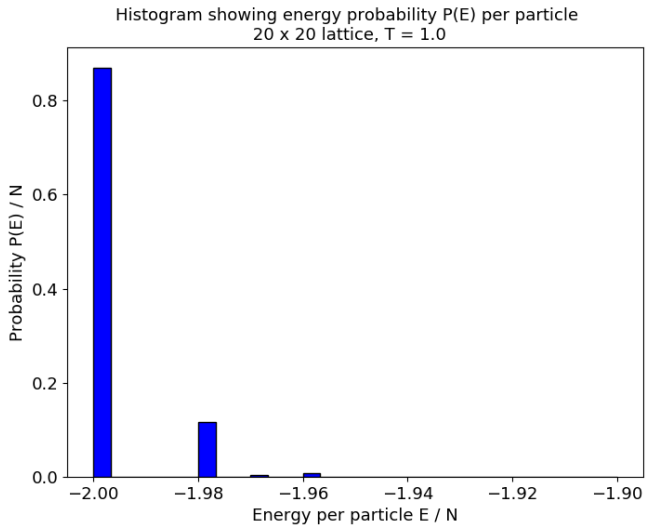

Figure 7. Histogram showing the energy probability at temperature $T = 1.0$. The computed variance is $\sigma_E^2 = 0.023$ and the average $\langle E \rangle = -1.997$

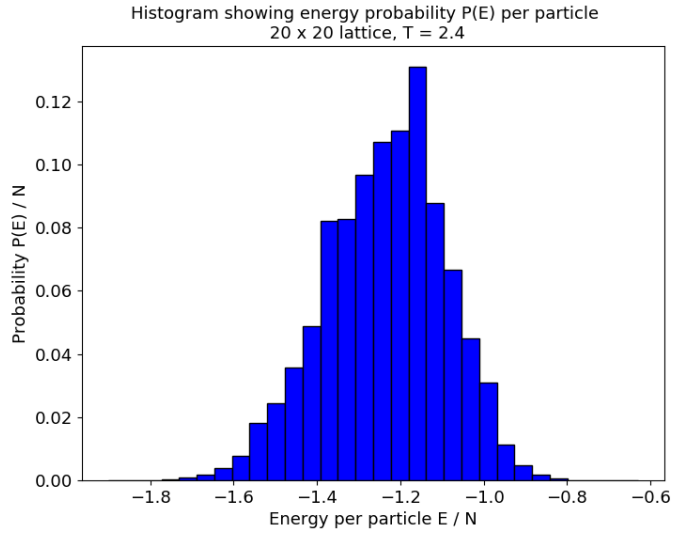

Figure 8. Histogram showing energy probability at temperature $T = 2.4$. The computed variance is $\sigma_E^2 = 8.12$ and the average $\langle E \rangle = -1.24$

Monte Carlo Cycles at Different Temperatures and Lattice Sizes

When we ran with larger system sizes we the values 40, 60, 80 and 100 for L. We tested with temperatures in the interval between 2.0 and 2.35, here we tested for $T = 2.0, 2.01, 2.02, \ldots, 2.35$. For every temperature we ran with 10^7 Monte Carlo cycles. In Figure 9 we have plotted the mean energy from these simulations, Figure 10 is a plot over the heat capacity with the cubic spline used to estimate T_C and in Figure 11 we have plotted the magnetization.

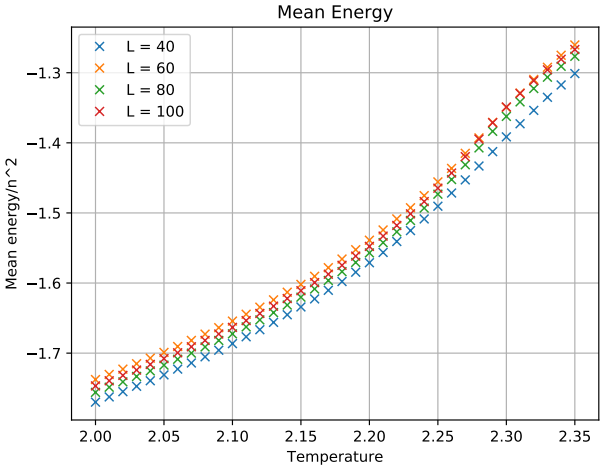

Figure 9. Mean energy as a function of temperature, for several system sizes.

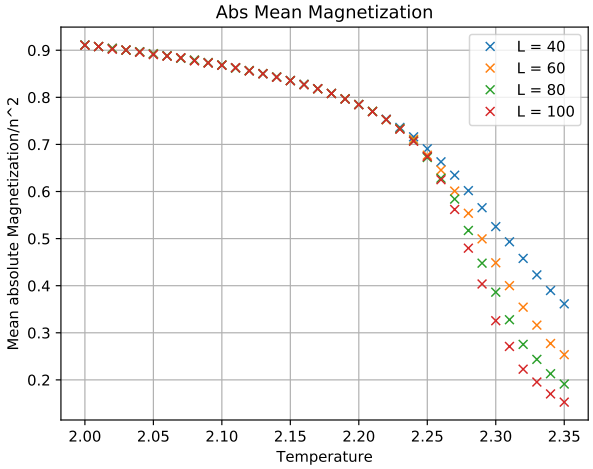

Figure 11. Mean magnetization as a function of temperature, for several system sizes.

We also plotted the magnetic susceptibility χ for each simulation in Figure 12. When plotting the temperature where the cubic spline was highest for each system size we got the plot in Figure 13, plotted here as the critical temperature for the data from the heat capacity and from the susceptibility. Both lines had an intercept of 2.270 ± 0.004.

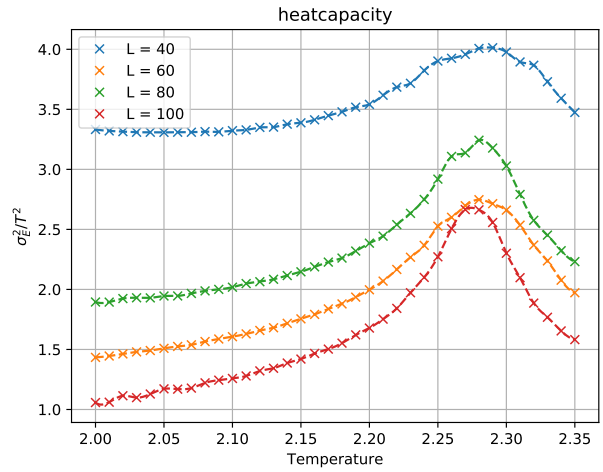

Figure 10. Heat capacity as a function of temperature, for several system sizes. A cubic spline of the data points is added as a dashed line

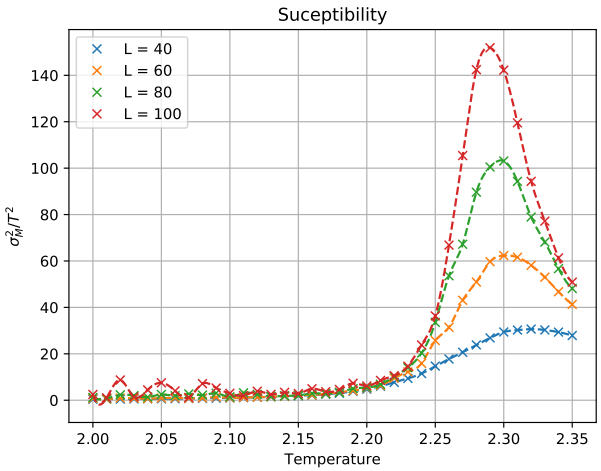

Figure 12. Magnetic susceptibility as a function of temperature, for several system sizes. A cubic spline of the data points is added as a dashed line.

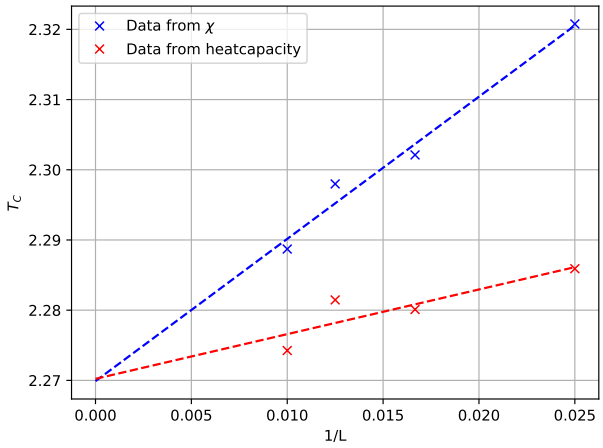

Figure 13. The estimated critical temperature for each system size, plotted vs $1/L$. The plot includes data from the susceptibility and heat capacity. A linear fit for each data set is added with a dashed line.

We also tested the time it took to run our simulation, with a varying number of cores. We tested for the system sizes of $L = 40$ and $L = 100$, and the temperatures $T = 1.5$ and $T = 2.3$. For each configuration of T and L we averaged the time over 100 runs, for 1 to 4 cores with 10^5 Monte Carlo cycles. The results are plotted in Figure 14. The theoretical best time, given the time used by one core is given by the dashed line. The standard deviation of the mean time was also calculated and added as error bars, but these are too small to see.

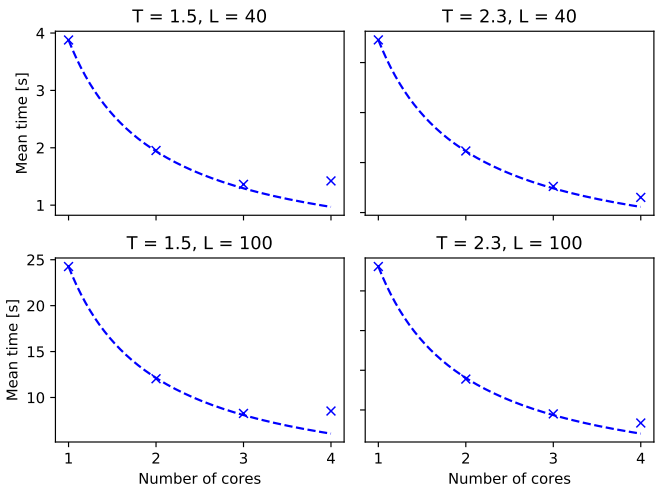

Figure 14. The time used to run simulations with 10^5 Monte Carlo cycles. The dashed line is the theoretical best improvement, given by the time used by one core divided by the number of cores.

DISCUSSION

Comparison of Analytical and Numerical Results

From the results in table II and table III we can see that for both 10^6 and 10^8 Monte Carlo cycles we get results that correspond with up to 4 decimal places with the analytical solutions for the mean energy and the absolute mean magnetization. However, there is a larger gap between in the heat capacity and the susceptibility. This is for a 2x2 lattice. The values will be quite close for less Monte Carlo cycles and will then fluctuate around the analytical value. This means that our choice of using 10^7 MC cycles for the heavier computations is a good compromise between speed and results.

For the larger lattice sizes, we see from Figure 10 that the system exhibits signs of a phase transition around a temperature of 2.25 to 2.30, as there are discernible peaks in the data, for all system sizes. This is also something we see in Figure 12, where we also see some peaks, these are also somewhat sharper than those in the heat capacity plot. In Figure 11 one also see signs of a phase transition, but here it is shown as a more negative slope. One thing to note from Figure 10 is that at a given temperature, the heat capacity seems to strongly depend on the system size, with $L = 40$ having the highest heat capacity, then $L = 80$, $L = 60$ and $L = 100$. This order seems somewhat strange, as one would expect it to either increase or decrease with system size, if it changed at all. We do not have a good explanation for this result, however from Figure 13 we see that the plots of susceptibility and heat capacity predict the same value for $T_C(L = \infty)$, but disagrees on all other values for L, which is an indication of the plot for heat capacity not being completely wrong, as the peaks seem to converge towards the correct value for $T_C(L = \infty)$. This value predicted by both the peaks from the susceptibility data and those from the heat capacity data agrees well with the result by Onsager of $2/\ln(1+\sqrt{2}) \approx 2.269$ for $J = 1$ [1], with both results ending up 0.2σ away from this value. This is then a strong indication that the peaks happen at the correct values. In future work on could possibly improve on these values by simulating for a smaller temperature step size, and adding more Monte Carlo cycles.

Time Needed to Reach Equilibrium

From the figures 1, 2, 3 and 4 we see that with a only 2000-4000 Monte Carlo cycles the values for the energy and magnetization start to oscillate around the analytical value. We also see from these figures that the random starting configuration for both temperatures used more time to stabilize and has larger oscillations, thus will have larger deviations from the analytical values. For future work we could run the disordered for longer (more MC cycles) to see if there is a point where the system stabilizes. For instance we see from figure 2 that the energy and especially the magnetization might stabilize with a higher number of MC cycles.

We also take a look at the number of accepted spin flips at

different temperatures. Firstly, If we compare figure 5 and figure 6 we see that they both scale linearly, i.e the number of moves accepted scale linearly with the number of MC sweeps over the lattice. In addition, we clearly see that for the same number of MC sweeps the number of spin flips by the metropolis algorithm is two orders of magnitude higher at $T = 2.4$, as opposed to $T = 1.0$. Our intuition tells us that this is due to the higher energy availability in the system which means that a move (spin flip) becomes more probable. This is also something we see in the next section.

Energy Probability

Based on the histograms seen in figure 7 and 8 we see that the most probable energy (peak) is also the mean energy we compute after the Monte Carlo cycles. This statistical behaviour is what we would expect from a normal distribution and tells us that the energies are somewhat normally distributed.

Furthermore, we see that the mean energy per particle/spin at $T = 1$ is fairly close to the analytical value of $\langle E \rangle = 1.995$, whereas we get $\langle E \rangle = 1.997$, which tells us that the numerically found energies are near the analytical values. We also notice that the peak at $T = 1$ is quite narrow which to be coherent with the small variance of $var(E) = \sigma_E^2 = 0.023$. In comparison, looking at figure 8 we see that the energy is more widely spread $var(E) = \sigma_E^2 = 8.12$, presumably because of the higher temperature $T = 2.4$ which makes multiple spin configurations available in the 20 x 20 lattice system. The much larger computed variance at $T = 2.4$ is also corresponds with what we see in the figure 8. A much greater probability spread. It is worth mentioning that this was the result of one MC sweep of the system. For future work one could perform multiple runs with 10^7 or higher number of Monte Carlo cycles to get better statistical data.

Parallelization

From Figure 14 we see that the time used to simulate the system generally decreases as the number of cores increase. However, when increasing from 3 to 4 cores, the increase is marginal for $T = 2.3$, and for $T = 1.5$ it even seems to increase somewhat. Since $T = 2.3$ is closer to the critical temperature than $T = 1.5$, and we see from Figures 5 and 6 that the number of sweeps required is higher close to this temperature, it then seems that for a higher number of sweeps, parallelization makes more of a difference. However the total size of the system does not seem to affect how parallelizable the system is. From Figure 14 we also see that in this case, increasing from 1 to 2 or 3 cores gives a speed up which is close to optimal, while 4 is somewhat above. One possible explanation for this, other than the program not being parallelizable is that we tested this on a computer with four cores. If we assume the computer always need some CPU power to background processes, then all 4 cores will not be fully available. The speed up of parallelization is then a topic which could be further investigated, using a system with more cores available to make this effect smaller.

CONCLUSION

To summarize, we have numerically implemented the Ising model and compared it to analytical results. First, we solved the 2 x 2-case that served as a benchmark for our results. Afterwards we moved on to a 20 x 20 lattice and found out that it takes about 2000-3000 MC cycles before the system reaches equilibrium depending on the temperature and starting configuration (random or ordered). Then we looked at how many spins that were flipped by our sampling rule, the metropolis algorithm. We saw that for higher temperatures there is a considerable increase, up to two orders of magnitude higher number of accepted spin flips.

By counting the number of energy occurrences we were able to make an energy probability histogram showing $P(E)$ at different values E. From this we saw a normal distribution behaviour as the mean energy also was the most probable energy.

Lastly we iterated around the critical temperature $T \in [2.00, 2.35]$ with a temperature step $\Delta T = 0.01$ and 10^7 Monte Carlo cycles for each step. This was done with varying lattice sizes, up to 100 x 100 and the data obtained from this was used to estimate the critical temperature T_C in the thermodynamic limit $L \to \infty$. The analytical result found by Lars Onsanger was $T_C(L = \infty) \approx 2.269$, while our numerical results gave us $T_C(L = \infty) \approx 2.270 \pm 0.004$, which means that the numerical value is within 0.2σ of the analytical value.

This way of implementing the Ising model numerically can be generalised so that one may apply it to other similar situations.

[1] L. Onsager, "Crystal statistics. i. a two-dimensional model with an order-disorder transition," *Phys. Rev.*, vol. 65, pp. 117–149, Feb 1944.

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[3] Hjort-Jensen M., "Computational Physics: Lecture Notes Fall 2015," *Lecture notes*, pp. 421–442, 2015.