FYS4150
Project 3, deadline October 25.

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Abstract

Introduction

The Ising model in two dimensions will be studied and discussed in this report. The model is widely used, both in the study of phase transitions and statistics (source). In this report, the Ising model will be used to study phase transitions. In particular, the transition from a system with magnetic moment, to a system with zero magnetic moment. The Ising model predicts a phase shift at a given temperature. The system studied in this report will be a two dimensional lattice, where each lattice point only can take two different values. These values represent the spin, up-spin or down-spin, but can be represented in many ways.

The report will start off by an analytical solution for the case with a 2×2 lattice before moving on to solving this system numerically. This will be done by using the Metropolis algorithm. The results computed with the Metropolis algorithm will be compared to the analytic solutions. The main emphasis will be put on the Metropolis algorithm, its efficiency and precision (tror jeg).

Method

It is possible to derive an analytic solution for the simplest of the two dimensional case. Namely a 2×2 lattice with periodic boundary conditions. The partition dunction is given by:

$$Z = \sum_{i=1}^{16} e^{-J*E_i\beta} \tag{1}$$

Where $\beta = \frac{1}{k_b T}$. There are 16 different states of energy. Luckily, a lot of these yield the same result. Summing up all of these gives:

$$Z = 2e^{-8\beta} + 2e^{8\beta} + 12 \tag{2}$$

The mean energy and magnetization is given by respectively:

$$E = \frac{1}{Z} \sum_{i=1}^{16} E_i e^{-J*E_i\beta} = \frac{-16e^{8\beta} + 16e^{-8\beta}}{Z} \tag{3}$$

and

$$M = \frac{1}{Z} \sum_{i=1}^{16} M_i e^{-J*E_i\beta} = \frac{8e^{8\beta} + 16}{Z} \tag{4}$$

The specific heat is given as the variance of energy divided by $k_b T^2$:

$$c_v = \frac{1}{k_b T^2} \left(\frac{128e^{8\beta} + 128e^{-8}\beta}{Z} - \left(\frac{-16e^{8\beta} + 16e^{-8\beta}}{Z} \right)^2 \right) \tag{5}$$

The variance of magnetism divided by $k_b T$ reveals the susceptibility.

$$X = \frac{1}{k_b T} \left(\frac{32^{\frac{8}{k_b T}} + 32}{Z} - \left(\frac{8e^{\frac{8}{k_b T}} + 16}{Z} \right)^2 \right) \tag{6}$$

This problem will be solved by using the Metropolis algorithm. The algorithm can be described in ten steps.

1. Establish an initial matrix with size $L \times L$ and compute the energy.

2. Position yourself at a random point in the lattice and flip one spin.

3. Compute the energy for this new state.

4. Compute $\triangle E$

5. If the energy is lowered, accept the new configuration and jump to step 9

6. If the energy is increased, compare $w = e^{-\beta \Delta E}$ with a random number.

7. If the random number is bigger than w, reject the new configuration and jump back to step 2.

8. If the random number is smaller or equal to w, accept the new configuration.

9. Update expectation values

10. Repeat $L \times L$ times to let every lattice point get a chance to get picked.

<div align="right">Hjorth-Jensen., 2015</div>

This algorithm has a lot of steps, but computations for lower L are quick. As stated earlier, one of the problems in this report will be to find a possible phase change. This will be done by computing for larger L. When increasing L, the computing time increases rapidly. To get a good result within the time-limit, the code has to be parallelized. This will be done by using MPI.

In order to find the critical temperature, it is possible to use this equation:

$$T_c(L) - T_c(L = \infty) = aL^{-\frac{1}{\nu}} \tag{7}$$

Where L is the size of the lattice, T_c is the critical temperature and ν is a constant equal to 1. $T_c(L)$ is found graphically, so all we need to do is solve for $T_c(L = \infty)$ and a numerically by using this equation:

$$T_c(L) = T_c(L = \infty) + aL^{-\frac{1}{\nu}} \tag{8}$$

Taking a closer look at equation 8 reveals that it in fact has the simple form $Y = Ax + B$. Where $T_c(L = \infty)$ is equal to the constant B, and $\frac{a}{L}$ is equal to the term Ax, where L is the variable. As $T_c(L)$ is found graphically, it is a simple process to do a linear regression, and find where this graph crosses the y-axis. This means that $\frac{a}{L} = 0 \Rightarrow L = \infty$ and the value at the crossing pint is equal to $T_c(L = \infty)$

Results

The 2×2 matrix will serve as a benchmark to test the program in this report. This can be done as the analytic equations can be derived for this simple case.

Table 1: Mean energy and specific heat for $T = 1.0$

Monte Carlo cycles	Mean E random matrix	Mean E up matrix	C_v random matrix	C_v up matrix
10^1	-8	-8	0	0
10^2	-7.92079	-8	0.627389	0
10^3	-7.97602	-7.97602	0.191233	0.0638722
10^4	-7.9808	-7.984	0.121357	0.108604
10^5	-7.98952	-7.98424	0.13093	0.118817
10^6	-7.9836	-7.98339	0.127234	0.128955
Numerical	-7.9839	-7.9839	0.1282	0.1282

The Mean energy moves quickly towards the analytic result. The mean is in fact accurate up to three leading digits even for 10^4 monte carlo cycles for both a random matrix and a all up initial matrix. The specific heat in this case is the same as the variance ($C_v = \frac{Variance}{k_b T^2}$ with $k_b T^2 = 1$)This property is more sensitive, and it is needed 10^6 monte carlo cycles before reaching an accuracy of two leading digits for the random matrix, and three leading digits for the all up initial matrix. The results varied when running the program, which is to be expected for a probability influenced system.

Table 2: Mean absolute value of the magnetization and susceptibility for $T = 1.0$

Monte Carlo cycles	Mean $|M|$ random matrix	Mean $|M|$ up matrix	X random matrix	X up matrix
10^1	4	4	0	0
10^2	3.94059	3.9604	0.115283	0.156847
10^3	3.998	3.99401	0.00399201	0.0199441
10^4	3.9952	3.9924	0.0127757	0.0239399
10^5	3.99382	3.99396	0.0178416	0.0188433
10^6	3.99456	3.9949	0.0164823	0.0150619
Numerical	3.9946	3.9946	0.0160	0.0160

The results for magnetization and susceptibility tell much of the same story. The mean absolute value of the magnetization is accurate with three leading digits for 10^3 monte carlo cycles in both the random and all up case. As for the specific heat, the susceptibility is here equal to the variance of magnetism. The susceptibility is not stable before being computed with 10^6 Monte Carlo cycles, and even then it is not accurate over two or one leading digits.
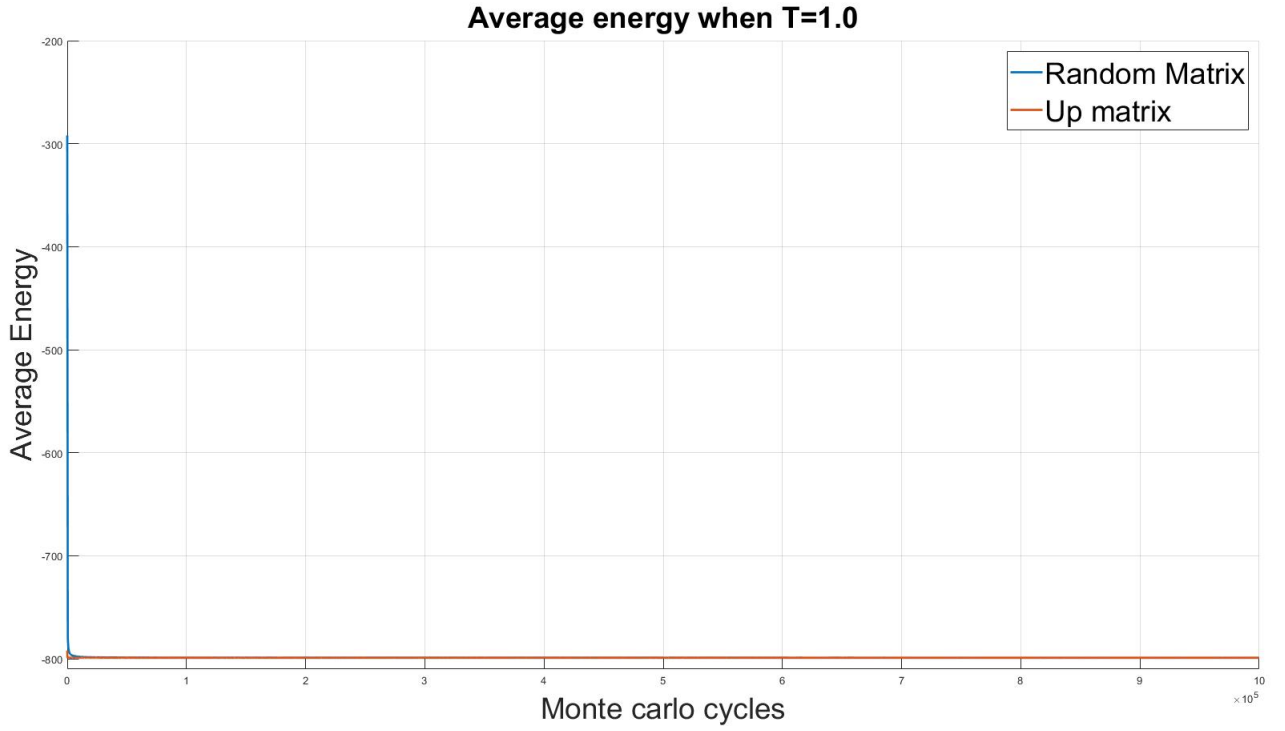
Figure 1: Development of average energy as a function of Monte Carlo cycles. Plotted at T=1.0 with an ordered and random matrix
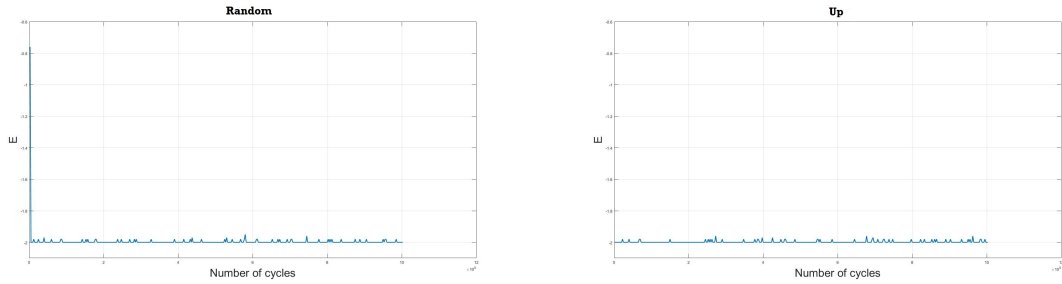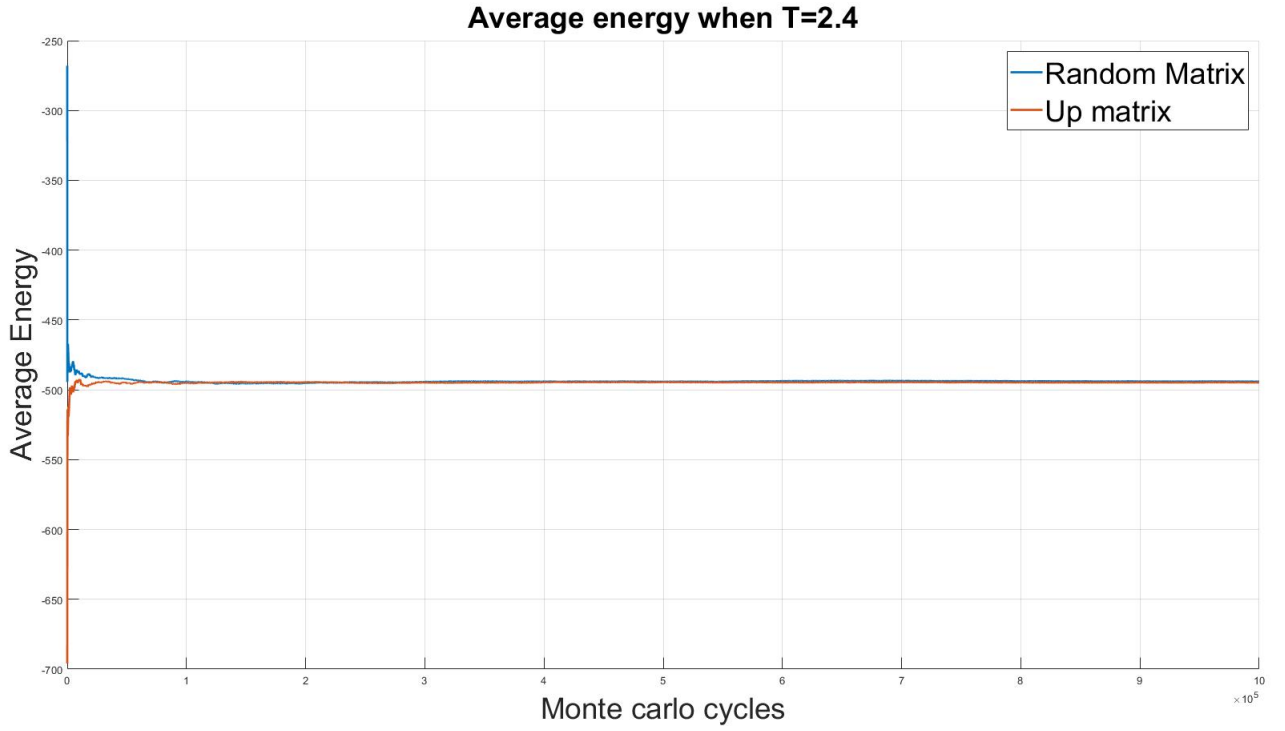

Figure 2: Energy per cycle of random and all up initial configuration for $T = 1$

It is clear to see in figure 1 and figure 2 that the energy quickly converges to a steady state around -2 per spin, or -800 for the entire system. For the all up initial configuration, it is already at this steady state (figure 2). This equilibrium state is confined to a small number of energy levels, and after as low as 10^4 cycles both seem to have reached the equilibrium. The nature of this low temperature system will be discussed later in the report.

Figure 3: Development of average energy as a function of Monte Carlo cycles. Plotted at T=2.4 with an ordered and random matrix
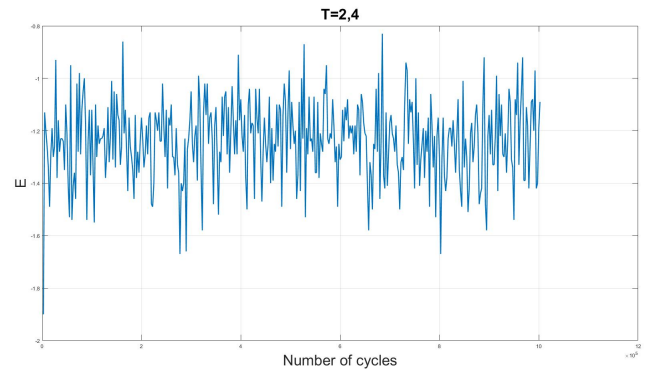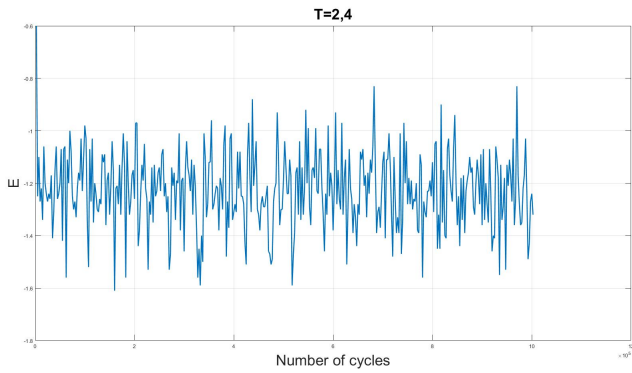

Figure 4: Energy per cycle of a random and all up initial matrix for $T = 2.4$

For $T = 2.4$ the energy also converges to an equilibrium state, but the energy fluctuates more than for lower temperature. This is to be expected, because there is more energy in the system, and will be elaborated further later in the report. The equilibrium is located at a higher energy than in figure 1. As an effect of this, the all up initial matrix is not already at the energy equilibrium. After about 10^5 cycles, it is safe to say that the equilibrium is reached (figure 3).
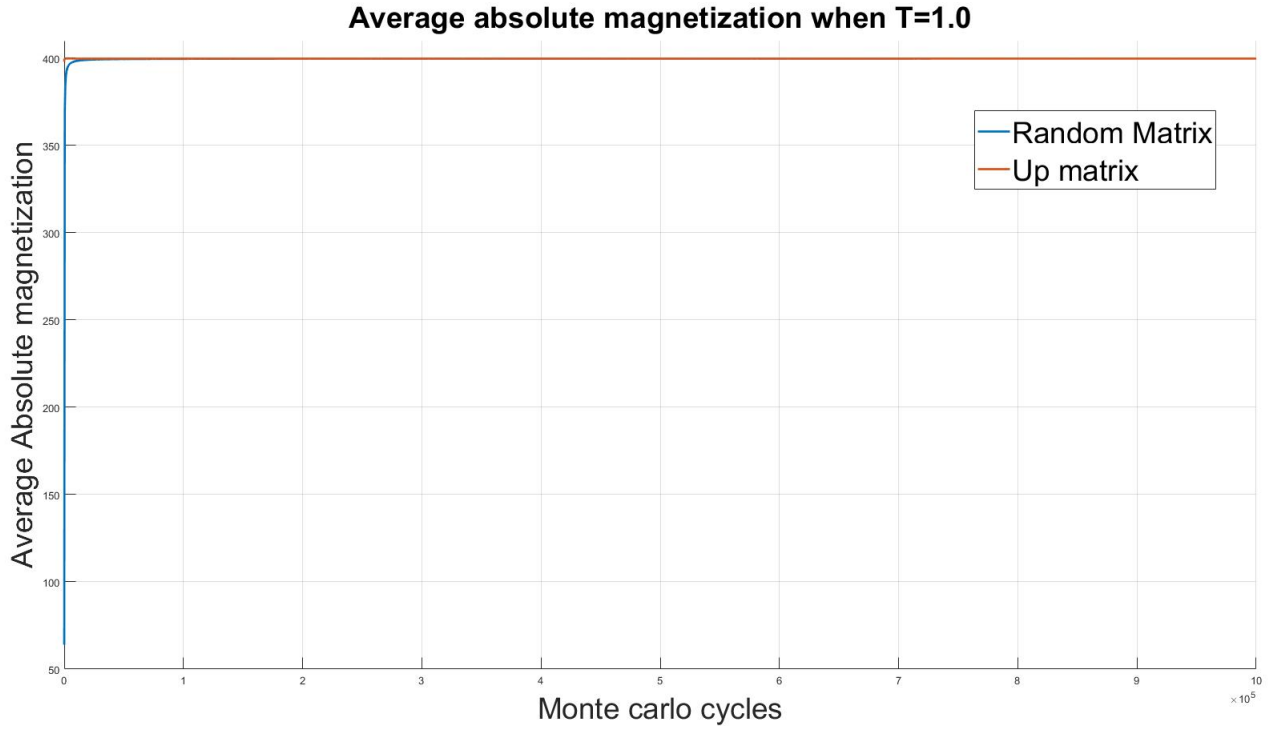
Figure 5: Development of average absolute magnetization as a function of Monte Carlo cycles. Plotted at T=1.0 with an ordered and a random matrix
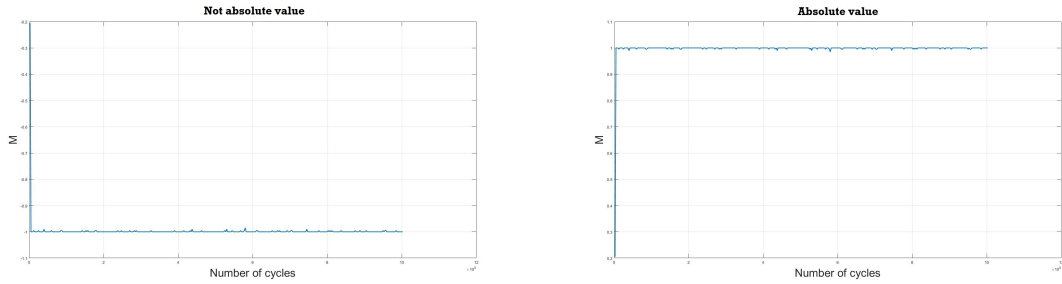

Figure 6: Development of magnetization and absolute magnetization per cycle with random starting matrices for increasing Monte Carlo cycles.

As with the energy shown in figure 1, the magnetization also converges quickly when the temperature is low (figure 5). It seems to have reached an equilibrium after $\approx 10^4$ cycles. The absolute magnetization behaves differently than the normal magnetization (figure **??**). This difference is not possible to see in the energy plots, and indicates that there are more than one configuration that serve as an energy minimum. There is no point in including the all up initial matrices, as it is already an energy minimum of all spins pointing up, and the absolute value would yield the same result.
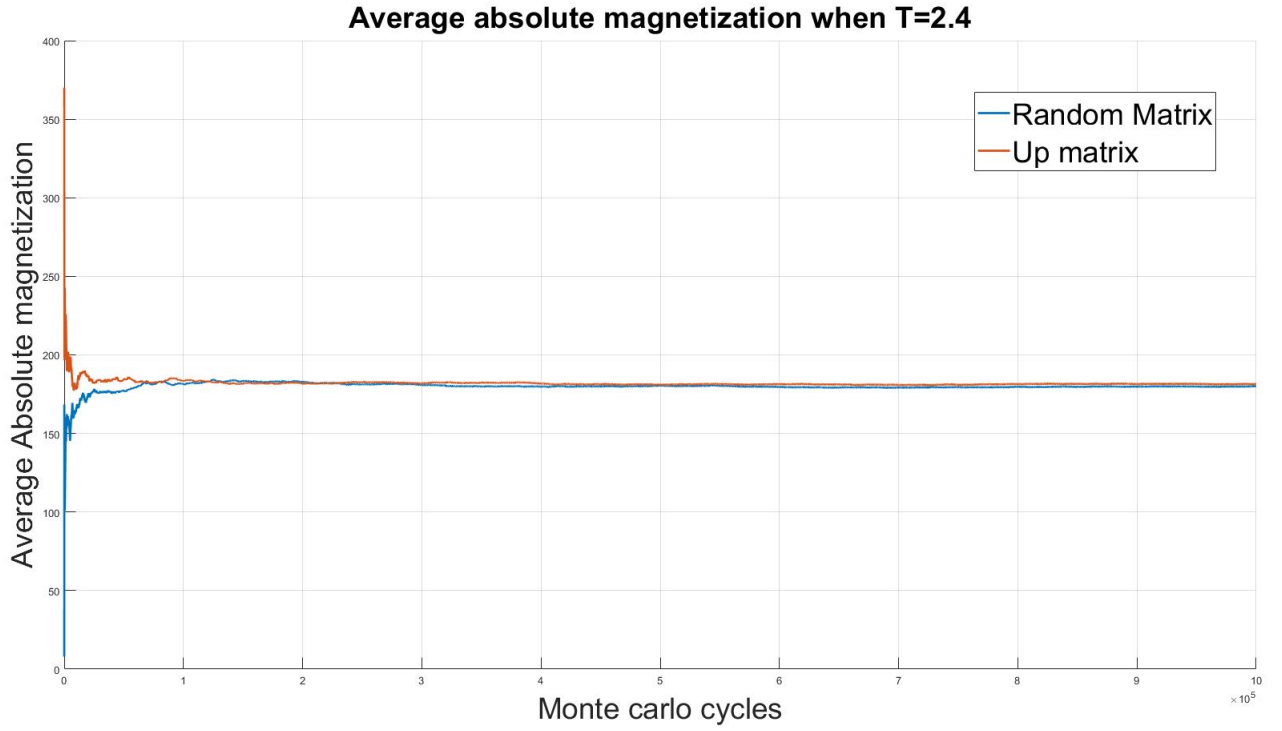
Figure 7: Development of average absolute magnetization as a function of Monte Carlo cycles. Plotted at T=2.4 with an ordered and random matrix
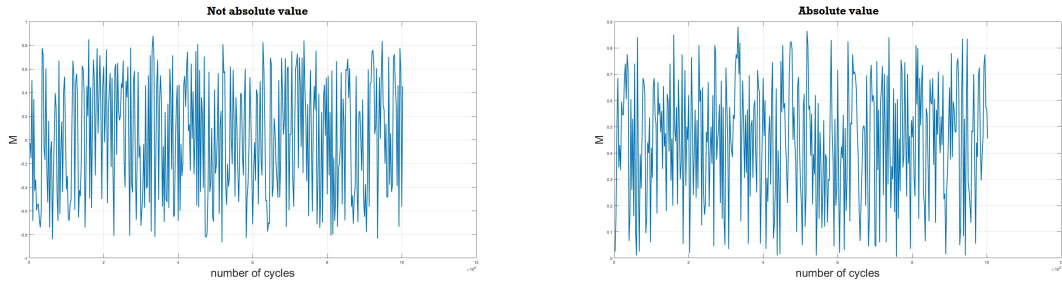

Figure 8: Development of magnetization and absolute magnetization per cycle with random starting matrices for increasing Monte Carlo cycles

As in the energy case for $T = 2.4$, none of the initial configurations are at the equilibrium. After about 10^5 Monte Carlo cycles they seem to have reached the equilibrium. When $T = 2.4$ the magnetization fluctuates between being positive and negative (figure 8) By looking at the absolute magnetization it soon becomes clear that the magnitude of the magnetization is limited to a finite range. The fluctuations are big, but this is to be expected, as there is more energy in the system.
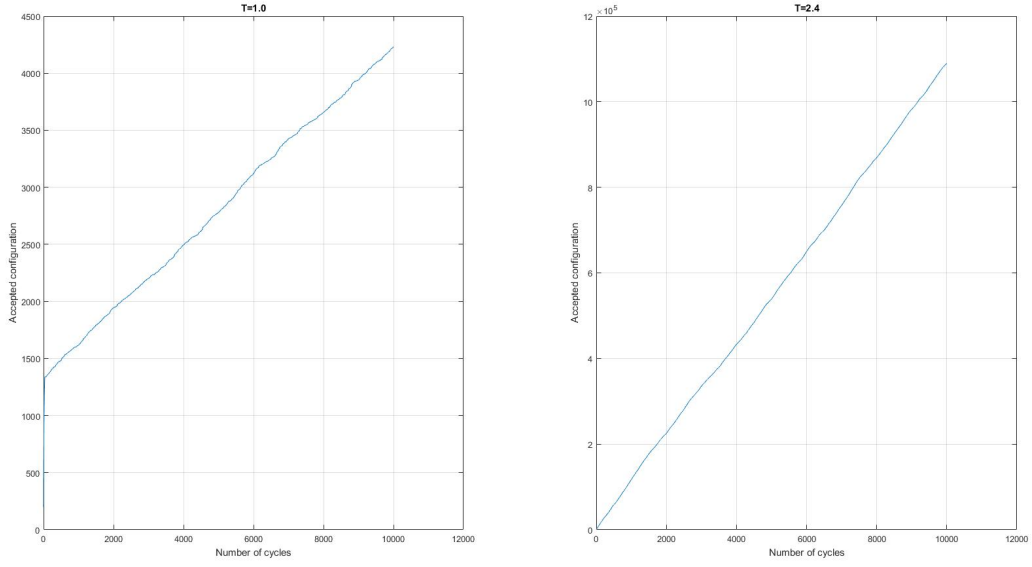
Figure 9: Number of accepted configurations for a random initial matrix computed with 10^4 Monte Carlo cycles for $T = 1.0$ and $T = 2.4$.
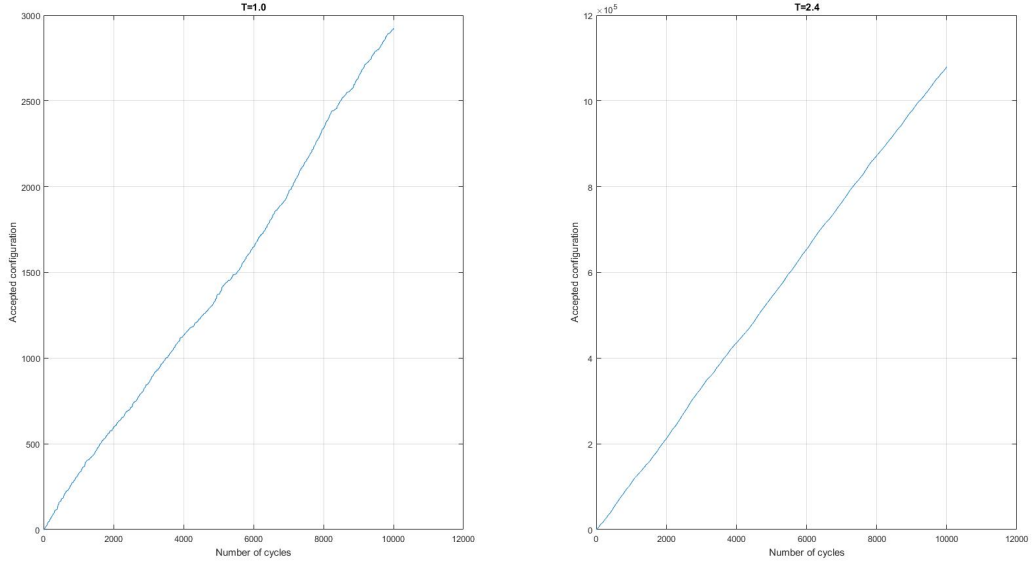

Figure 10: Number of accepted configurations for an all up initial matrix computed with 10^4 Monte Carlo cycles for $T = 1.0$ and $T = 2.4$.

The system with a random initial matrix at $T = 1.0$ accepts many flips in the first few Monte Carlo cycles (figure 9). This is because it initially is not at the equilibrium state. After it has reached equilibrium, it accepts far fewer moves, and follows the same pattern as figure 10 for $T = 1.0$. The total number of accepted configurations for the all up initial matrix at $T = 1.0$ is the same as the accepted configurations for the random case after it has reached the equilibrium. The total number of accepted configurations is much higher when $T = 2.4$, and the difference is negligible between the two. At this temperature, none of starting configurations are at the

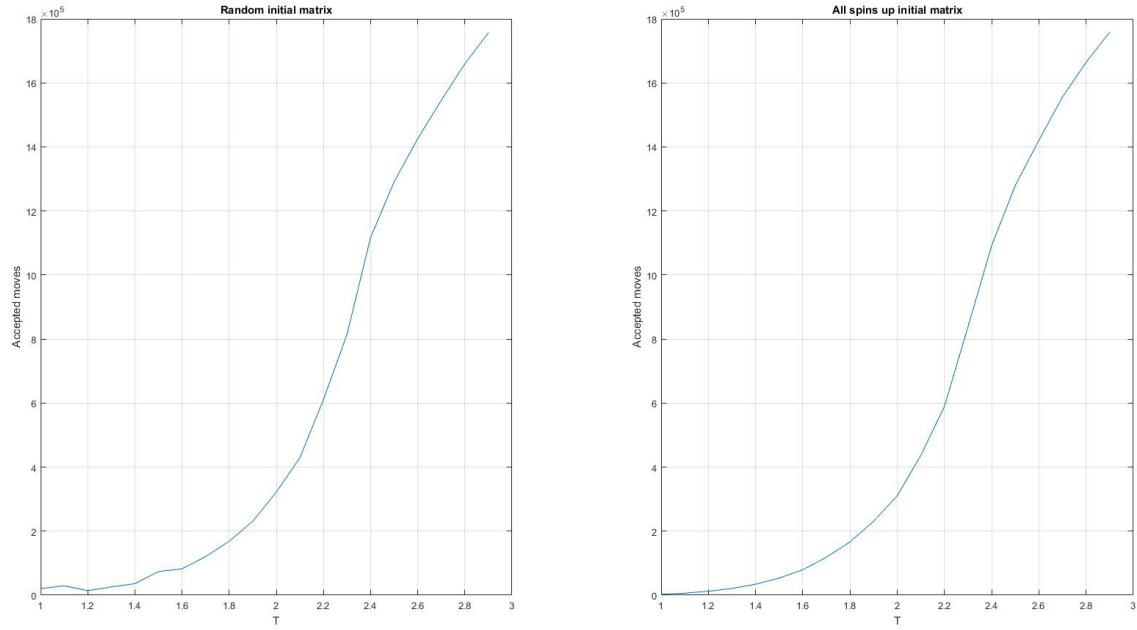equilibrium, and will both accept many flips in the first cycles.

Figure 11: Total number of accepted configurations as a function of temperature

The number of configurations grows exponentially with temperature. The smooth nature of the all spins up initial matrix is contrasted by the graph for a random initial matrix. The uneven nature of this graph is a result of the random initial matrix.
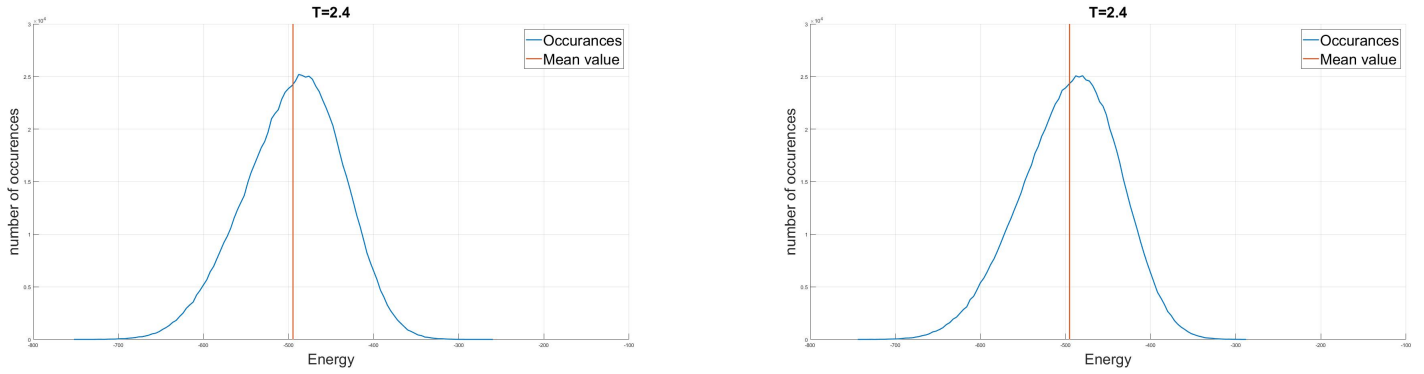

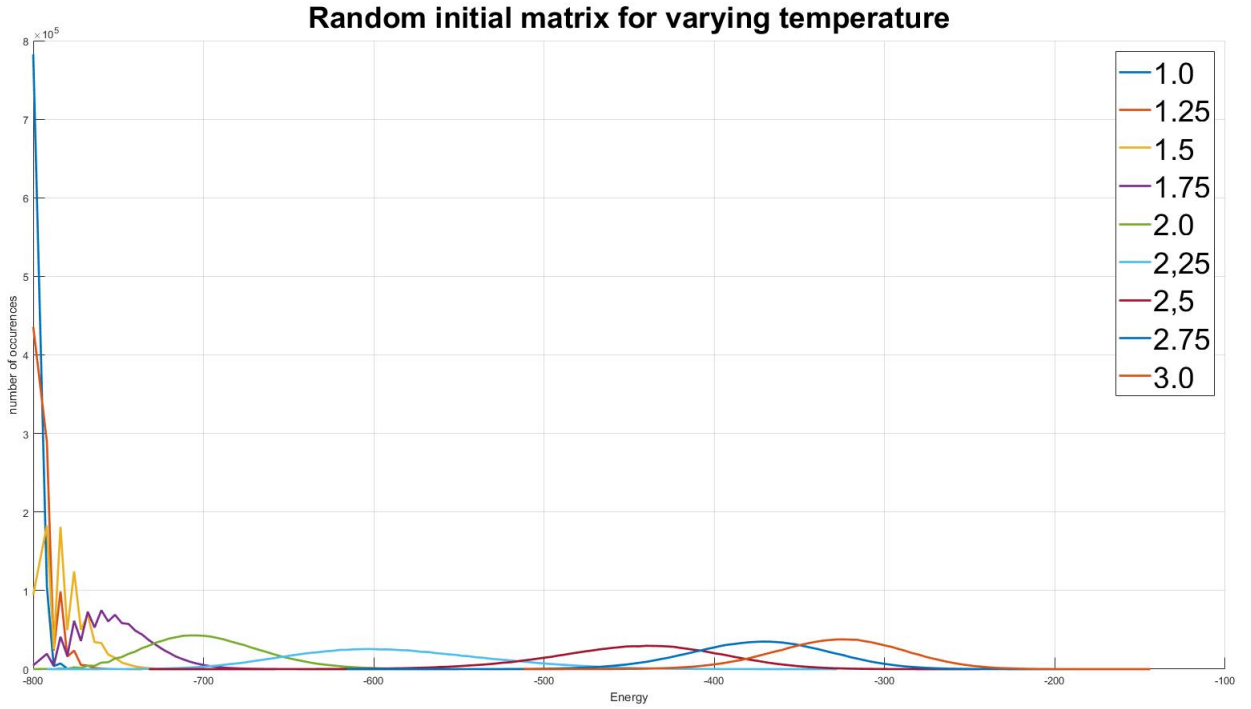Figure 12: Probability distribution for T=2.4 for a random and an all up initial matrix.

Figure 13: Probability distribution for varying temperature. Computed with 10^6 Monte Carlo cycles.

Table 3: Variance in energy for different temperatures computed with a random matrix for different temperatures and 10^6 Monte carlo cycles.

Temperature	Variance
T=1.0	0.0227441
T=1.25	0.129337
T=1.50	0.444368
T=1.75	1.18547
T=2.0	2.88226
T=2.25	7.89626
T= 2.50	6.18416
T=2.75	4.25249
T=3.0	3.61595

The probability distribution shown in figure 13 show that higher energies are to be expected when the temperature is increased. When the temperature is low, there are only a few possible energy states. This is in accordance with the energyplots in figure 2 and figure 4. The variance in table 3 is increasing up to $T = 2.25$ before decreasing again. This is also shown in figure 13. The graph representing $T = 2.25$ is much wider than all the other graphs. The probability distribution for $T = 2.4$ is shown in figure 12. The graph is negatively skewed (right modal), and there are no significant differences between starting from a random or all up initial configuration (figure 12).
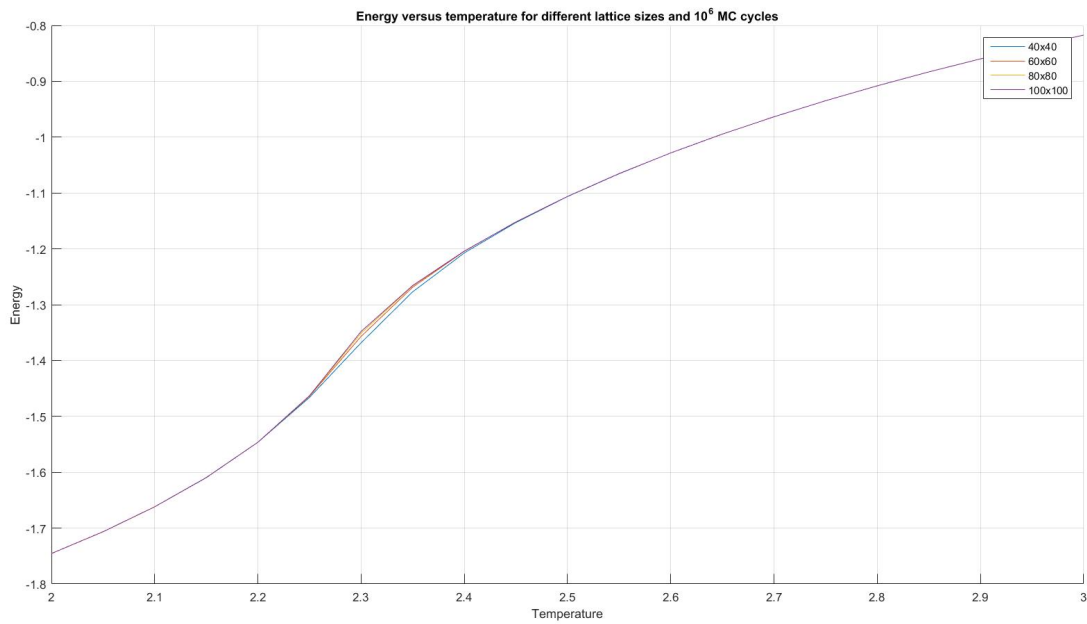
Figure 14: Mean energy per lattice point plotted against temperature for different lattice sizes

Even when computed for different lattice sizes, the energy at different lattice sizes stay relatively equal. There is one major anomaly though, this occurs around $T = 2, 3$ i.e close to the critical temperature.
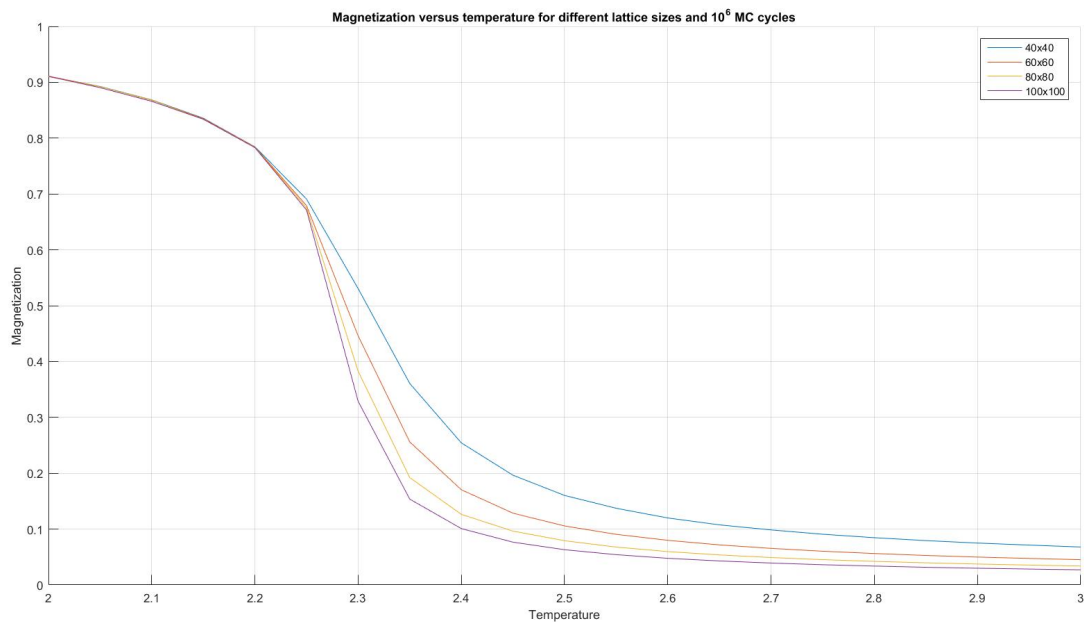

Figure 15: Mean absolute magnetization per lattice point plotted against temperature for different lattice sizes

The magnetization starts off relatively equal, but splits when getting closer to the critical tem-

perature. In contrast to the energy, the magnetization does not rejoin. The magnetization also decreases drastically, and goes toward zero.
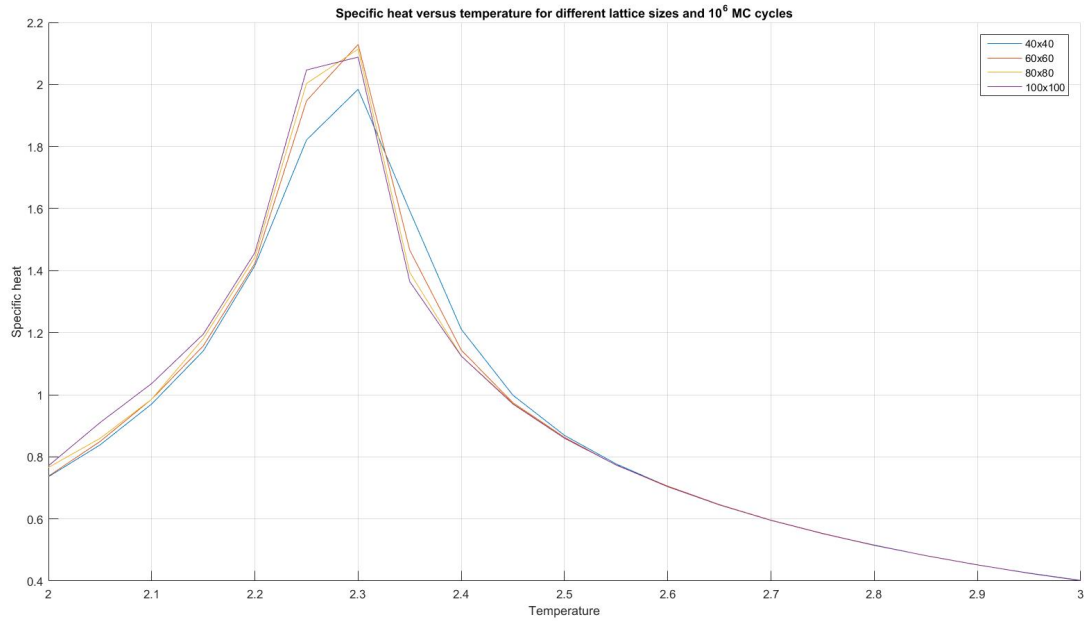

Figure 16: C_v per lattice point plotted against temperature for different lattice sizes

On all the graphs for specific heat, there is a peak at 2.3. There is however a difference; for $T = 2.25$ the specific heat seems to be growing when the lattice size increases.
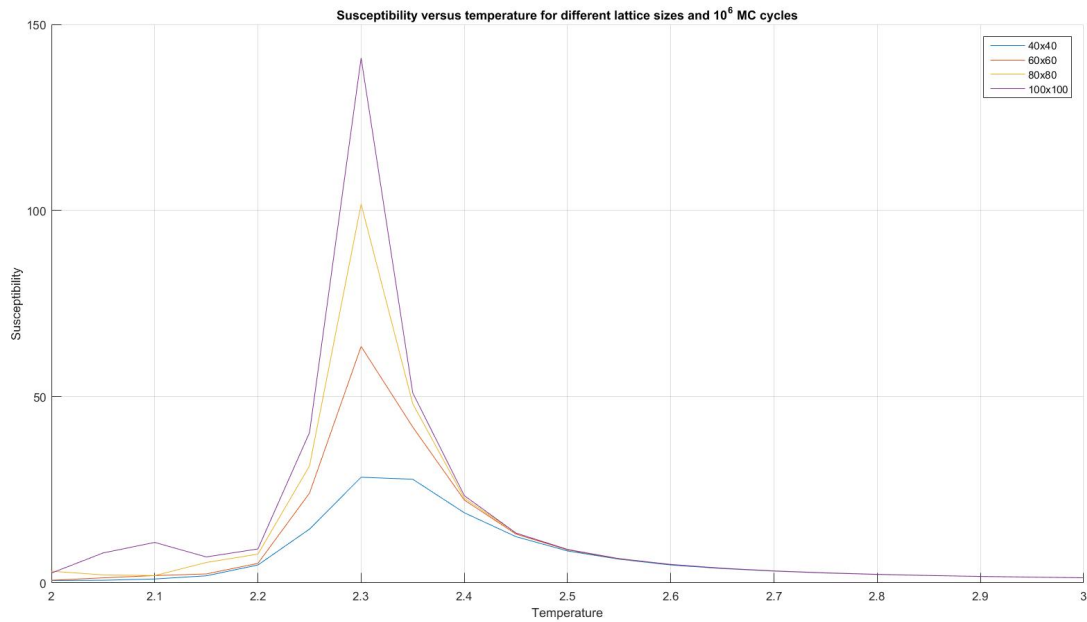

Figure 17: Susceptibility per lattice point plotted against temperature for different lattice sizes

As in figure 16, the susceptibility also has a peak at $T = 2.3$.

The results from figure 14, figure 15, figure 16 and figure 17 were used to extract the critical temperature. The anomalies in all of these figures occur around $T = 2.3$. In figure 16 and figure 17, these anomalies are clear, and manifest as big peaks. All of the peaks in these two figures occur on $T = 2.3$, so running the linear regression presented earlier would only yield:

$$T_c(L = \infty) = 2.3$$

From the literature, it is known that the real critical temperature is equal to:

$$T_c(L = \infty) = \frac{2}{ln(1 + \sqrt{2})} \approx 2.269$$

Possible ways to fix this will error will be presented.

Errors and timing

As the system being examined is based upon probability, there will always be some degree off error. This problem would only be solved if there was a way to obtain an infinite amount of Monte Carlo cycles. On account of this not being possible, the results obtained by the program agree to a reasonable extent. This is true for all but the critical temperature. The program was run with a temperature step of 0.05. This was clearly not enough to get a proper result. There are two ways to fix this, either to decrease the temperature step, or to run for bigger lattice dimensions. Considering increase in computation time, the preferred one would probably be to decrease the temperature step. figure 16 shows that the specific heat at $T = 2.25$ increases in relation to at $T = 2.3$. If the program was run an additional time with a lattice size bigger than 100×100, the result would be closer to what found in the literature. The best way to fix these problems would probably be a combination of decreasing the temperature range, to save time, decreasing the temperature step and increasing the lattice sizes to increase accuracy.

Table 4: Run time for computation of different matrix sizes with paralellized code. The program was in this instance run from $T = 2.0 \Rightarrow T = 3.0$ with temperature step of 0.05

Lattice size	Run time in seconds
60x60	3996.57
80x80	7081.15
100x100	18630.9

As stated earlier, the computation of bigger dimension lattices takes long time. Therefore, the code was paralellized using MPI. The computer used for this, had 8 cores, effectively making the computations 8 times faster. Without paralellization, the program would have used about 40 hours to run for a 100×100 lattice over the 20 temperature steps (Table 4).

Discussion

For the 2×2 case, the expection values showed distinct sensitivities (table 1,2). The mean energy and mean absolute magnetization converged quickly towards the analytic value. Both were accurate with three leading digits for as few as 10^4 Monte Carlo cycles. When increasing the number of Monte Carlo cycles to 10^6 the relative error decreases to a fraction of a ‰. The specific heat and susceptibility were both sensitive. The specific heat was accurate up to two or three leading digits, depending on the starting matrix, when computed with 10^6 Monte Carlo cycles. The specific heat was accurate up to only one or two leading digits with 10^6 Monte Carlo cycles. The program did not produce the same results for each run. This is due to the random nature of the system being examined.

The 20×20 case was studied with an emphasis on when the most likely state is reached. As shown in figure 1 and figure 5 the graphs converge quickly towards an equilibrium when $T = 1$. This is contrasted by the mean energy and mean absolute magnetization when the temperature is 2.4(figure 3,figure 7). This system is governed by the Boltzmann distribution:

$$e^{-\frac{\Delta E}{k_b T}} \tag{9}$$

To increase the energy, the random number used in the Monte Carlo test must be lower than $e^{-\frac{\Delta E}{k_b T}}$ (step 6). At low temperatures, the system will allow fewer energy increases compared to for higher temperatures. This results in faster converging towards the equilibrium for lower temperatures.

Another way to look at this is through a pure physical perspective. There is, by definition, more energy in the system when the temperature is higher. This will lead to more flips, and a higher degree of disorder. With less energy in the system, it is less likely to flip, hence faster converging to an equilibrium.

When starting with a random matrix, there are generally more flips (figure 9,figure 10). When the number of Monte Carlo cycles are increased, this difference becomes almost negligible (figure **??**). When the equilibrium is reached, the increase in accepted flips will behave in a similar fashion. This can be read out of figure 9 and figure 10 for $T = 1$, as after the first few cycles, the growth of accepted configurations grow at the same rate. For increasing temperature, the number of accepted configurations start growing exponentially. This true for both a random and ordered starting matrix. This is in line with what is to be expected, as the Boltzmann distribution is depending on the temperature (equation 9). Another interesting thing to look at is how both the random and all up initial matrix accept many moves in the first few cycles for $T = 2.4$. This is not shown clearly in figure 9 and figure 10, as the total number of accepted configurations become exceedingly high. Nonetheless, it can be read out of the average energy and mean absolute magnetization plots (figure 3, figure 5). None of the initial configurations are at the equilibrium, hence they will accept many flips the first few cycles to converge to the equilibrium.

The probability distribution for $T = 2.4$ seem to have av negative skewness (right-modal)(figure 12). This means that the majority of the energy occurrences happen to the left of the mean value. This again means that the system prefers to jump down in energy, which is to be expected,as it always wants to be at the lowest possible energy state. Another interesting thing to look at, is how the probability distribution behaves for different temperatures (figure 13). For lower temperatures, there are only a few lower energy levels that are are occurring frequently. The probability distributions are shifted towards higher energies as the temperature increases. The distributions become wider moving towards the critical temperature, before narrowing again. This is mirrored by the variance shown in table 3.

The critical temperature was calculated to be 2.3. This differs somewhat for the reasons explained in the errors part. It is still clear that something extraordinary occurs in this region. This is

the only place the energies differ (figure 14). The susceptibility and specific heat has a peak (figure 16, figure 17), and the magnetization goes rapidly towards zero. As the graphs tend to get steeper for increasing lattice sizes, it is okay to assume that this sudden shift from finite mean absolute magnetization, to almost zero magnetization will be even more rapid for an infinite lattice. Moreover, the graphs also indicate that the mean absolute magnetization would get even closer to zero with an infinite lattice (figure 15). This is confirmed by looking at the literature, where it is stated that the slope of the magnetization would become infinite for an infinite lattice (Hjort-Jensen,2015). The phase transition in the two dimensional Ising model is of second order. It manifests itself as an abrupt change from a mean magnetization $M \neq 0$ below T_c, to $M = 0$ above T_c.

Concluding remarks The metropolis algorithm has proved to

Reference list

Hjort-Jensen,M., 2015. Computational physics, accessible at course github repository. 551 pages