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 $\beta = \frac{1}{k_b T^2}$. There are 16 different states of energy. Luckily, a lot of these yield the same result. Summing up all of these gives:

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

The mean energy and magnetization is given by respectively:

$$E = \frac{1}{Z}\sum_{i=1}^{16} E_i e^{-J*E_i\beta} = \frac{-8e^{\beta 8J} + 8e^{-\beta 8J}}{e^{-\beta 8J} + e^{\beta 8J} + 6} \tag{3}$$

and

$$M = \frac{1}{Z}\sum_{i=1}^{16} M_i e^{-J*E_i\beta} = \frac{4e^{\beta 8J} + 8}{e^{-\beta 8J} + e^{\beta 8J} + 6} \tag{4}$$

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

$$c_v = \frac{64}{k_b T}\frac{1 + 3cosh(8\beta)}{(cosh(8\beta) + 3)^2} \tag{5}$$

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

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

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.

Hjorth-Jensen., 2015

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

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

This was done using the least squares rule for linear regression.

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.

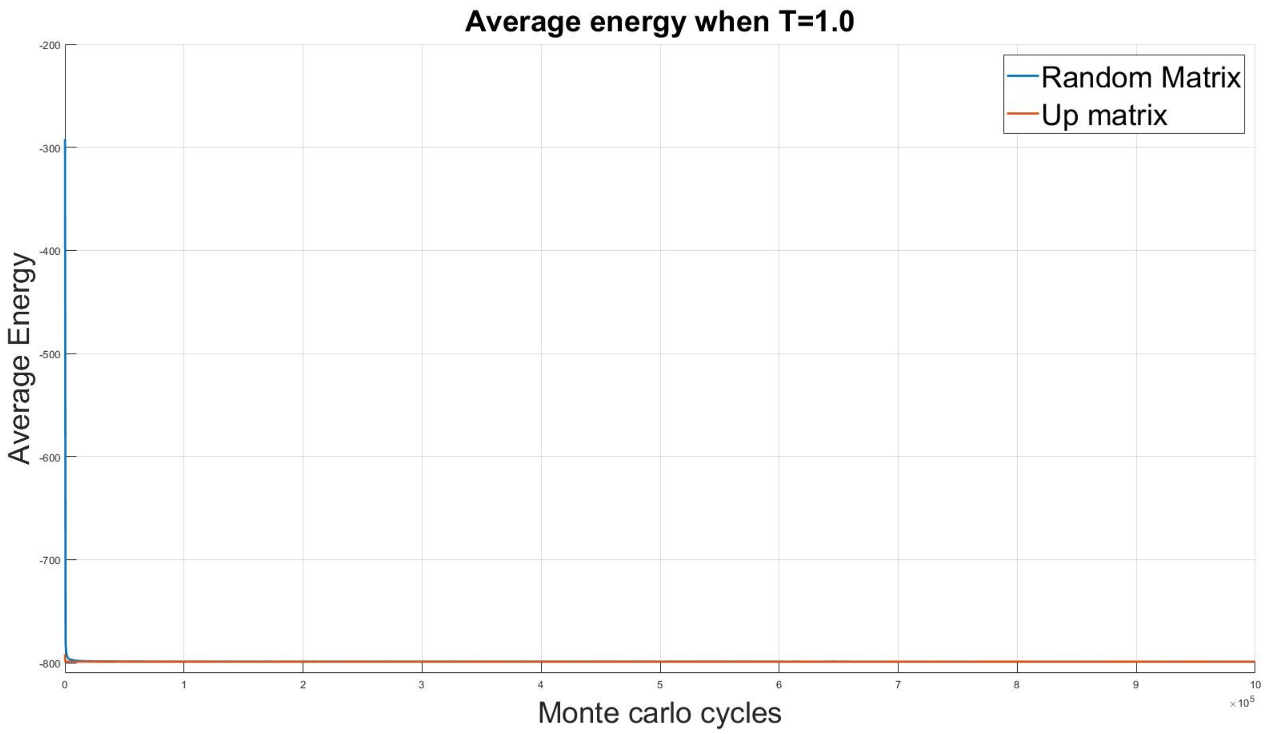
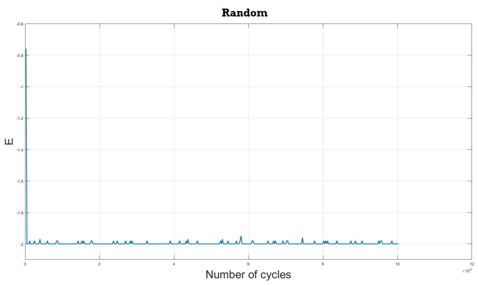


Figure 1: Development of average energy as a function of Monte Carlo cycles. Plotted at T=1.0 with an ordered and random matrix



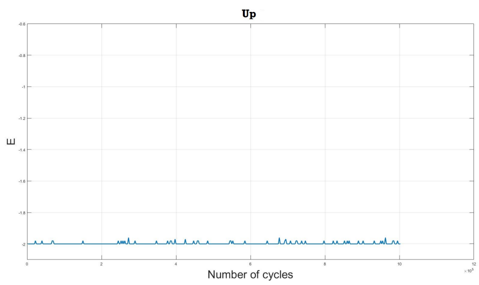


Figure 2: Energy of random initial matrix per lattice point plotted against number of monte carlo cycles for T=1.0 and T=2.4

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.

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.

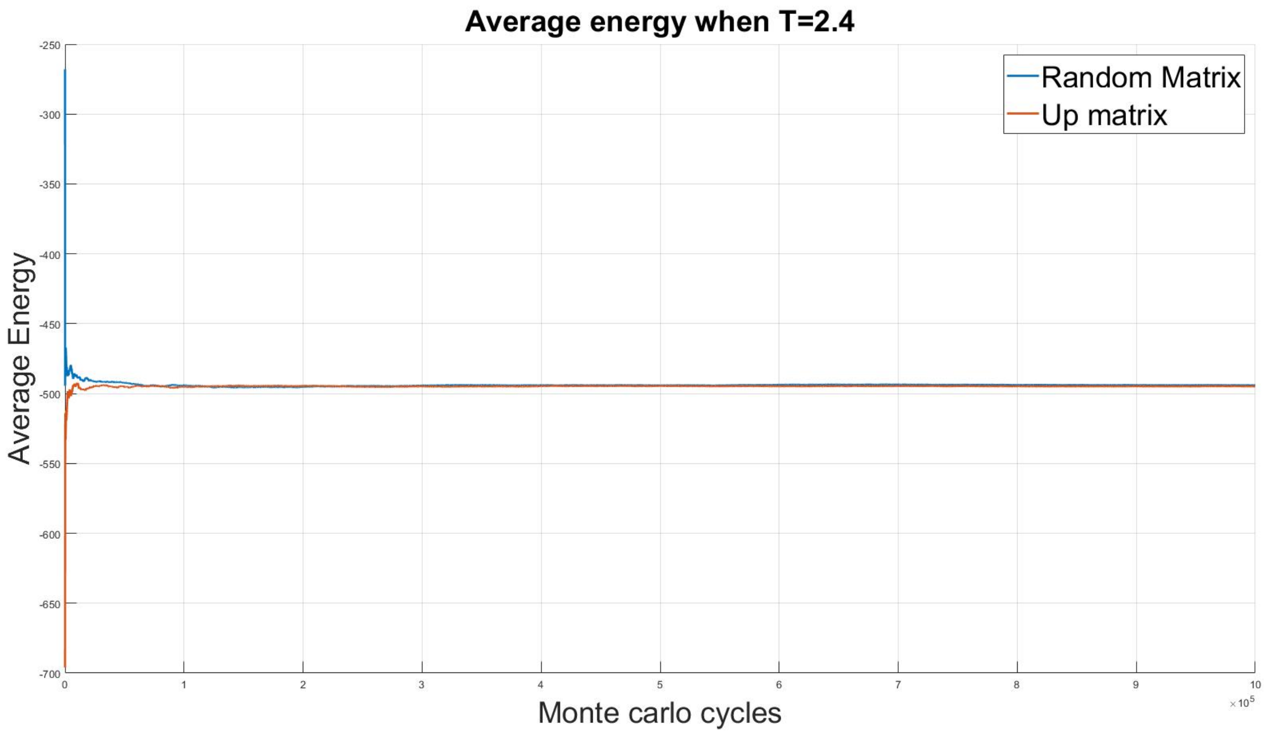
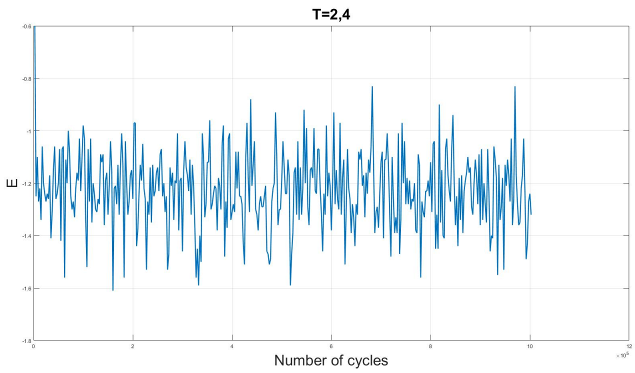


Figure 3: Development of average energy as a function of Monte Carlo cycles. Plotted at T=2.4 with an ordered and random matrix



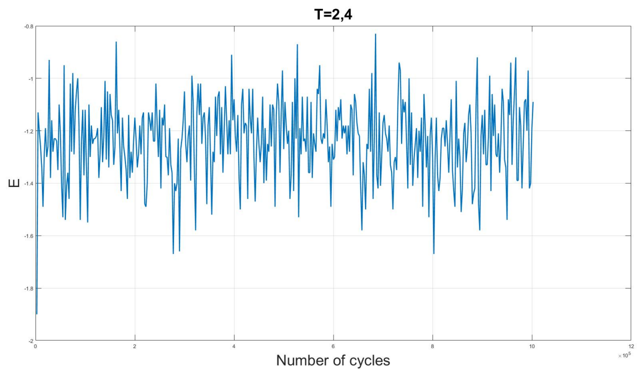


Figure 4: Energy of all spins up inititial matrix plotted against number of monte carlo cycles

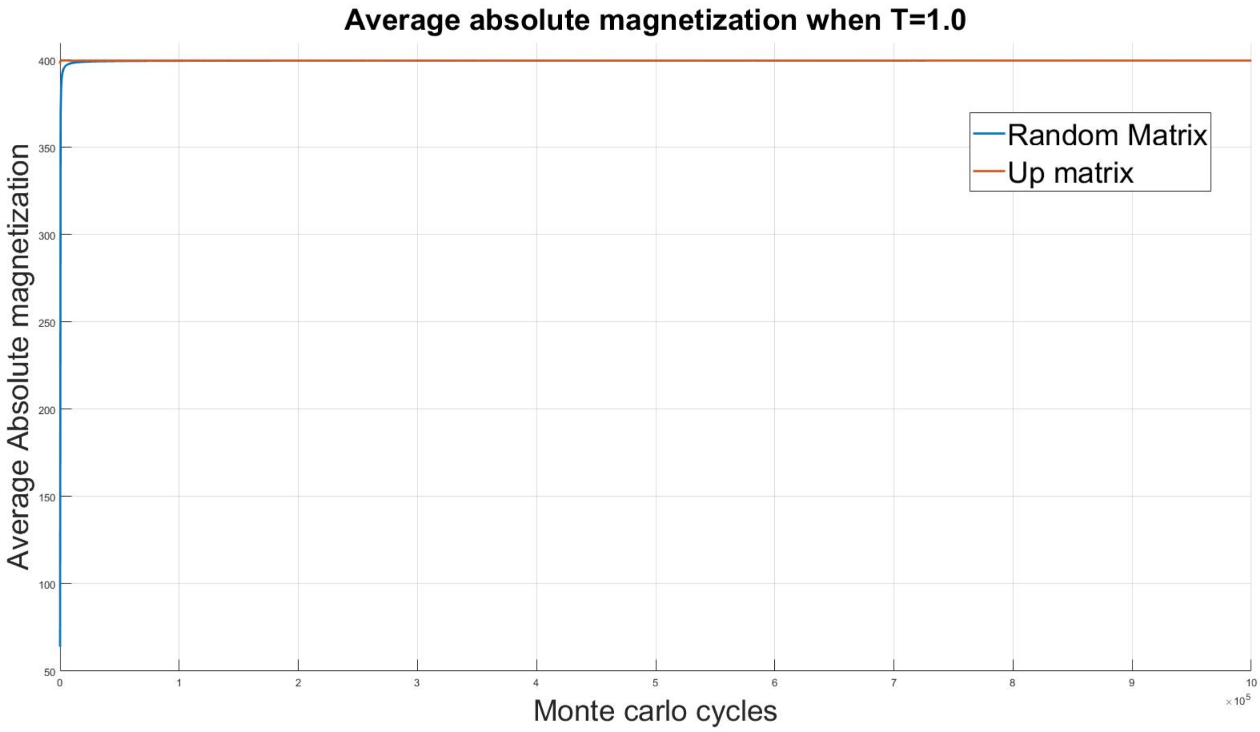


Figure 5: Development of average absolute magnetization as a function of Monte Carlo cycles. Plotted at T=1.0 with an ordered and random matrix

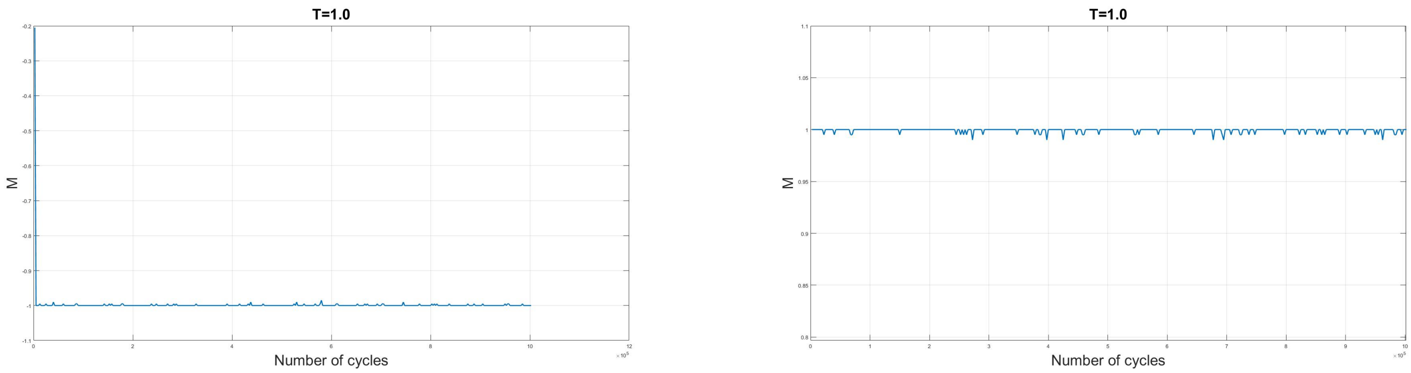


Figure 6: Development of magnetization with random starting matrices for increasing monte carlo cycles.

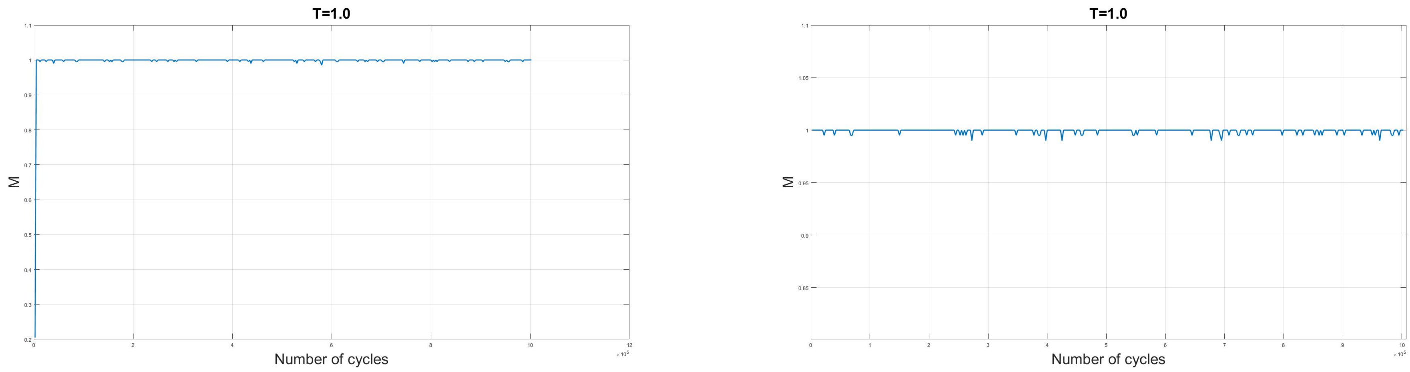


Figure 7: Development of absolute magnetization with random starting matrices for increasing Monte Carlo cycles.

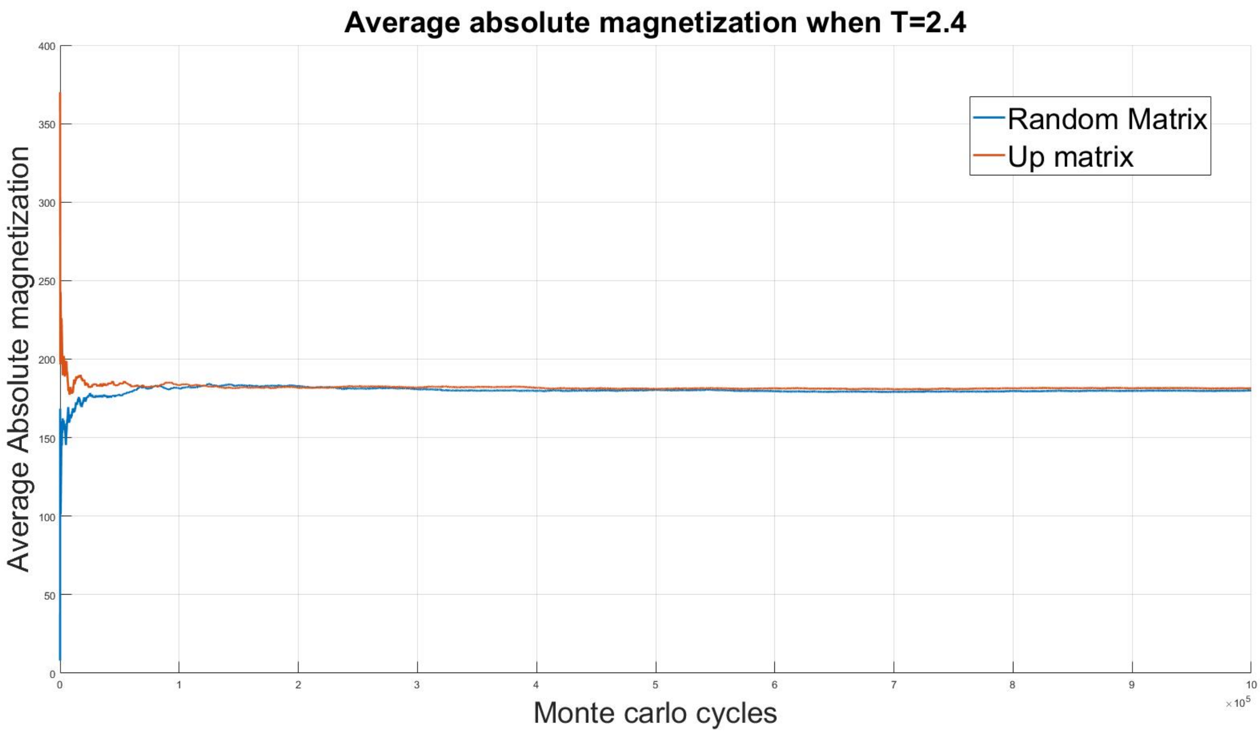


Figure 8: Development of average absolute magnetization as a function of Monte Carlo cycles. Plotted at T=2.4 with an ordered and random matrix

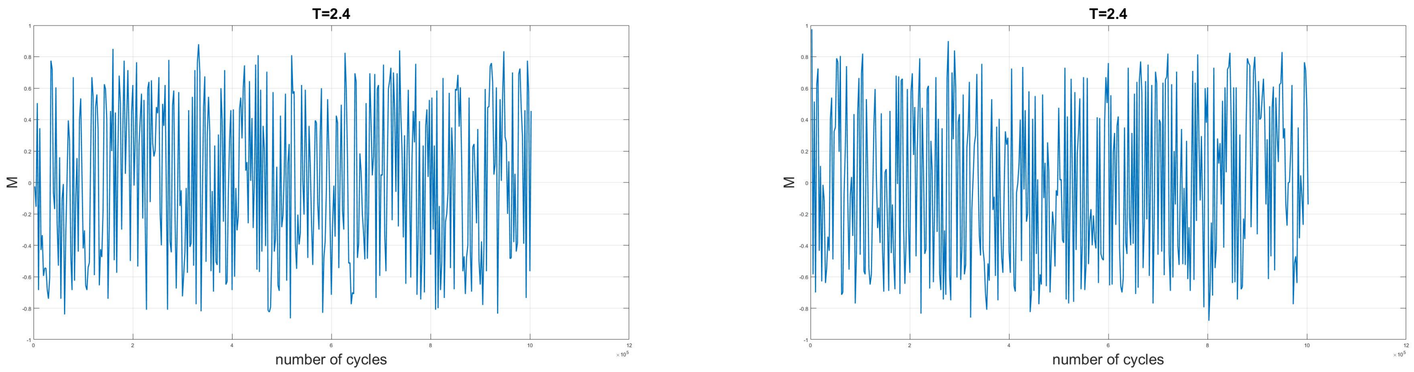


Figure 9: Development of magnetization with all up starting matrices for increasing Monte Carlo cycles

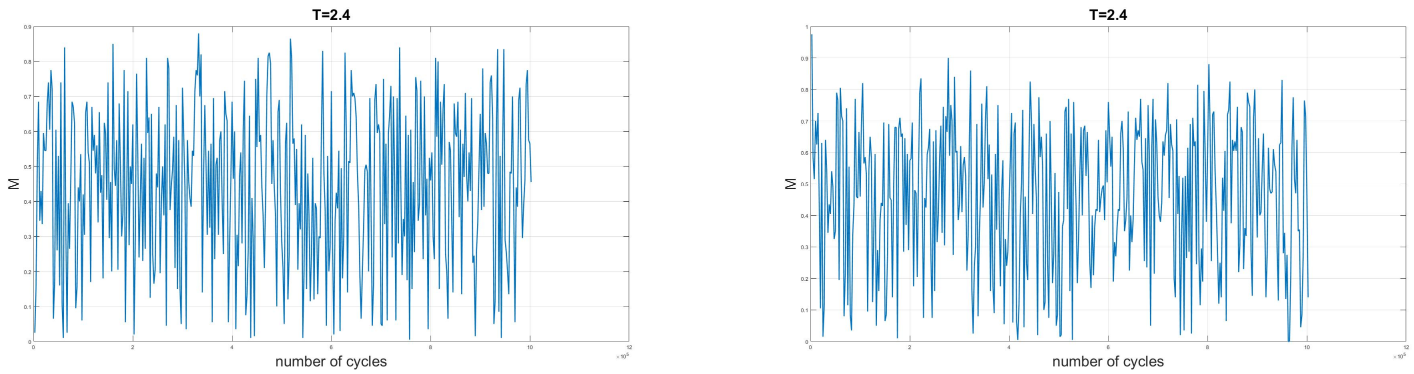


Figure 10: Development of absolute magnetization with all up starting matrices for increasing Monte Carlo cycles.

All figures of energy and magnetization were plotted with 1 000 000 Monte Carlo cycles and written to file for every 2500 points
figure 6, figure 7, figure 9 and figure 10 shows that the magnetization behaves similarly for $T = 1.0$ in all the cases. There is no difference at all when taking the absolute value for the all up initial matrix, because the magnetism is continuously positive to begin with. When the starting matrix is random, the first Monte Carlo cycles is used to reach the equilibrium state. As the random matrix in this instance is closer to an equilibrium state where all the spins point down, it will tend towards this state instead of the configuration with all spins up. These two states have the same energy, hence both states serve as a valid energy equilibrium.

When $T = 2.4$ the magnetization fluctuates between being positive and negative in both the ordered and random case. 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 compared to when $T = 2.4$.

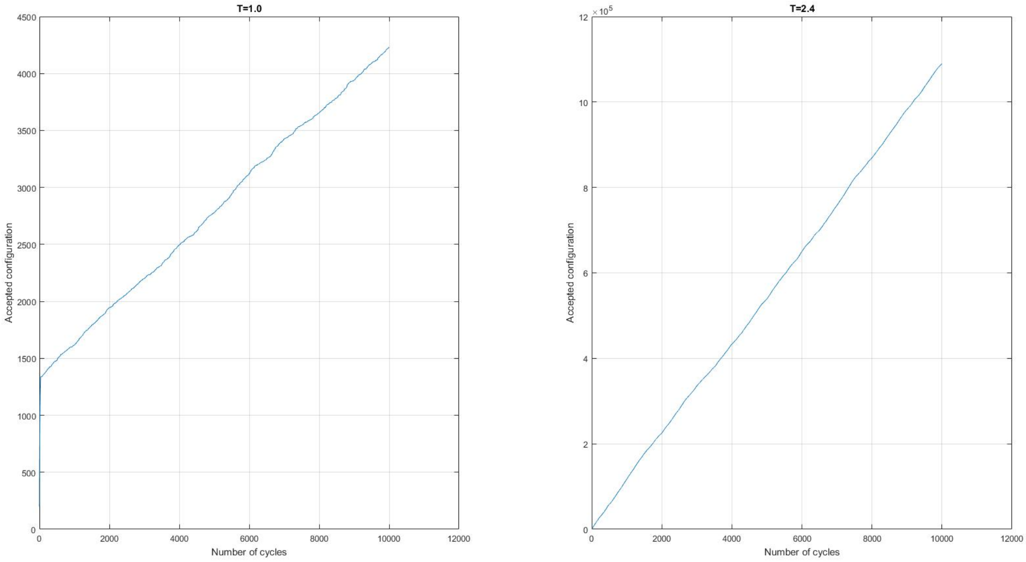


Figure 11: Number of accepted configurations for a random initial matrix computed with 10^4 Monte Carlo cycles for $T = 1.0$ and $T = 2.4$.

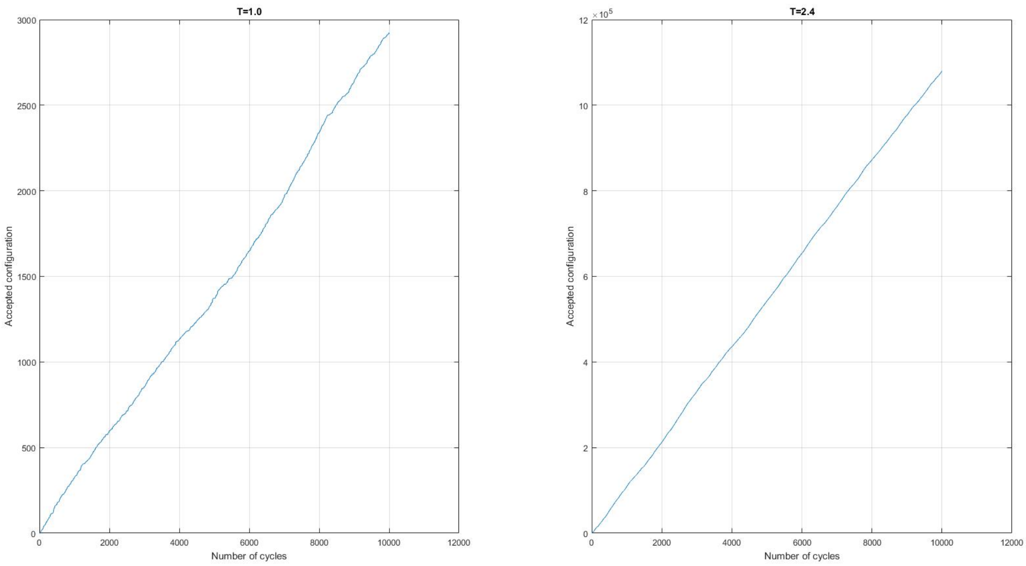


Figure 12: Number of accepted configurations for an all up initial matrix computed with 10^4 Monte Carlo cycles for $T = 1.0$ and $T = 2.4$.

The system with a random initial matrix at $T = 1.0$ accepts many flips in the first few Monte Carlo cycles (figure 11). 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 12 A. When subtracting the number of accepted configurations from the first few cycles in figure 11 A from the total number of accepted configurations, the answer is the same number of accepted configurations as in figure 12 A. The total number of accepted configurations is much higher when $T = 2.4$, and the difference is negligible between the two.

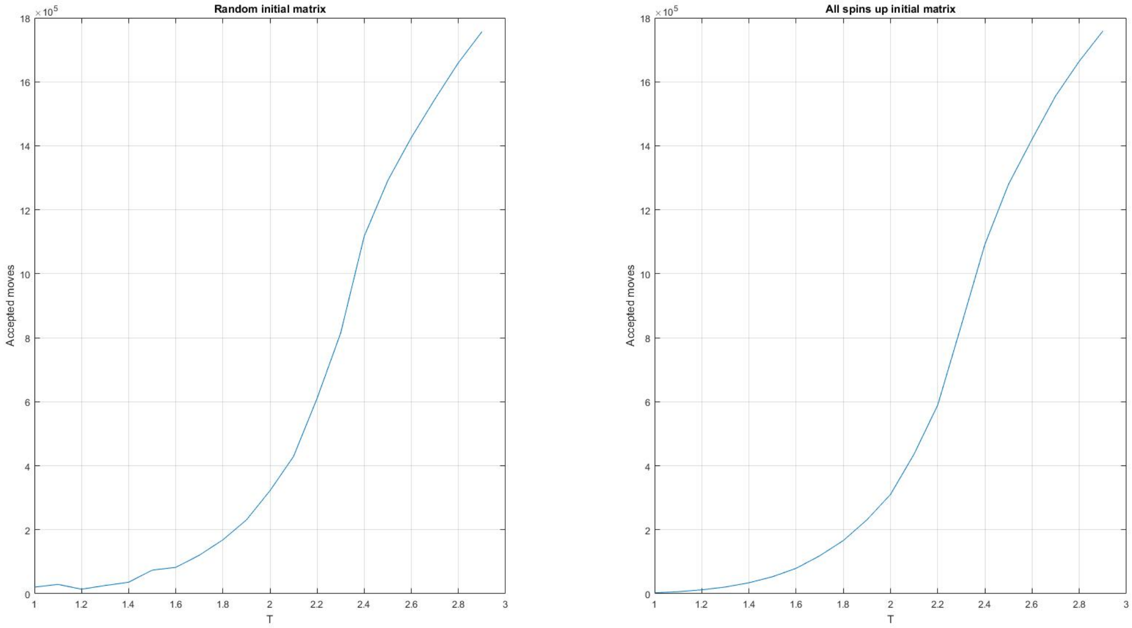


Figure 13: Total number of accepted configurations as a function of temperature

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.

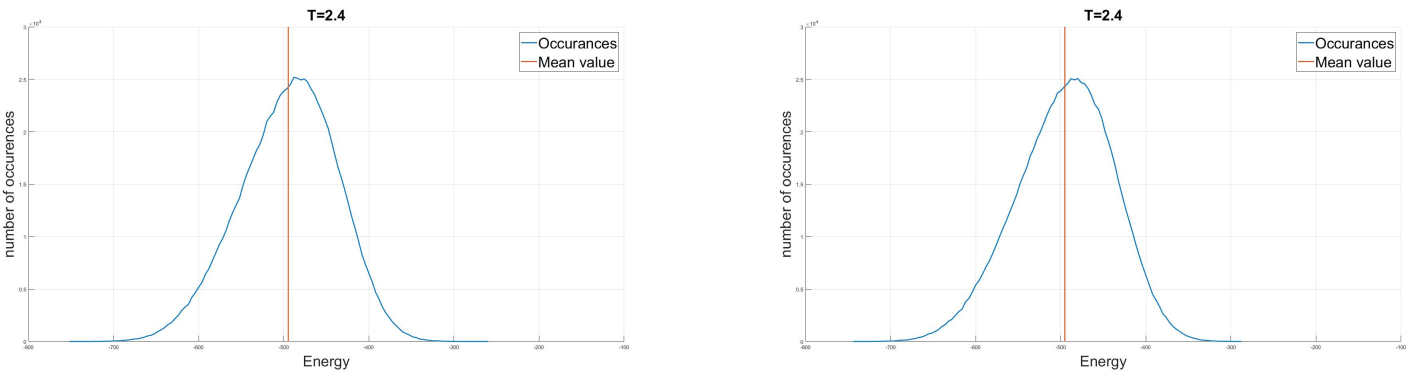


Figure 14: Probability distribution for T=2.4 for a random and an all up initial matrix.

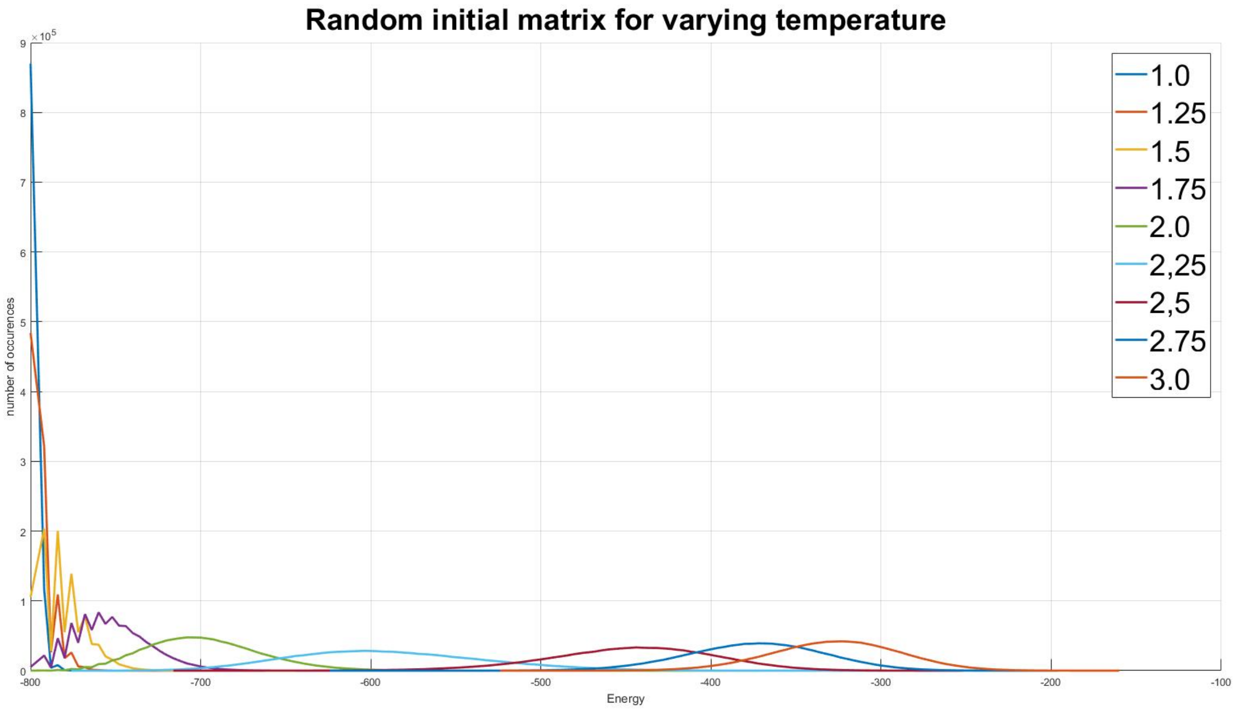


Figure 15: Probability distribution for varying temperature. Computed with 10^6 Monte Carlo cycles.

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	10.1076
T=1.25	52.9558
T=1.50	181.261
T=1.75	478.219
T=2.0	1157.08
T=2.25	3145.36
T= 2.50	2479.22
T=2.75	1690.69
T=3.0	1445.91

The probability distribution shown in figure 15 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 **??** and figure 4. The variance in table 3 is increasing up to $T = 2.25$ before decreasing again. This is also shown in figure 15. 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 14. The graph is skewed towards higher energies. WHY ARE THEY SKEWED?

For T mindre og lik 2.25 er de skewed positivt, og negativt for t større enn 2.25

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 8). This system is governed by the Boltzmann distribution:

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

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. When there are high temperatures, by definition, there is more energy in the system. 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 11,figure 12). When the number of Monte Carlo cycles are increased, this difference becomes almost negligible. When the equilibrium is reached, the increase in accepted flips will behave in a similar fashion. This can be read out of figure 11 and figure 12 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, and is in line with what is to be expected, as the Boltzmann distribution has an exponential relation with temperature.(ER DETTE GREIT Å SKRIVE (skriv om uansett)).

The probability distribution for $T = 2.4$ seem to have av negative skewness (right-modal)(figure 14). 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 15). 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 temperatures increase. The distributions become wider moving towards the critical temperature, before narrowing again. This is mirrored by the variance shown in table 3.

Conclusion

Reference list

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