1 Results

1.1 2×2 lattice, analytical expressions

If we scale the value of β from $1/k_BT$ to $1/J$ (Scaling factor k_BT/J) in the analytical expression from section **??**, we will get a good benchmark for computer computations to come. These values are listed in table 1 below. Note that all values are divided by four, since we want the values per bond, and not for the entire lattice.

Mean energy, $\langle \mathbf{E} \rangle$	-1.9960
Mean absolute magnetization, $\langle \lvert \mathcal{M} \rvert \rangle$	0.9987
Specific heat capacity, $\mathbf{C_V}$	0.0321
Susceptibility, χ	3.9933

Table 1: Analytically calculated benchmark for material characteristics per bond for a 2×2 lattice

1.2 2×2 lattice, numerical results

Using $T = 1.0$, like in the analytical calculations, the program /code/Ising/ gives the results listed in table 2:

	Set initialization	**Random initialization**
Mean energy, $\langle \mathbf{E} \rangle$	-1.9955	-1.9958
Mean absolute magnetization, $\langle \lvert \mathcal{M} \rvert \rangle$	0.9985	0.9986
Specific heat capacity, $\mathbf{C_v}$	0.0358	0.0337
Susceptibility, χ	3.9925	3.8237

Table 2: Computed values of material characteristics per bond for a 2×2 lattice.

The values correspond very well with each other and the analytical.

1.3 Ising model: simulation over temperature

We ran the program for different amounts of Monte Carlo cycles and plotted the error (analytical − simulated) in figure 1 below. Using 10^7 Monte Carlo cycles, we seem to be getting pretty accurate results.

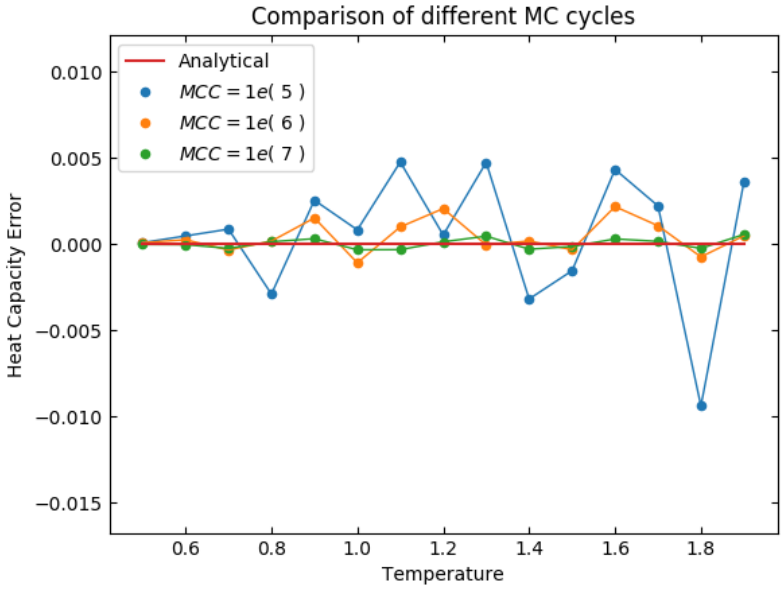

Figure 1: Shows the accuracy of different amount of MC cycles over temperature.

This shows that our computed results are quite close to our analytical results for the 20×20 lattice. This is a good indication of a successfull simulation.

1.4 20×20 lattice

Ordered spin orientation

Initializing the spin structure, we first set every spin up for $T < 1.5$ and every spin down for $T \geq 1.5$. In figure 2, the computed values for the mean magnetization and energy are plotted against the number of MC cycles, at $T = 1.0$ and $T = 2.4$:

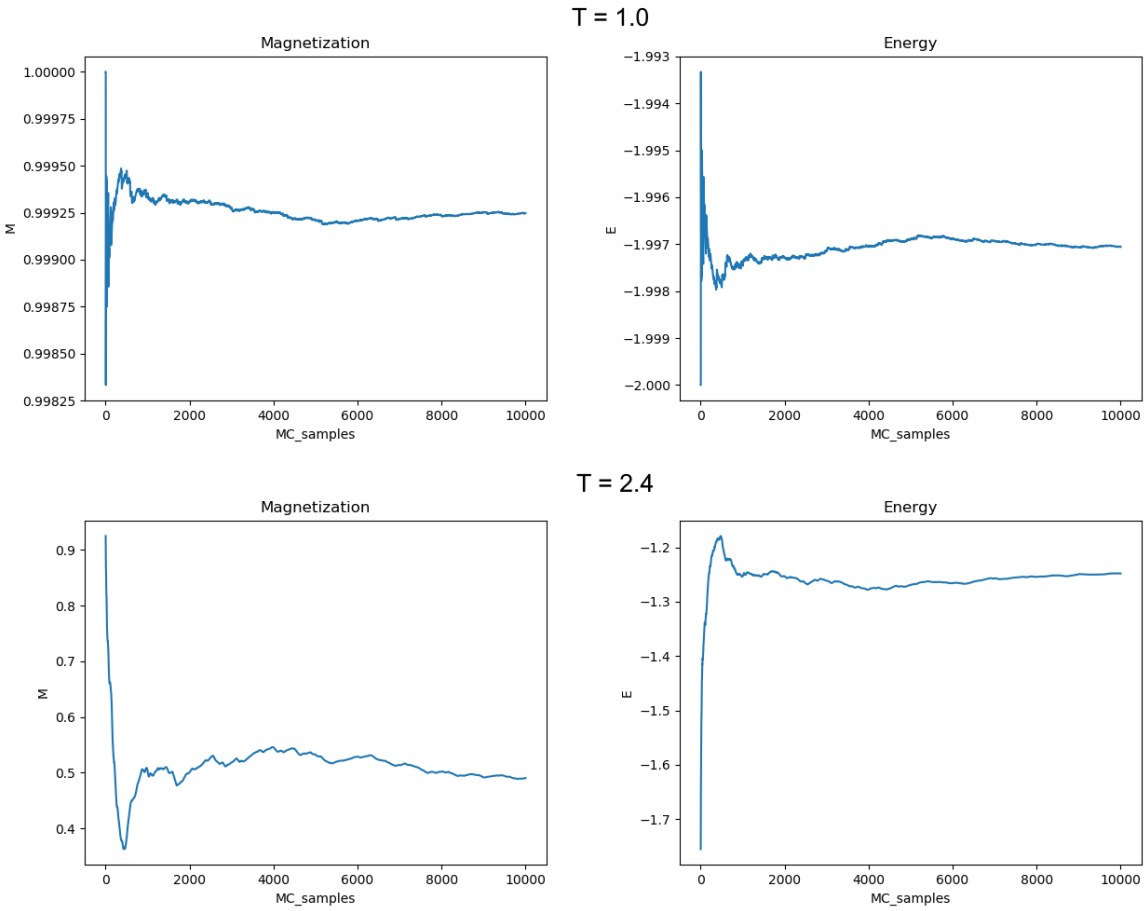

Figure 2: Shows the computed value for the mean magnetization and energy, with ordered initialization, against the number of MC cycles. The scaled temperature is $T = 1.0$ and $T = 2.4$ respectively.

All the plots pretty much stabilize into a value after 8000-1000 MC cycles. For $T = 1.0$, the magnetization stabilizes around the value 0.99950 and the energy around the value -1.997. This corresponds pretty good with the analytically calculated values. For $T = 2.4$, the magnetization stabilizes around the value 0.5 and the energy around the value -1.25.

Random spin orientation

Following the ordered initialisation, we also initialized the crystal randomly. In figure 3, the computed values for the mean magnetization and energy are plotted against the number of MC cycles, at $T = 1.0$ and $T = 2.4$:

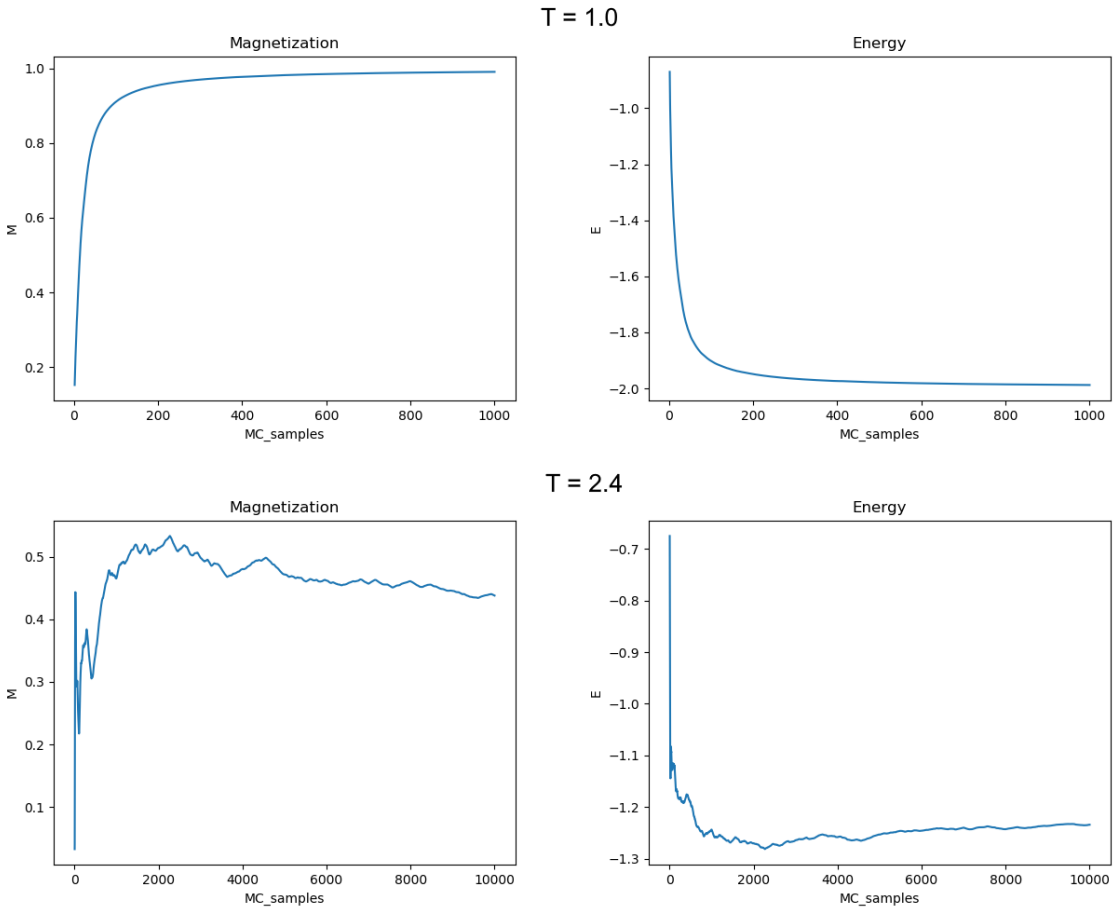

Figure 3: Shows the computed value for the mean magnetization and energy, with random initialization, against the number of MC cycles. The scaled temperature is $T = 1.0$ and $T = 2.4$ respectively.

The plots for $T = 1.0$ follow a clean exponential curve, while the other plots pretty much stabilize after 8000-1000 MC cycles - like the previous ones. For $T = 1.0$, the magnetization ends on the value 1.0 and the energy on the value -2.0. This is similar to the analytical values, but does not have the same accuracy. For $T = 2.4$, the magnetization stabilizes around the value 0.45 and the energy around the value -1.25.

1.5 Analyzing the probability distribution

In figure 4 you can see the probability distribution for low and high temperature respectively. We can see that for a low temperature, the system tends to settle

in the lowest energy state, while for the higher temperature the energies are a bit more spread. In table 3 you will see the computed variance. Note that we calculated standard deviation of the histogram with NUMPY.STD, and took the square root of this to get the variance.

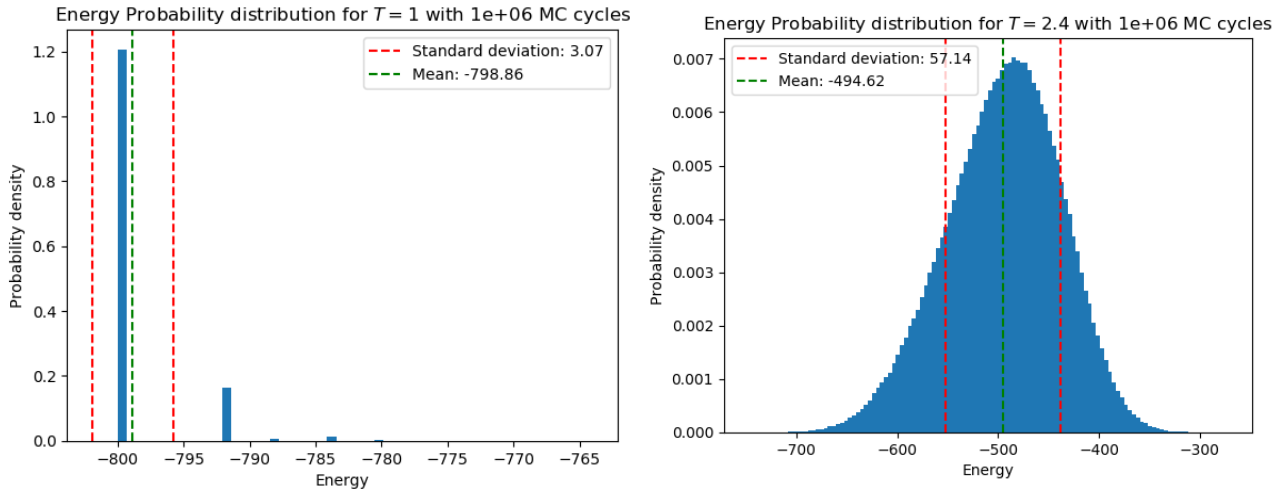

Figure 4: Shows probability distribution for low and high temperature.

Temperature	calculated variance	from histogram	deviation
1	9.375	1.752	81%
2.4	8.053	7.550	6.2%

Table 3: Computed variance

1.6 Numerical studies of phase transitions

After playing around with the domain of the temperature we found that the domain used in figure 5 and 6 nicely presents the phase change of the material. We used 10^6 Monte Carlo Cycles for each temperature step, which had a stepsize of $\Delta T = 0.005$. As shown in the figures we can clearly see that something is happening around $T = 2.3$.

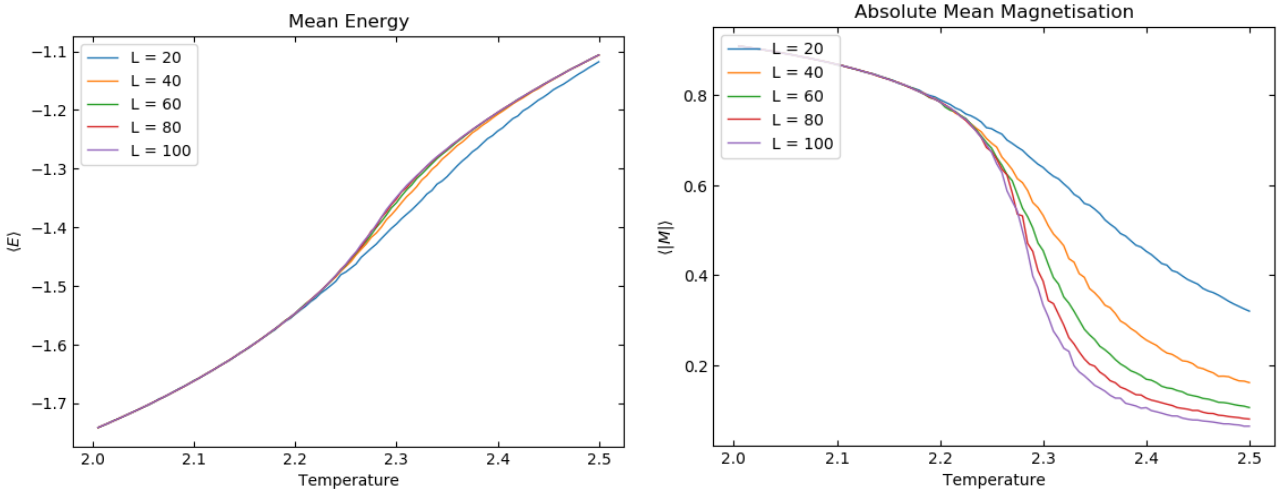

Figure 5: Mean energy and magnetisation over temperature interval $T \in [2.0, 2.5]$ with lattice sizes $L = 20, 40, 60, 80, 100$.

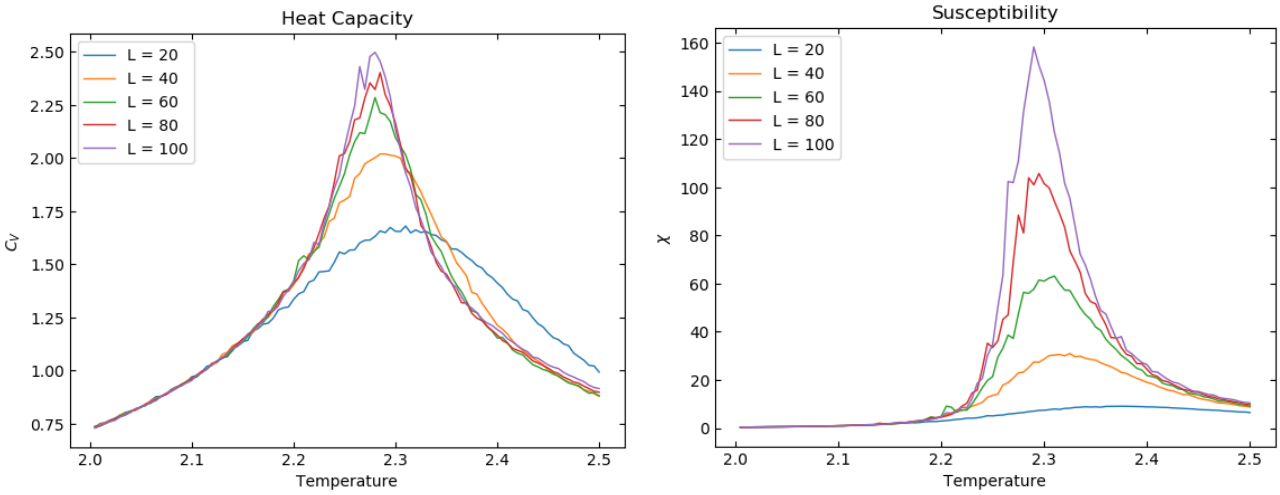

Figure 6: Heat capacity and Susceptibility over temperature interval $T \in [2.0, 2.5]$ with lattice sizes $L = 20, 40, 60, 80, 100$.

The simulations were run on an 16-core AMD Ryzen 1700x with 3.4GHz clock speed. It took approximately 3 hours to complete. To compare parallelized time to using a single core, we ran calculations for the 20x20 lattice with 10^5 Monte Carlo cycles and $T \in [2.0, 2.5]$ with step size $\Delta T = 0.05$. The time is shown in table 4.

Cores	Time spent
1	42s
2	26s

Table 4: Time spent on calculations for different thread-count.

1.7 Extracting the critical temperature

The critical temperatures of the different sized arrays was found by taking the averange of the full width half maximum of the heat capacity and the susceptibility. This resulted in the critical temperatures found in table 5.

Lattice size, L	T_C
40	2.318
60	2.301
80	2.291
100	2.284

Table 5: Critical temperatures of different lattice sizes.

By using equation (**??**), and (**??**). we find the constant a, and thereafter the critical temperature for an infinitely large lattice.

Parameter	Value
a	2.26667
T_C	2.261

Table 6: Numerical values for the parameter a, and the critical temperature.

For reference, the exact result for the criticalt temperature for $L \to \infty$ is $kT/J = 2/ln(1+\sqrt{2}) \approx 2.269$ after Lars Onsager.[**larsonsager**]