FYS4150 Project 4: Numerical integration

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1. Introduction

In this project we study the Ising model in two dimensions, without an external magnetic field. In its simplest form the energy is expressed as

$$E = -J \sum_{<kl>}^{N} s_k s_l \tag{1}$$

with $s_k = \pm 1$, N is the total number of spins and J is a coupling constant expressing the strength of the interaction between neighbouring spins. The symbol $< kl >$ indicates that we sum over nearest neighbours only. We will assume that we have a ferromagnetic ordering, viz $j > 0$. We also assume periodic boundary conditions. This project will be solved using the Metropolis algorithm.

2. Analytical solution

To start with we assume that we only have two spins in each direction, such that $L = 2$, giving us a total of 4 spins. This gives a partition function

$$Z = 12 + 4\cosh(8J\beta) \tag{2}$$

where $\beta = 1/kT$. An expectation value for energy

$$< E > = -\frac{32J\sinh(8J\beta)}{Z} \tag{3}$$

A variance for the energy

$$\sigma_E^2 = \frac{2^{10}(1 + 3\cosh(8J\beta))}{Z^2} \tag{4}$$

Expectation value for the magnetization

$$< M > = 0. \tag{5}$$

Expectation value for the absolute value of the magnetization

$$< |M| > = \frac{8(e^{8J\beta} + 2)}{Z} \tag{6}$$

Variance of the magnetization

$$\sigma_M^2 = \frac{2^5(e^{8J\beta} + 1)}{Z} - < |M| >^2 \tag{7}$$

$$C_V = \frac{\sigma_E^2}{kT^2} \tag{8}$$

and magnetic susceptibility

$$\chi = \frac{\sigma_M^2}{kT} \tag{9}$$

All these values will prove very useful for verifying that the program simulating larger systems is running correctly.
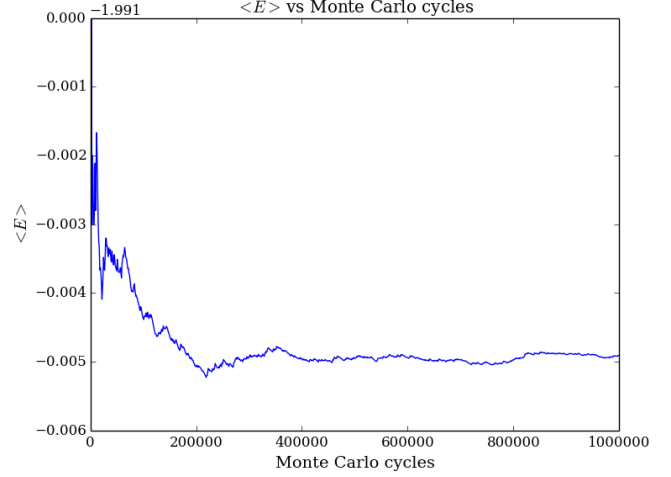

Fig. 1. Plot shows he computed $< E >$ versus the number of Monte Carlo cycles. In this case $T = 1$ (in units of kT/J), and L=2

	Analytical	Numerical
$< E >$	-1.996	-1.996
$< |M| >$	0.999	0.999
C_V	0.032	0.032
χ	0.004	0.004

Table 1. Table of values from the analytial calculations for a system with L=2 and T = 1 in units of (kT/J). Note the precision of the numerical result.

3. Simulating the L=2 system

It is now time to simulated the system using the Metropolis algorithm. The program we write computes the mean energy $< E >$, mean magnetization $< |M| >$, the specific heat C_V and the susceptibility χ as functions of T. To start with we want to check that our program works correclty by checking our results against the ones for the L=2 system. We do this for temperature $T = 1$ (in units kT/J).

By looking at the expectation values versus the number of Monte Carlo cycles we can estimate how many cycles are needed before we get a value close to the analytical one. Depending on what one defines as a "good" approximation we get either a very good match from the beginning, or a good match after about 300,000 cycles. Note that both expectation values for energy and magnetization vary only by one thousandth. See figures 1 and 2.

Comparing the output from the program with the values we calculated earlier gives the following table

4. Larger systems

Since we have now verified that our program runs correctly we want to increase the size of the lattice. We start by increasing the number of spins to $L = 20$ in each direction. We did not study how many cycles were needed to reach the most likely
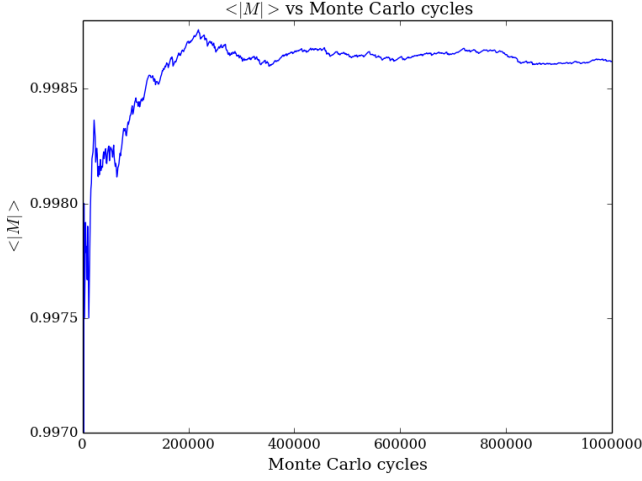
Fig. 2. Plot shows he computed $<|M|>$ versus the number of Monte Carlo cycles. In this case $T = 1$ (in units of kT/J), and L=2

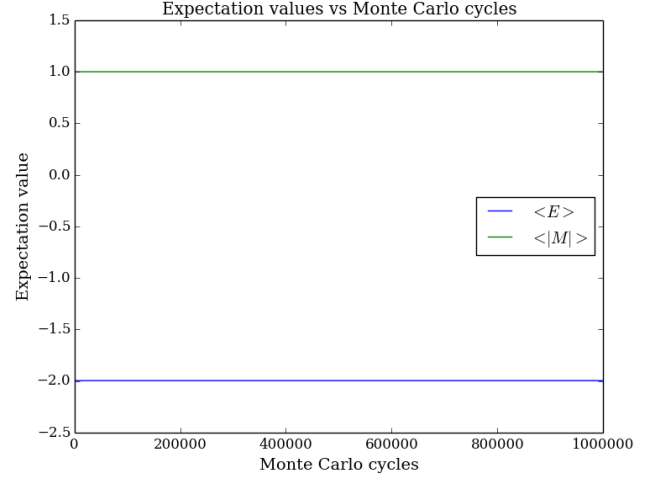**Fig. 3.** The figure shows the expectation values for energy and the absolute value of the magnetization. Note that with such a low temperature the values stabilize from the start, and the variations are too small to see at this scale.

Fig. 4. Plot of specific heat and the magnetic susceptibility as a function of Monte Carlo cycles.

Fig. 5. The figure shows the expectation values for energy and the absolute value of the magnetization for the case with $L = 20$ at $T = 1$ (still in units of kT/J). Note that with such a low temperature the values stabilize from the start, and the variations are too small to see at this scale exactly as we saw for the $L = 2$ case.
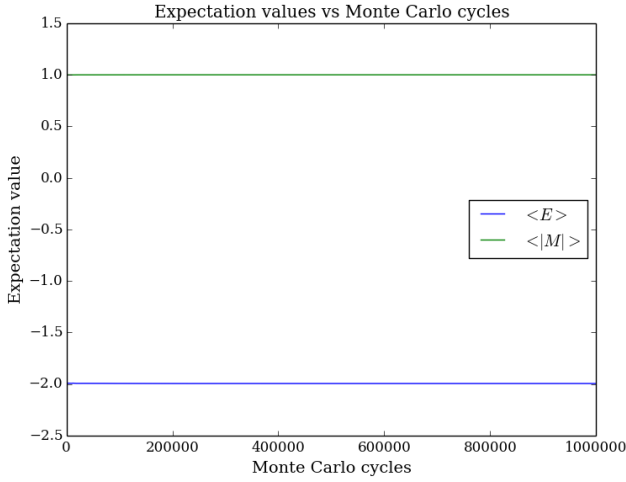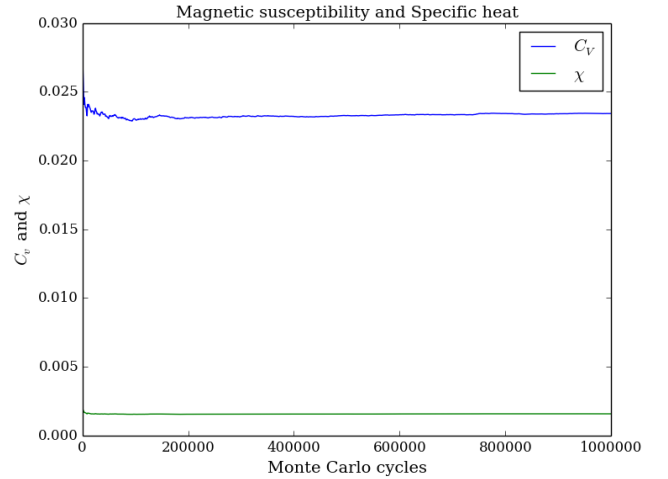

Fig. 6. Plot of specific heat and the magnetic susceptibility as a function of Monte Carlo cycles. In this case $L = 20$, corresponding to 400 spins.
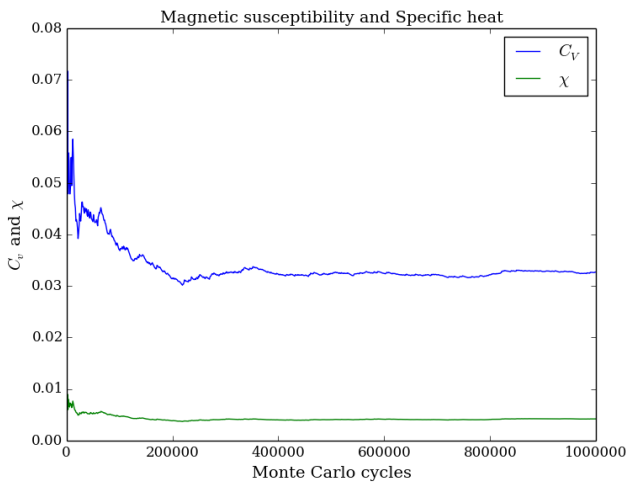
state in the last section. This is something we should study so that we know how much time is needed to reach an equilibrium state, and so how long we have to wait before we start computing our expectation values. We start by making an estimate by plotting the the expectations values as function of the number of Monte Carlo cycles. This is done for $T = 1$. Figure 5 show the expectation values for energy and mangetization, while figure 6 shows the susceptibility and the specific heat. We see that we need about 200,000 Monte Carlo cycles for the values to stabilize.

So far we have only looked at the evolution of a system that starts in an orderes state with all spins pointing up. Next we study the same system, but this time we start in a random state. Figure 7 shows the evolution of this system. If one compares this to the same system with an ordered intial state (figure 6) the difference is remarkable.(The expectation values stabilize too quickly to see any difference at this temperature.)
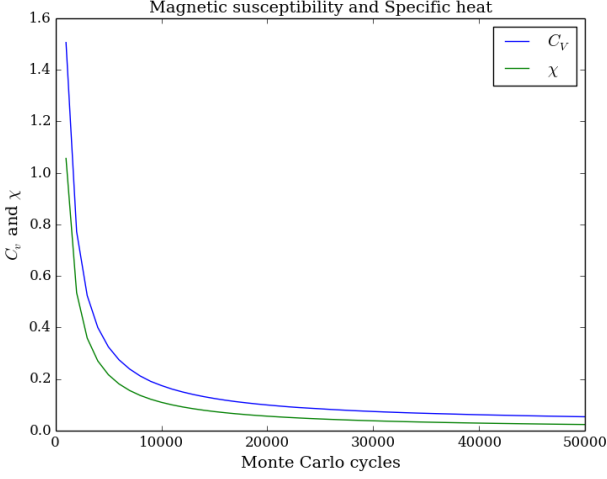
Fig. 7. Plot of specific heat and the magnetic susceptibility as a function of Monte Carlo cycles. In this case $L = 20$, corresponding to 400 spins. This time with a disordered initial state, and $T = 1$.
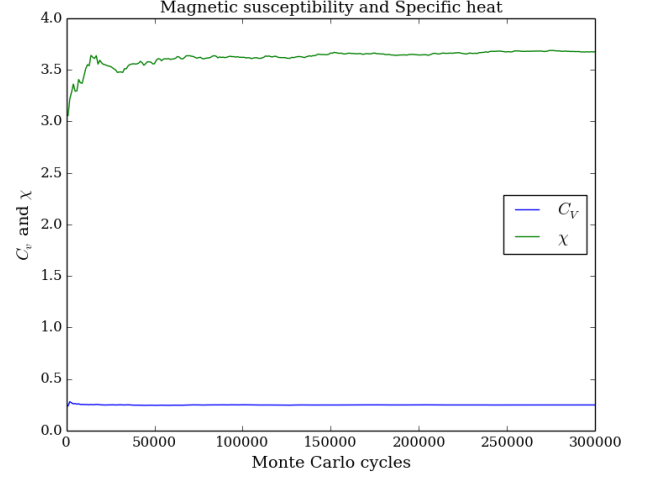

Fig. 9. Plot of specific heat and the magnetic susceptibility as a function of Monte Carlo cycles. In this case $L = 20$, corresponding to 400 spins. This time with a disordered initial state, and $T = 2.4$.
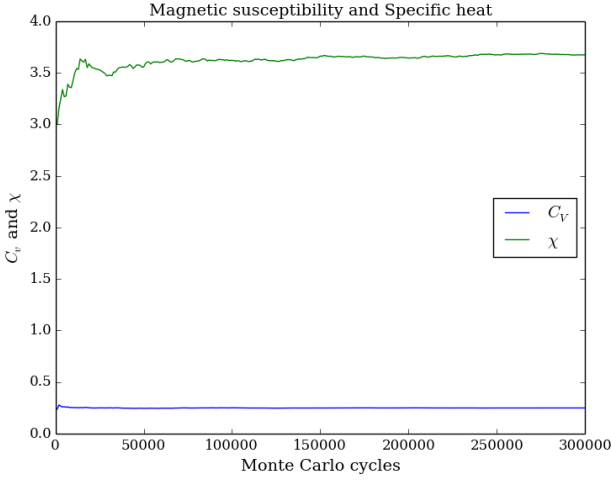

Fig. 8. Plot of specific heat and the magnetic susceptibility as a function of Monte Carlo cycles. In this case $L = 20$, corresponding to 400 spins. This time with an ordered initial state, and $T = 2.4$.
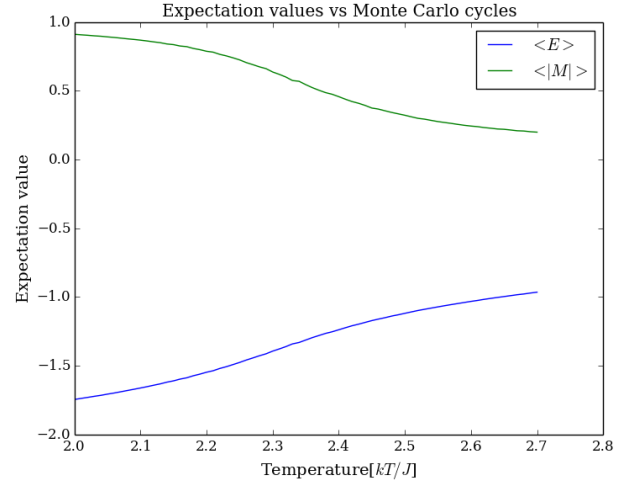

Fig. 10. Plot of the expectation values for magntization and energy for the temperature range $T = [2.1, 2.7]$. In this case our lattice has size $L = 20$. This plot was made with a temperature step 0.01, and 1,000,000 Monte Carlo cycles for each step.

The next step is to increase the temperature. In figure 8 and 9 you can see the magnetization and specific heat with an ordered, and a disordered initial state using $T = 24$.

Note that at this temperature the figures become almost identical. There is actually a small difference in the beginning but it changes so quickly that it is nearly impossible to see with the eye.

In our algoritm there are two processes competing. There is the constant attempt to reach a lower energy state, and there is the metropolis part which accepts moves to higher energies if a random number we pick is lower than $exp(-\Delta_E \beta)$.

This means that if we increase the temperature the probability of reaching a high energy state gets lower and lower. Because of this there is a tansition point where we go from having a lattice that is magnitized to one which is not. Note that increasing the temperature further has noe effect other than minimizing the magnetization even further. To study this we plot the expectation values for energy and magnetization, as well as the specific heat and the susceptibility for $T = [2.1, 2.7]$. The first attempt

uses $L = 20$. The results of this can be seen in figure 11 and 10. We see that the susceptibility goes us up between $T = 2.3$ and $T = 2.4$. This could indicate a phase transition. Looking at the expectation value for the magnetization this would seem to be the case. We should do the same with a larger lattice to be certain.

Plotting exactly the same as before, still with 1,000,000 Monte Carlo cycles for each temperature step for $L = 40$ results in figure 13 and 12. Here the spike in susceptibility is very clear, and the change in magnetization becomes more sudden

We also include the same figures for $L = 60$ (figure 15 and 14) and $L = 80$ (figure 17 and 16).

Phase transitions: The Ising model was motivated by the physical phenomenon ferromagnetism. In order to have ferromagnetism, atoms must have permanent magnetic moments induced by a large number of electrons which spin in the same direction. As the temperature increase, the electron spins gets distorted and the magnetism is reduced. In contrast, decreasing the
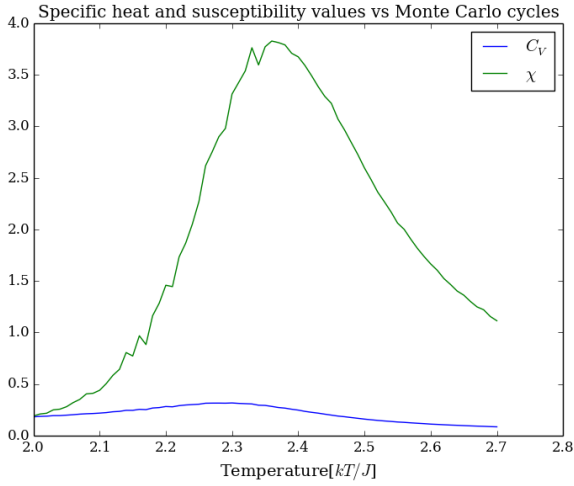
Fig. 11. Plot of specific heat and the magnetic susceptibility as a function temperature. In this case $L = 20$, corresponding to 400 spins. This was made with a temperature step 0.01, and 1,000,000 Monte Carlo cycles for each step.
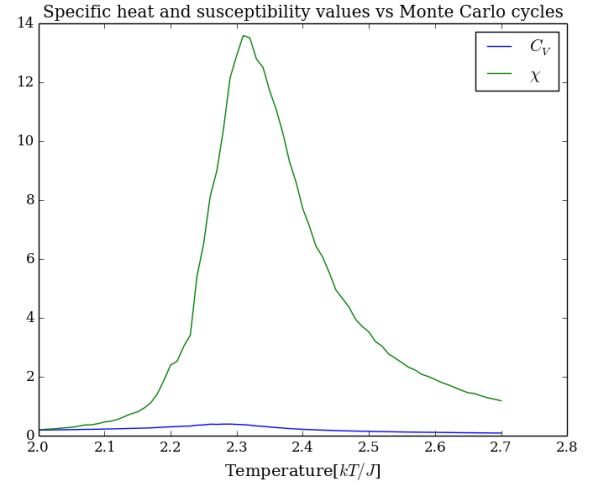

Fig. 13. Plot of specific heat and the magnetic susceptibility as a function temperature. In this case $L = 40$, corresponding to 400 spins. This was made with a temperature step 0.01, and 1,000,000 Monte Carlo cycles for each step.
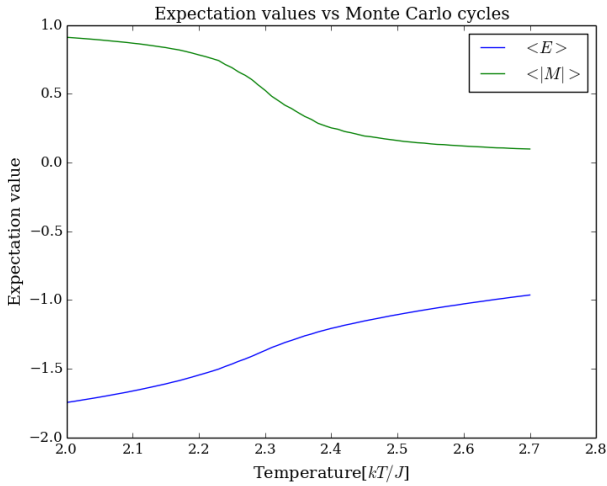

Fig. 12. Plot of the expectation values for magntization and energy for the temperature range $T = [2.1, 2.7]$. In this case our lattice has size $L = 40$. This plot was made with a temperature step 0.01, and 1,000,000 Monte Carlo cycles for each step.
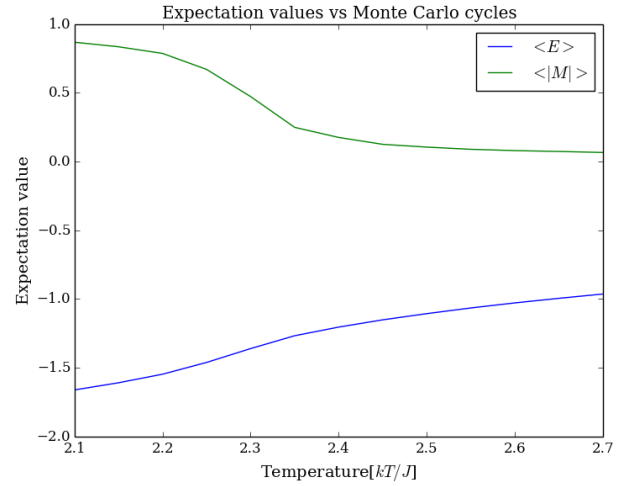

Fig. 14. Plot of the expectation values for magntization and energy for the temperature range $T = [2.1, 2.7]$. In this case our lattice has size $L = 60$. This plot was made with a temperature step 0.01, and 1,000,000 Monte Carlo cycles for each step.

7. References

Computational Physics, Lecture notes Fall 2015, Morten Hjorth-Jensen

temperature will induce magnetic behavior. The electrons have stronger influence on its neighbours, and the spins align. Such transition between magnetic and non magnetic properties in a system is a phase transition. It happens at a certain temperature T_C. Below T_C we have magnetic behaviour. The Ising model allows identification of such transitions.

5. Conclusions

6. Source code

The source code for this document, the c++ project, and the python program for plotting can be found at `https://github.com/pederfo/Project4`.
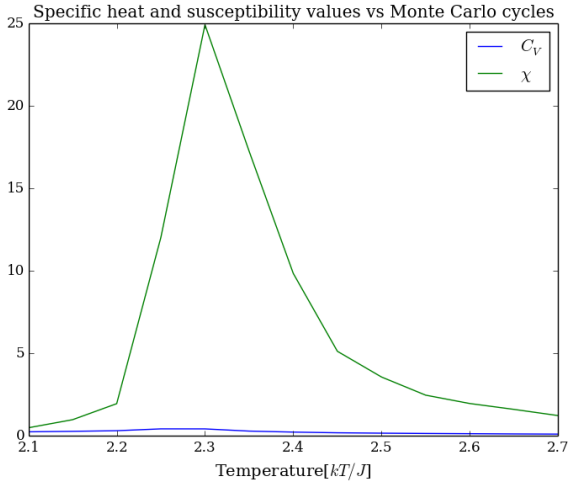
Fig. 15. Plot of specific heat and the magnetic susceptibility as a function temperature. In this case $L = 60$, corresponding to 400 spins. This was made with a temperature step 0.01, and 1,000,000 Monte Carlo cycles for each step.
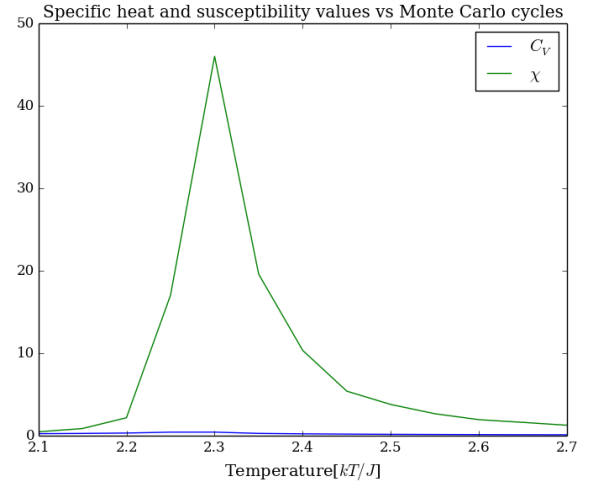

Fig. 17. Plot of specific heat and the magnetic susceptibility as a function temperature. In this case $L = 80$, corresponding to 400 spins. This was made with a temperature step 0.01, and 1,000,000 Monte Carlo cycles for each step.
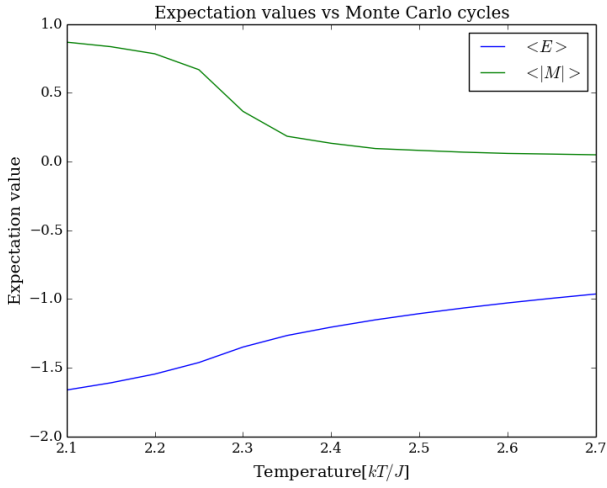

Fig. 16. Plot of the expectation values for magntization and energy for the temperature range $T = [2.1, 2.7]$. In this case our lattice has size $L = 80$. This plot was made with a temperature step 0.01, and 1,000,000 Monte Carlo cycles for each step.