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

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

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

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

A variance for the energy

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

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.

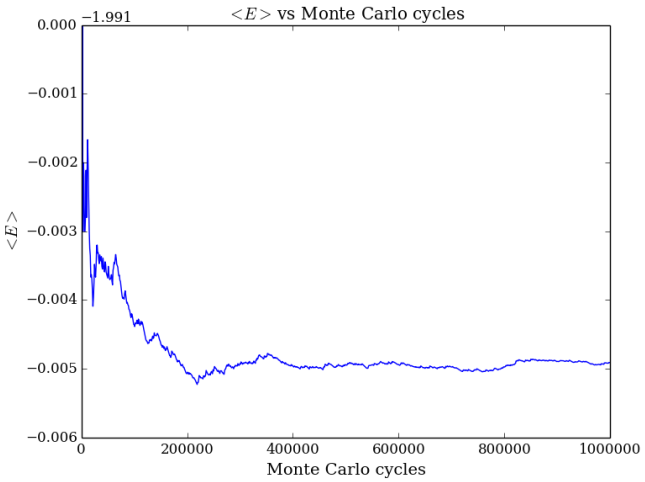

Fig. 1. Plot shows he computed $< E >$ versus the number of Monte Carlo cycles.In this case $T = 1$ (in units of kT/J), and L=2

	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

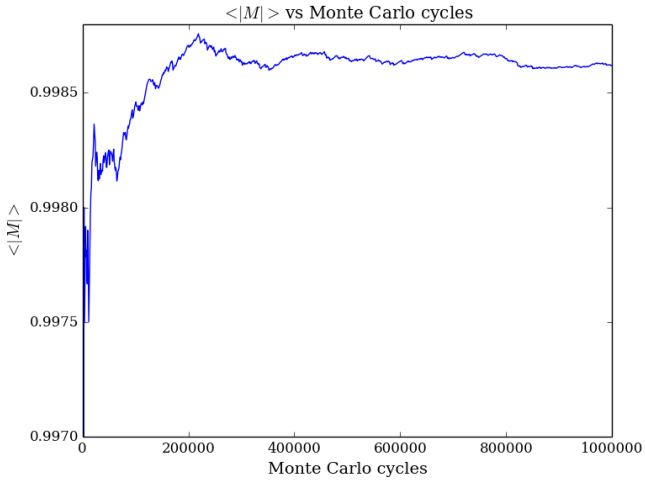

Fig. 2. Plot shows he computed $< |M| >$ versus the number of Monte Carlo cycles. In this case $T = 1$ (in units of kT/J), and L=2

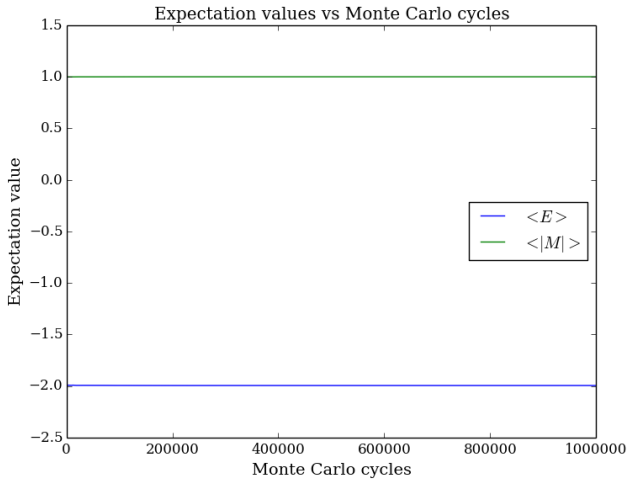

Fig. 3. The figure shows the expectation values for energy and the absolute value of the magnetization. Note that with such a low temperature the values stabilize from the start, and the variations are too small to see at this scale.

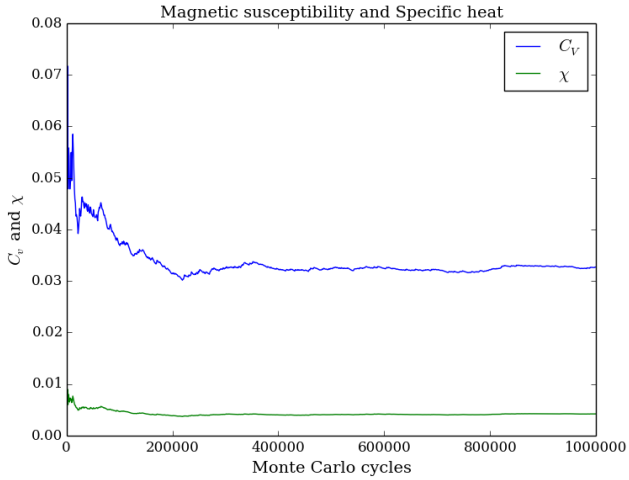

Fig. 4. Plot of specific heat and the magnetic susceptibility as a function of Monte Carlo cycles.

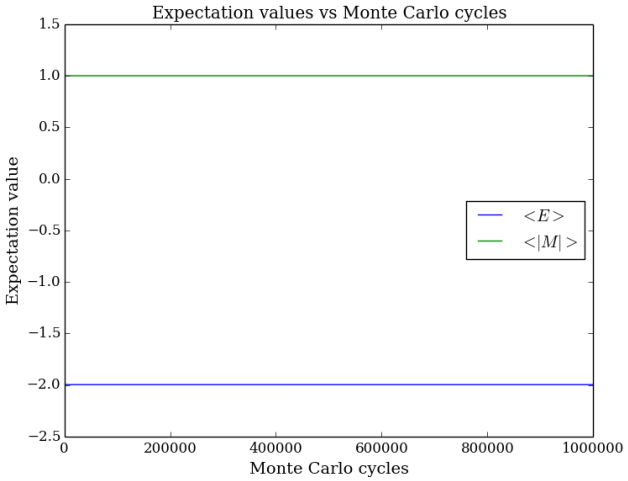

Fig. 5. The figure shows the expectation values for energy and the absolute value of the magnetization for the case with $L = 20$ at $T = 1$ (still in units of kT/J). Note that with such a low temperature the values stabilize from the start, and the variations are too small to see at this scale exactly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

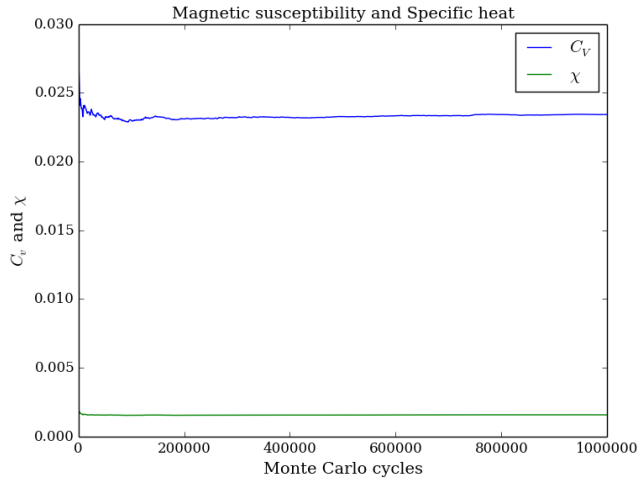

Fig. 6. Plot of specific heat and the magnetic susceptibility as a function of Monte Carlo cycles. In this case $L = 20$, corresponding to 400 spins.

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 XXXXXXXX SOME NUMBER XXXXXXXXXX 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 **??** and **??** shows the evolution of this system.

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.

7. References

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