Project 4, FYS4150

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About the problem

The aim of this project is to simulate the development of a system of spins fixed in a position in the plane. The particles can have spin up or down represented by the values ± 1. We simulate using the simplest form of the Ising model in 2D where the energy of a particle is given by $E = -J \sum_{\langle kl \rangle} s_{kl}$. The notation on the summation sign indicates a sum over the nearest neighbours of the paricle in question. J is here a coupling constant which we will set equal to 1 throughout the project. We will also limit ourselves to using only the Metropolis algorithm with periodic boundary conditions meaning that at the boundary (say the right boundary) the neighbouring partice to the right of a particle at the boundary is the particle on the left boundary with the corresponding coordinates.

The algorithm

The algorithm of choise here is the Metropolis algorithm combined with Monte Carlo (MC) cycles. What we end up doing in the final program is to run some N MC cycles and for each cycle we run trough the entire $n \times n$ grid, pick a spin at random and flip it. We then use the Metropolis principle to estimate wehter or not the flip is accepted. We calculate the change in energy ΔE caused by the flip. If the change in energy is negative the energy of the system is reduced, and the flip is accepted. Should the flip however increase the energy of the system we need to compare the probability of this happening to some other probability. In this case a random number drawn from the uniform distribution. The increase in energy for the system is not a non-physical move, it is simply a very unlikely one. However, this unlikeliness decreases when the temperature becomes large, thus more energy states will become avalible for the system at larger temperatures.

Analytic solution

In the case where we have a lattice size of 2×2 we are able to find a closed form solution for all the important parameters in this project. We will start off by finding the energy of the system for all $2^4 = 16$ possible microstates of the system:

configuration	multiplicity (Ω)	E	$\|M\|$	M	M^2
$\uparrow\uparrow$ $\uparrow\uparrow$	1	-8J	4	4	16
$\uparrow\downarrow$ $\uparrow\uparrow$	4	0	2	2	4
$\uparrow\uparrow$ $\downarrow\downarrow$	4	0	0	0	0
$\uparrow\downarrow$ $\downarrow\uparrow$	2	8J	0	0	0
$\uparrow\downarrow$ $\downarrow\downarrow$	4	0	2	-2	4
$\downarrow\downarrow$ $\downarrow\downarrow$	1	-8J	4	-4	16

Table 1: All the possible spin configurations for a 2×2 system of spins with periodic boudarys.

From this we can find the partition function of the 2×2 system through the well known formula for the partition function

$$Z = \sum_E \Omega(E)e^{-\beta E} = 12 + 2e^{-8\beta J} + 2e^{8\beta J} = 4\left(3 + \cosh(8\beta J)\right)$$

We can now find the energy of the system through the relation

$$\langle E \rangle = -\frac{\partial \ln(Z)}{\partial \beta} = -\frac{1}{4\left(3 + \cosh(8\beta J)\right)} \cdot \frac{d}{d\beta} 4\left(3 + \cosh(8\beta J)\right)$$
$$\langle E \rangle = \frac{-8\beta J \sinh(8\beta J)}{(3 + \cosh(8\beta J))}$$

And by differentiating this expression one more time with respect to β we can find the heat capacity

$$\begin{aligned}\langle C_V \rangle &= \frac{1}{k_B T^2} \cdot \frac{\partial^2 \ln(Z)}{\partial^2 \beta} = \frac{-(8J)^2}{k_B T^2} \cdot \left(\frac{\cosh(8\beta J)(3 + \cosh(8\beta J)) - \sinh^2(8\beta J)}{(3 + \cosh(8\beta J))^2}\right) \\ &= \frac{-(8J)^2}{k_B T^2} \cdot \frac{3\cosh(8\beta J)}{(3 + \cosh(8\beta J))^2}\end{aligned}$$

We can also find the expectation value of the absolute magnetization

$$\langle |M| \rangle = \frac{1}{Z}\sum_{i=1}^{N} |M_i| e^{-\beta E_i} = \frac{1}{Z}\left(2 \cdot 4e^{8\beta J} + 2 \cdot (4 \cdot 2)\right) = \frac{2e^{8\beta J} + 4}{3 + \cosh(8\beta J)}$$

And finally we can find the magnetic sucepitbility $\chi = \frac{\sigma_M^2}{k_B T} = \frac{\langle M^2 \rangle - \langle M \rangle^2}{k_B T}$. We find the relevant values of $\langle M^2 \rangle$ and $\langle M \rangle^2$ from table .

$$\begin{aligned}\chi &= \frac{1}{Z}\sum_{i=1}^{N} M_i^2 e^{-\beta E_i} - \left[\frac{1}{Z}\sum_{i=1}^{N} M_i e^{-\beta E_i}\right]^2 \\ &= \frac{1}{Z}\left(2 \cdot 16e^{8\beta J} + 2 \cdot 4^2\right) - \left[\frac{1}{Z}\left(4e^{8\beta J} - 4e^{8\beta J} + 2 - 2\right)\right]^2 = \frac{8(e^{8\beta J} + 1)}{3 + \cosh(8\beta J)}\end{aligned}$$

Results

As a verification of the program we can check that it reproduces the analytical results for a 2×2 grid with periodic boundary conditions. Now, the analytical solution is for the entire system, while the program gives the results per particle, so we will need to divide the analytical solution by 4 to get corresponding numbers. As mentioned in the introduction we use the values $k_B = J = 1$ and futhermore we will do the verification for the temperature $T = 1$ where T is in units of $\frac{k_B T}{J}$. The results of the verification are found in table 2

-	$\langle E \rangle$	$\langle \lvert M \rvert \rangle$	C_V	χ
analytical	-1,995982086	0,998660733	0,032075159	3,993303776
numeric	-1.99606	0.998681	0.0314933	3.98768

Table 2: verification of the program for a 2×2 grid with 1 000 000 Monte Carlo cycles.

As we can see there is a fair compliance between the analytical results and the results from the program.

We would also like to see if the initial configuration of spins has a lot to say with regard to how fast the system reaches equilibrium. We do this for a 20×20 grid starting out with $T = 1$.

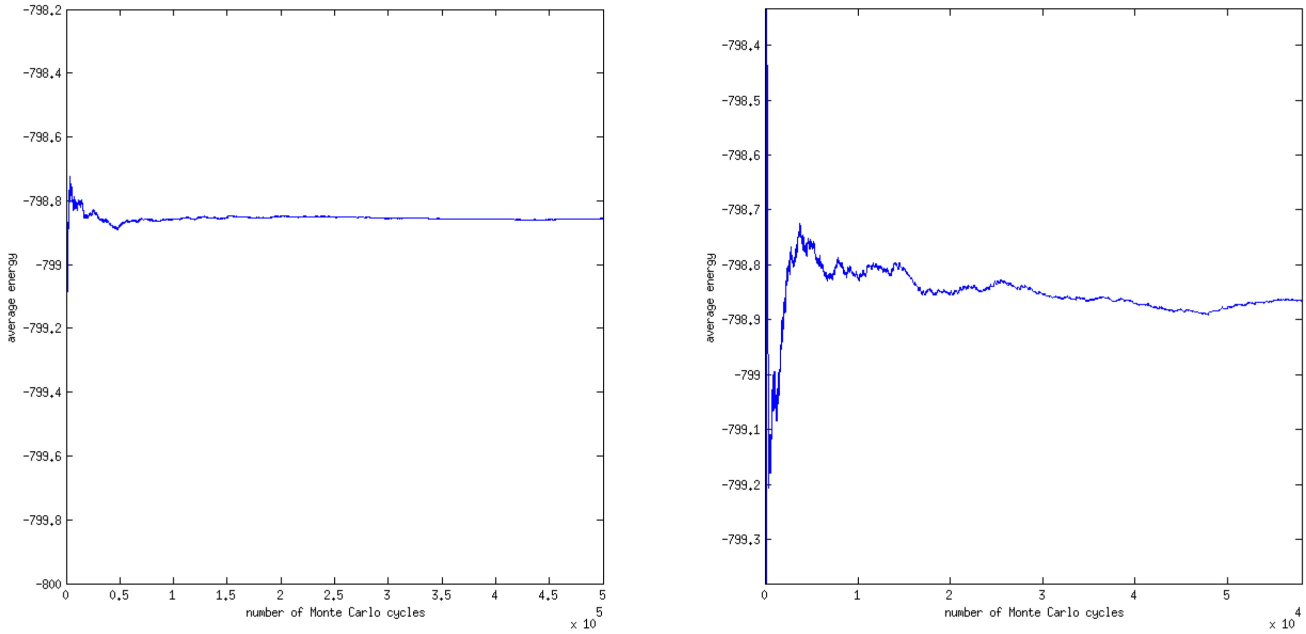

Figure 1: Convergence of the total energy 20×20 grid temperature is 1, all spins pointing up initially.

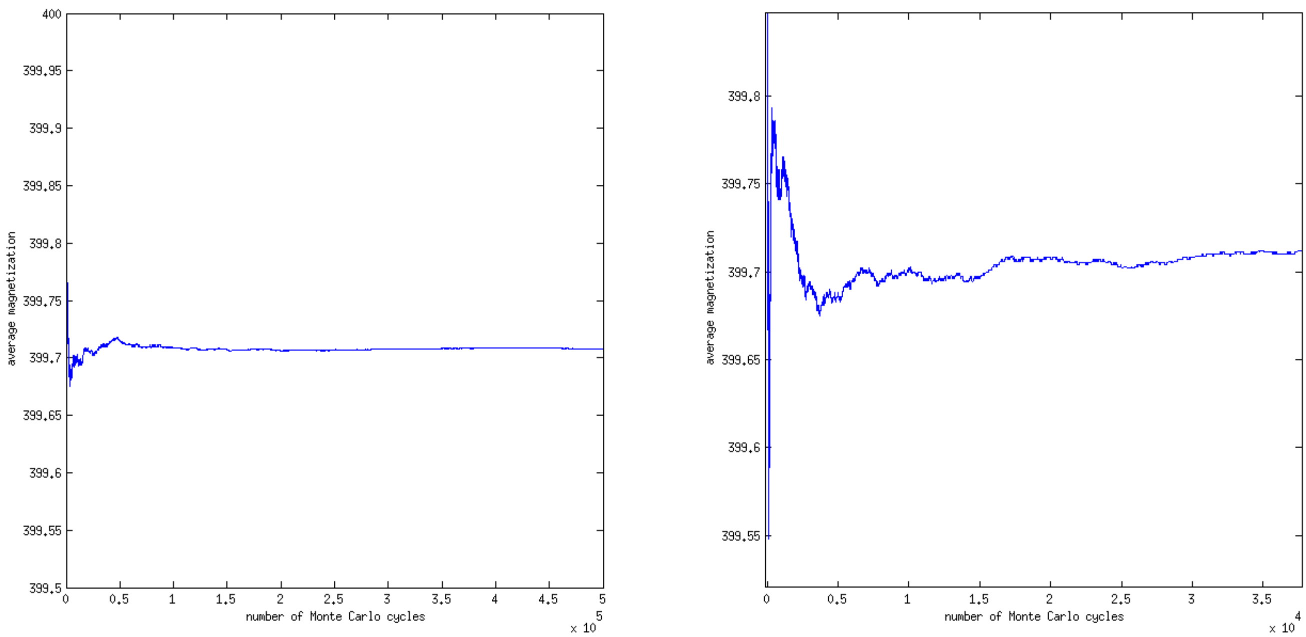

Figure 2: Convergence of the total magnetization 20×20 grid temperature is 1, all spins pointing up initially.

In both figure 1 and 2 the picture on the right is simply a closeup of the interesting part of the left picture. We can see that it takes roughly $5 \cdot 10^4 = 50000$ MC cycles for the energy to reach equilibrium which is 10% of the total amount of MC cycles in this run. Of course when we look at the magnetization at equilibrium, the starting point could not have been better. So what happens if we should start out with a random distribution. We can see the results in figure 3. Surprisingly this seems like a much better starting point even though the initial distribution of spins is far from the equilibrium at the relevant temperature. Figures 4 and **??** show the same plots for the temperature 2.4. We can see from theese plots that it does not seem to matter too much which configuration we start out with. This is because there is no well defined equilibrium configuration of spins at this temperature. The stable (equilibrium) configuration is the random one (we can see this from the magnetization plot when we know that the absolute value of the magnetization is plotted). Thus every initial configuration is equally close to the equilibrium configuration and as we saw for $T = 1$ starting close to equilibrium means slow convergence.

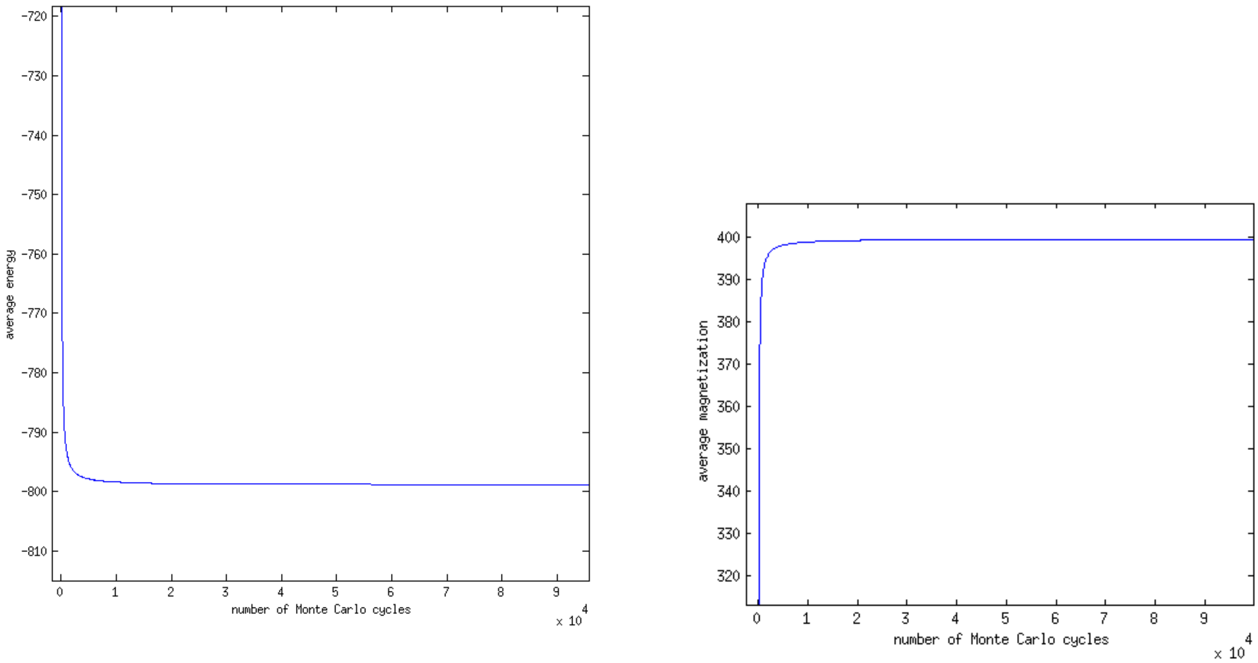

Figure 3: Convergence of the total energy and magnetization 20×20 grid temperature is 1,random initial configuration.

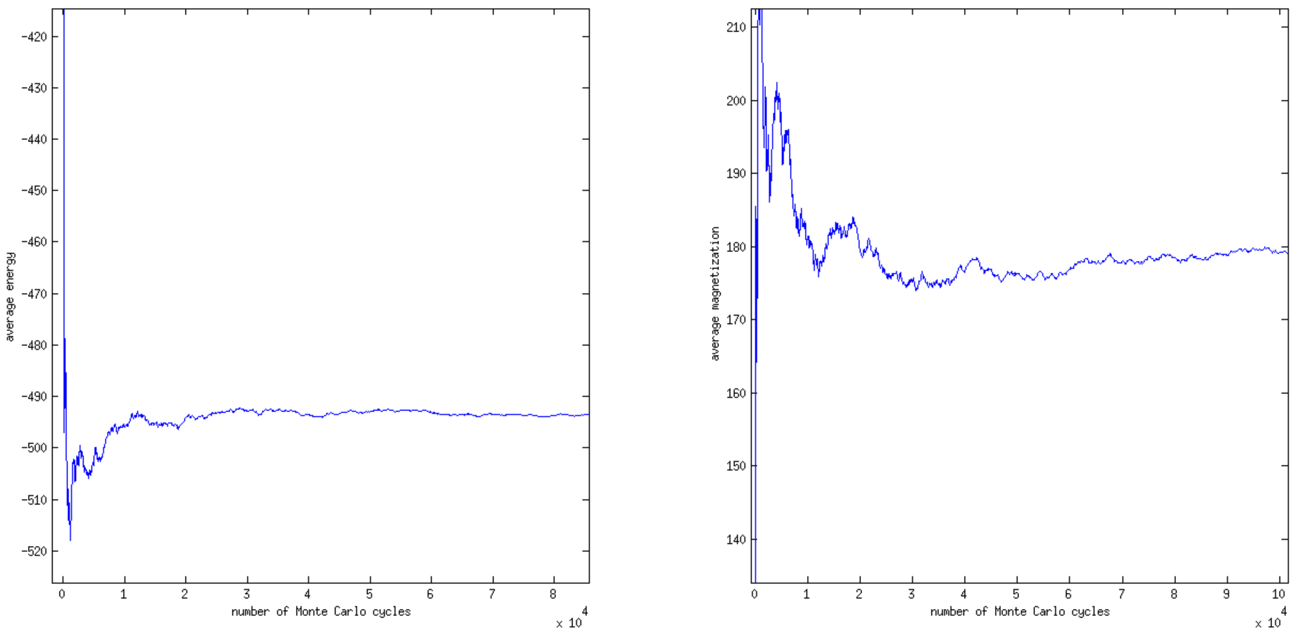

Figure 4: Convergence of the total energy and magnetization 20×20 grid. temperature is 2.4, random initial configuration.

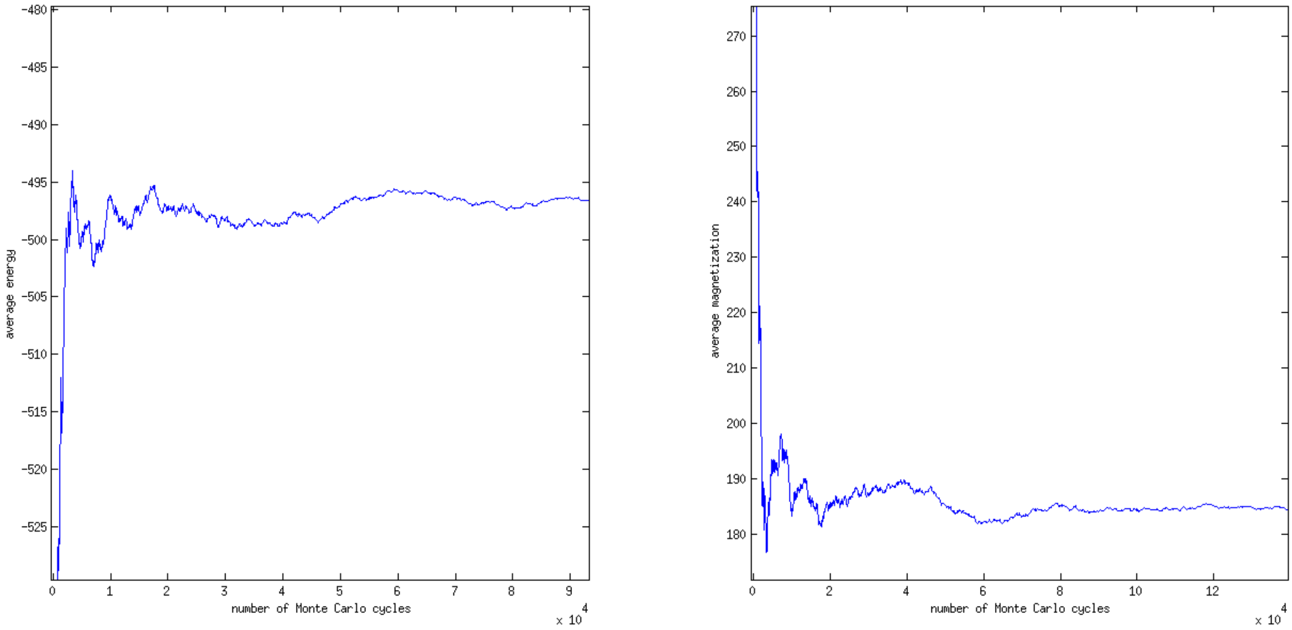

Figure 5: Convergence of the total energy and magnetization 20×20 grid. Temperature is 2.4 all spins initially point up.

One of the things the Ising model can predict is a phase transition, and we can see this in our simplified version too, if we know what to look for. A (second order) phase transition is characterized by a divergence in the heat capacity and in the magnetic suceptibility. Unfortunately theese quantities will only truly diverge in the thermodynamic limit ($n_{spins} \to \infty$), however we can see a discontinuity if we plot them around the critical temperature were the phase transistion takes place. This discontinuity will become more clear for larger grid sizes, as we can see in figures 6

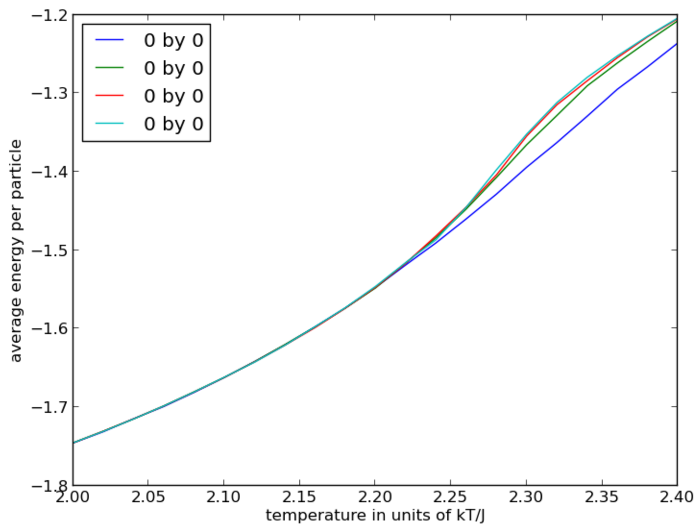

Figure 6: Energy at phase transition

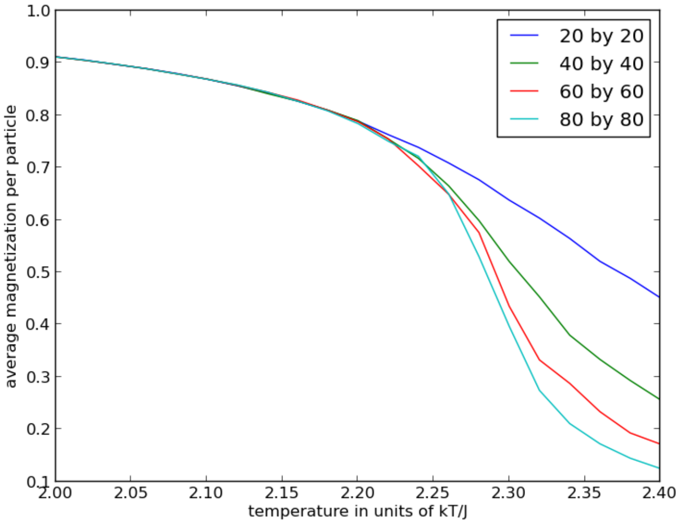

Figure 7: Magnetization at phase transition

Stability and precision

Final comments