

**FYS4150**  
**Project 4, deadline November 15.**



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**Abstract**

# Introduction

In this project we will study phase transitions in magnetic systems. We will use the widely popular Ising model in two dimensions.

# Method

Before starting on the program we need to find analytical expressions for the partition function  $Z$  and the corresponding energy values  $E$ , the mean magnetization  $|M|$ , the specific heat  $C_v$  and the susceptibility  $\chi$  as functions of the temperature  $T$  using periodic boundary conditions.

The partition function is given by:

$$Z = \sum_{i=1}^M e^{-\beta E_i}$$

Where  $M$  is the total number of configurations,  $\beta$  is the inverse temperature given by  $\beta = \frac{1}{kT}$  with  $k$  as the Boltzmann constant.  $E_i$  is the energy for different spin settings given by:

$$E = J \sum_{\langle kl \rangle}^N s_k s_l$$

where  $J$  is a constant which expresses the strength of the interaction between spins.  $N$  is the total number of configurations.  $\langle kl \rangle$  expresses that we only look at the nearest neighbours in the lattice.  $s_k$  and  $s_l$  are the spins of two neighbouring objects.

For now we work with a 2x2 lattice and the Ising model where the spins can only be in two states, giving a total number of  $2^4 = 16$  configurations.

Table 1: Energy with periodic boundary conditions and magnetization for different spin-configurations

Spin configuration	Energy	Magnetization
$\uparrow\uparrow$	$-2J$	2
$\uparrow\downarrow$	$2J$	0
$\downarrow\uparrow$	$2J$	0
$\downarrow\downarrow$	$-2J$	-2

From the table above one can observe that the energy is only non-zero on lattices where all objects have the same spin ( $-8J$ ) and when the diagonals have opposite spin ( $8J$ ). The magnetization of a 2x2 lattice is only zero when half of the objects have the same spin. We can now calculate the mean energy, the mean absolute magnetization, specific heat and susceptibility with these expressions:

Partition function:

$$Z = \sum_{i=1}^{16} e^{-\beta E_i}$$

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

$$Z = 4\cosh(8\beta J) + 12$$

Mean energy:

$$\begin{aligned}\langle E \rangle &= \frac{1}{Z} \sum_{i=1}^{16} e^{-\beta E_i} E_i \\ \sum_{i=1}^{16} e^{-\beta E_i} E_i &= -16J(e^{8\beta J} - e^{-8\beta J}) = -32J \sinh(8\beta J) \\ \langle E \rangle &= -\frac{8J}{\cosh(8\beta J) + 3} \sinh(8\beta J)\end{aligned}$$

Mean absolute magnetization:

$$\begin{aligned}\langle |M| \rangle &= \frac{1}{Z} \sum_{i=1}^{16} e^{-\beta E_i} |M_i| \\ \sum_{i=1}^{16} e^{-\beta E_i} |M_i| &= 8e^{8\beta J} + 16 \\ \langle |M| \rangle &= \frac{2e^{8\beta J} + 4}{\cosh(8\beta J) + 3}\end{aligned}$$

Specific heat:

$$\begin{aligned}C_v &= \frac{\beta}{T} (\langle E^2 \rangle - \langle E \rangle^2) \\ \langle E \rangle^2 &= \frac{64J^2}{(\cosh(8\beta J) + 3)^2} \sinh^2(8\beta J) \\ \langle E^2 \rangle &= \frac{1}{Z} \sum_{i=1}^{16} e^{-\beta E_i} E_i^2 = \frac{64J^2}{\cosh(8\beta J) + 3} \cosh(8\beta J) \\ \rightarrow C_v &= \frac{64\beta J^2}{T(\cosh(8\beta J) + 3)^2} (3\cosh(8\beta J) + 1)\end{aligned}$$

Susceptibility:

$$\begin{aligned}\chi &= \beta (\langle |M|^2 \rangle - \langle |M| \rangle^2) \\ \langle |M|^2 \rangle &= \frac{1}{Z} \sum_{i=1}^{16} e^{-\beta E_i} M_i^2 = \frac{8e^{8\beta J} + 8}{\cosh(8\beta J) + 3} \\ \rightarrow \chi &= \beta \left( \frac{8e^{8\beta J} + 8}{\cosh(8\beta J) + 3} - \frac{(2e^{8\beta J} + 4)^2}{(\cosh(8\beta J) + 3)^2} \right)\end{aligned}$$

Giving these values:

$$\langle E \rangle = -7.983928$$

$$\langle |M| \rangle = 3.994643$$

$$C_v = 0.128329$$

$$\chi = 0.016043$$

Notice that the terms in  $C_v$  and  $\chi$ ,  $\langle E^2 \rangle - \langle E \rangle^2$  and  $\langle |M|^2 \rangle - \langle |M| \rangle^2$ , respectively, are the variance of the energy and variance of the magnetization.

# Method

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# Results

After only 10.000 Monte Carlo cycles the numerical solutions for the mean energy and the mean magnetization are close to the values found analytical. They are only off by a value of  $10^{-3}$ . To get the same magnitude of agreement for the specific heat and susceptibility, 100.000 Monte Carlo cycles was needed. For fewer than 10.000 Monte Carlo cycles the values are irregular.

Table 2: Analytical and numerical solutions

	Analytical	Numerical	MC cycles
$\langle E \rangle$	-7.983928	-7.98472	10.000
$\langle  M  \rangle$	3.994643	3.99494	10.000
$C_v$	0.128329	0.122007	100.000
$\chi$	0.016043	0.015054	100.000

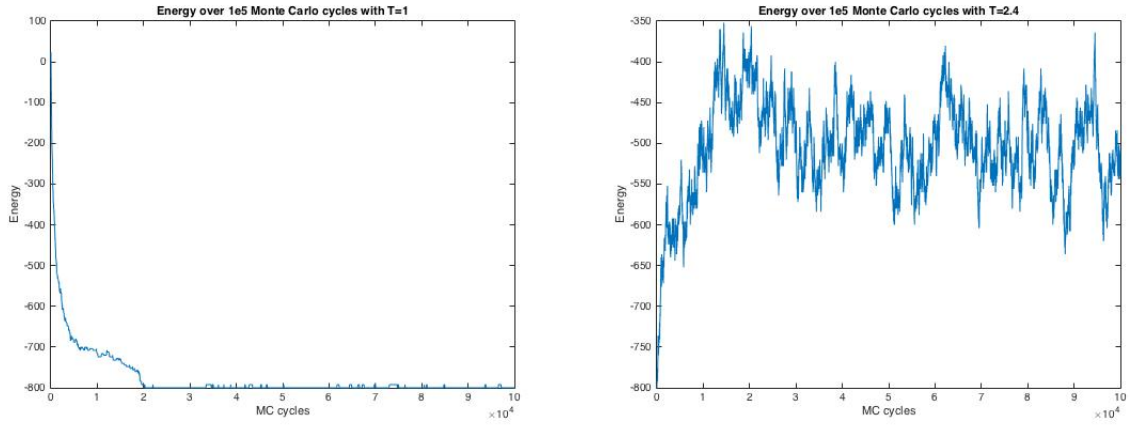


Figure 1: Energy vs. Monte Carlo cycles for  $T=1$ (left) and  $T=2.4$ (right) with random initial  $20 \times 20$  matrix

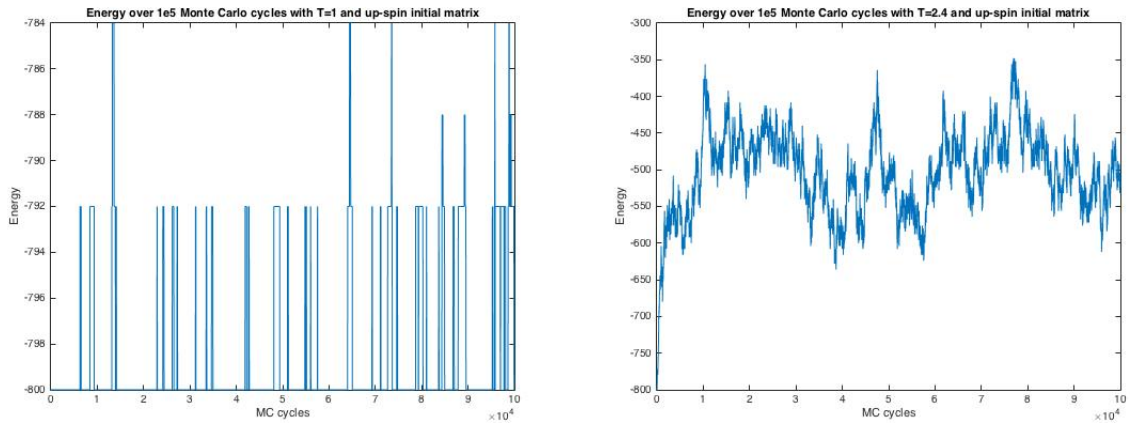


Figure 2: Energy vs. Monte Carlo cycles for  $T=1$ (left) and  $T=2.4$ (right) with initial up-spin orientated  $20 \times 20$  matrix

From figure 1 we notice that the random  $20 \times 20$  lattice with  $T=1$  reach an equilibrium situation after

$2 \times 10^4$  Monte Carlo cycles. For  $T=2.4$  the energy oscillates more, but the equilibrium is reached after about the same amount of Monte Carlo cycles. With an initial up-spin oriented matrix the equilibrium is reached more promptly as seen in figure 2, after about  $7 \times 10^3$  Monte Carlo cycles. The up-spin oriented matrix with a higher temperature oscillates more, but yet again the equilibrium is reached after the same amount of Monte Carlo cycles as for  $T=1$ .

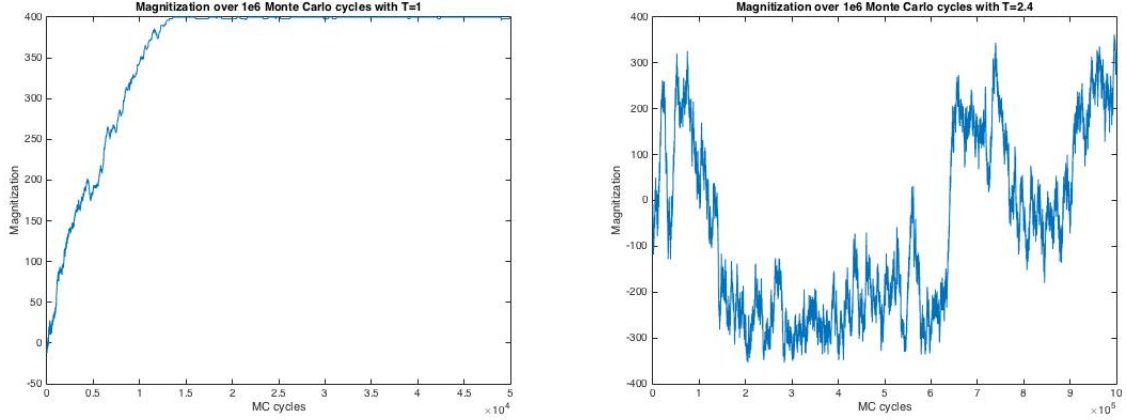


Figure 3: Magnetization vs. Monte Carlo cycles for  $T=1$ (left) and  $T=2.4$ (right) with random initial  $20 \times 20$  matrix

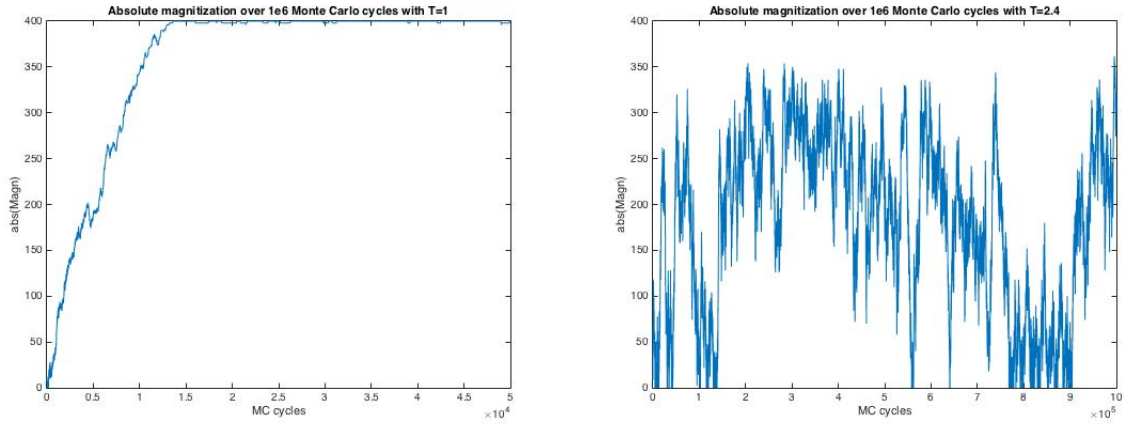


Figure 4: Absolute magnetization vs. Monte Carlo cycles for  $T=1$ (left) and  $T=2.4$ (right) with random initial  $20 \times 20$  matrix

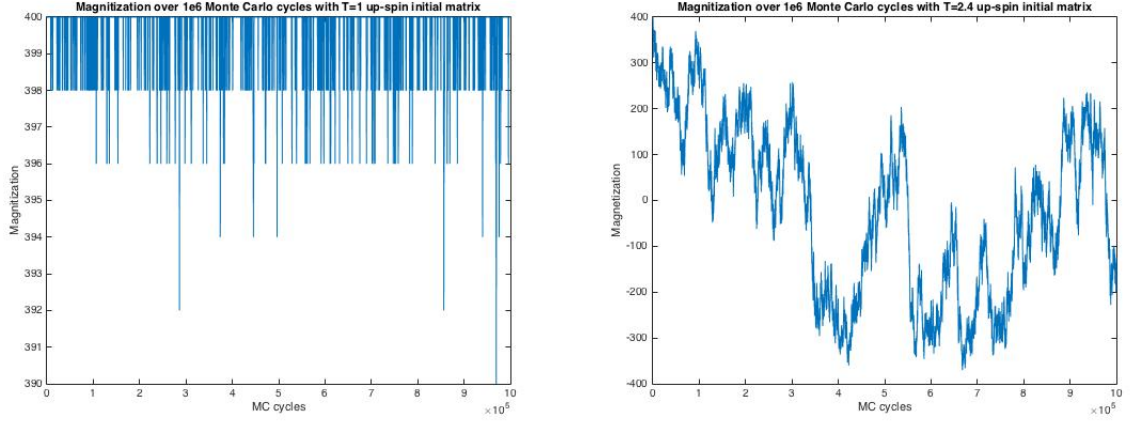


Figure 5: Magnetization vs. Monte Carlo cycles for  $T=1$ (left) and  $T=2.4$ (right) with up-spin initial  $20 \times 20$  matrix

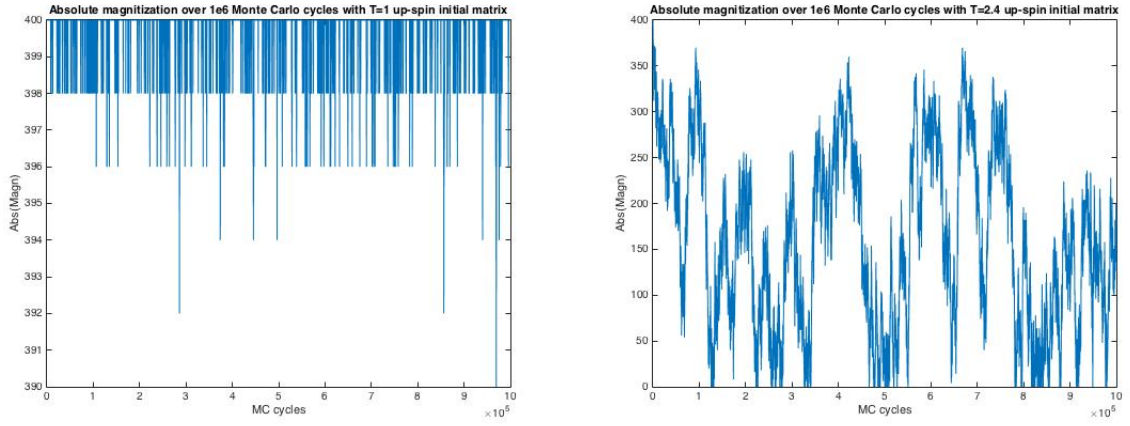


Figure 6: Absolute magnetization vs. Monte Carlo cycles for  $T=1$ (left) and  $T=2.4$ (right) with up-spin initial  $20 \times 20$  matrix

Table 3: Equilibrium values for  $T=1$   $T=2.4$  for random- and up-spin orientated matrix

Initial matrix:	Temperature:	Equilibrium	MC cycles
Random	1	Random	Random
Random	2.4	Random	Random
Up-spin	1	400	xx
Up-spin	2.4	0	xx

For a random initial matrix the equilibrium value differs depending on the initial matrix. One of them are shown in figure 3. This one reaches equilibrium after  $1.5 \times 10^4$  Monte Carlo cycles with a magnetization value of 400. After multiple runs with different initial matrices they all seem to reach equilibrium before  $3 \times 10^4$  Monte Carlo cycles, but the values varies.

The up-spin oriented initial matrix with  $T=1$  start with a magnetization equal to its equilibrium value of



400, and does not differ much. Notice the values on the y-axis. When  $T=2.4$  the magnetization oscillates more but blabla

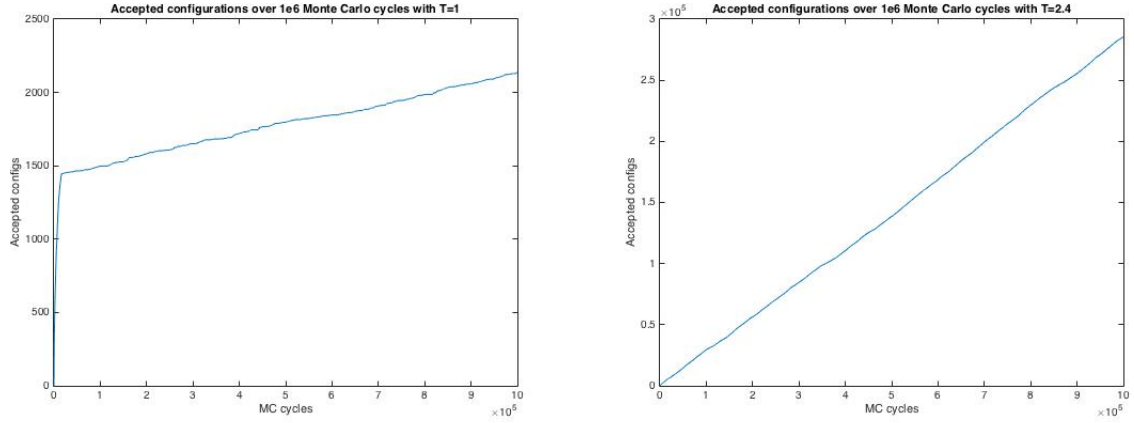


Figure 7: Accepted configurations over  $1e^6$  Monte Carlo cycles for  $T=1$ (left) and  $T=2.4$ (right) for a random initial  $20 \times 20$  matrix

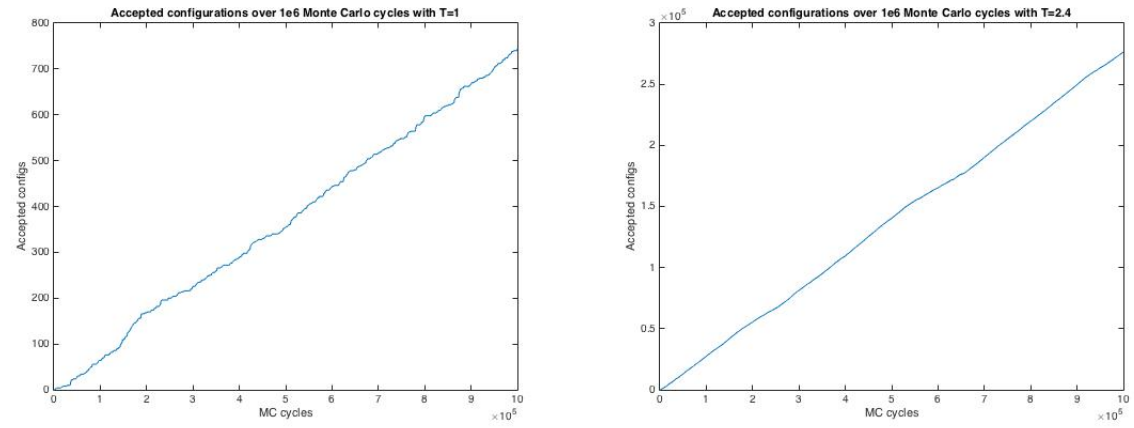


Figure 8: Accepted configurations over  $1e^6$  Monte Carlo cycles for  $T=1$ (left) and  $T=2.4$ (right) for an up-spin initial  $20 \times 20$  matrix

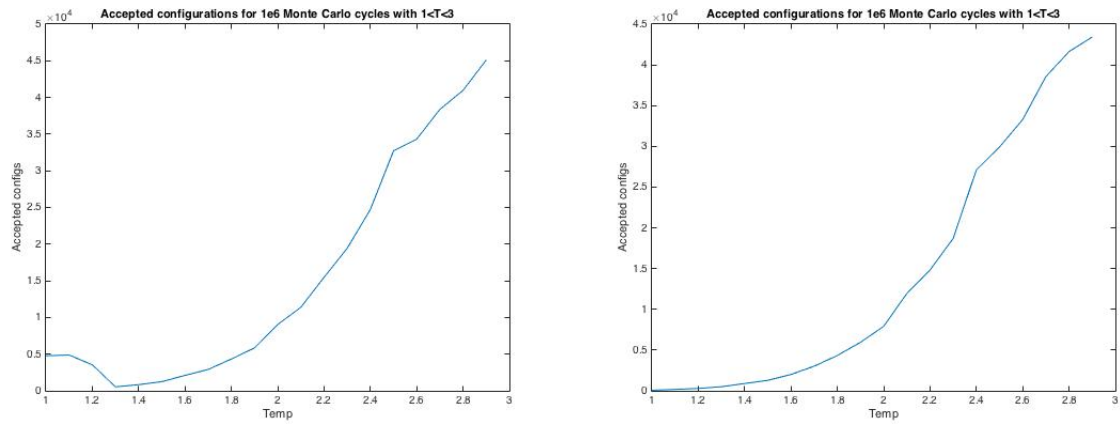


Figure 9: Accepted configurations for  $1e^6$  Monte Carlo cycles over  $1 < T < 3$  for a random- and up-spin initial  $20 \times 20$  matrix, respectively

As seen in figure 7, for a random initial 20x20 matrix and  $T=1$  a lot of configurations are accepted at the start, before quickly (less than  $10^5$  Monte Carlo Cycles) reaching an linear state where about the same amount of configurations are accepted. Here it behaves as the initial up-spin matrix seen in figure 8. For  $T=2.4$  the random- and up-spin initial matrices behaves the same. They both accept much more configurations and does not seem to reach a state of equilibrium(?).

Figure 9 shows us a exponential growth in accepted configurations for increasing temperatures. There does not seem to be big differences between a random- and a up-spin initial 20x20 matrix.

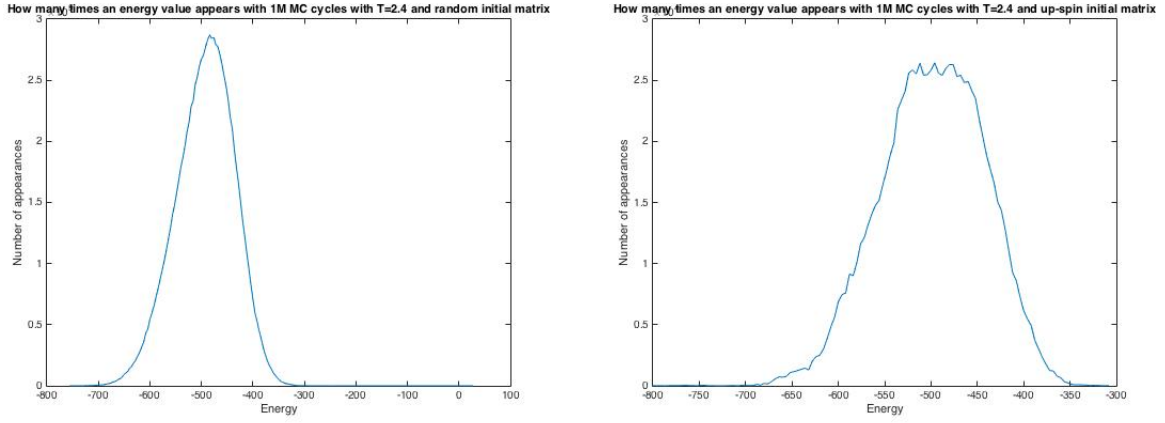


Figure 10: Probability distribution for  $T=2.4$ , random- and up-spin initial  $20 \times 20$  matrix, respectively

Table 4: Variance in energy found graphical and numerical

Initial matrix:	Temperature:	Variance graphical	Variance numerical(spe heat)
Random	1	496.65	496.65
Random	2.4	3178.2	3178.24
Up-spin	1	9.85	9.85
Up-spin	2.4	3151.8	3152.76

graphical in matlab and numerical in c++

For random- and up-spin initial matrix and  $T=1$  there are almost only the equilibrium value and a small variance. For  $T=2.4$  we notice a negative skewed probability distribution, with the mean value laying on the left side of the mode.