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FYS4150
Project 4 - deadline November 15

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Introduction

Method

To be able to start programming, one first needs to find the expressions for the partition function Z with its corresponding energy values E, the mean magnetic moment M, the specific heat C_V and the susceptibility X as functions of the temperature T. All of this using the periodic boundary condition. The partition function Z is giving by:

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

where β is the inverse temperature given by $\beta = \frac{1}{kT}$ where k is the Boltzmann constant and T is the temperature, so every expression containing β is dependent on the temperature T. E_i is the energy for different spin settings given by:

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

where J is the coupling constant and N is the total number of spins. s_k and s_l are the spins of two neighbouring objects in a lattice. Since we are working 2x2 lattice, the total number of combinations are given by $2^4 = 16$, considering we are working with the Ising model where the spins can only be -1 or 1.

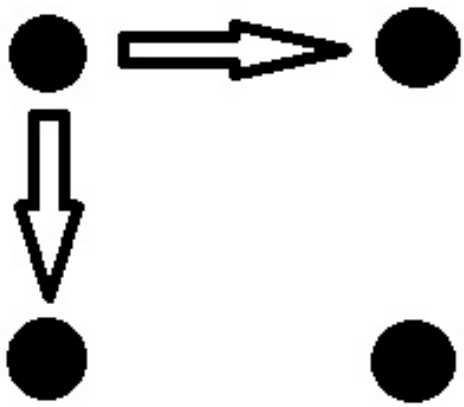


Figure 1: A two by two lattice and how they interact using the Ising model

From figure 1 we see how the Ising model works on a 2x2 lattice and from this the energy is calculated. One can observe that energy is non-zero on lattices where all the objects have the same spin $(-8J)$ and where the two diagonals have opposite spin from each other $(8J)$. All other settings have zero energy. Knowing the energy values we can calculate the mean energy $< E >$ with our specific partition function:

$$< E >= \frac{1}{Z}\sum_{i=1}^{M} E_i e^{-\beta E_i}$$

$$= \frac{1}{2e^{-8} + 2e^{8} + 12}\sum_{1}^{16} E_i e^{-\beta E_i}$$

$$= \frac{16e^{-8} - 16e^{8}}{2e^{-8} + 2e^{8} + 12} = -7.983928$$

Now we can simply put the same energy values into our partition function:

$$Z = e^{-\beta * -8J} + e^{-\beta * -8J} + e^{-\beta * 8J} + e^{-\beta * 8J} + 12 * e^{0}$$

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

The magnetization is given by:

$$M = \sum_{j=1}^{N} s_j$$

Unlike in the energy case, the magnetization does not depend the lattice having the same spin or that the diagonals have opposite spin. The only case where the magnetization is zero in a 2x2 lattice is when half of the objects in the lattice opposite spins. Therefore we get the magnetization values:

$$M_i = [4 + 2 + 2 + 2 + 2 + 0 + 0 + 0 + 0 + 0 + 0 + -2 + -2 + -2 + -2 + -4]$$

To calculate the mean magnetic moment or mean magnetization we use the equation below with our calculated magnetic moment and energy values:

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

$$= \frac{1}{2e^{-8} + 2e^{8} + 12}\sum_{1}^{16} M_i e^{-\beta E_i}$$

$$= \frac{8e^{8} + 16}{2e^{-8} + 2e^{8} + 12} = 3.994643$$

To calculate the the specific heat, one only needs to know the total number of spins of the lattice. In the 2x2 lattice case the total number of spins is 4, and remember also that $\beta J = 1$ and $k = 1$. The specific heat is then:

$$C_V = \frac{1}{kT^2}(< E^2 > - < E >^2)$$

$$= \frac{1}{kT^2}(\frac{128e^{-8} - 128e^{8}}{2e^{-8} + 2e^{8} + 12} - (\frac{16e^{-8} - 16e^{8}}{2e^{-8} + 2e^{8} + 12})^2)$$

$$= 0.128329$$

The term $< E^2 > - < E >^2$ is also called the variance of the energy and is precisely calculated just as shown above. The same variance calculation can be applied to calculating the susceptibility, but the energy terms have to be substituted for mean magnetization. Let's calculate the variance separate from the desired equation this time:

$$\sigma_M^2 =< M^2 > - < M >^2 = \frac{1}{Z}\sum_{i=1}^{M} M_i^2 e^{-\beta E_i} - (\frac{1}{Z}\sum_{i=1}^{M} M_i e^{-\beta E_i})^2$$

$$= \frac{32}{2e^{-8} + 2e^{8} + 12}(e^8 + 1) - (\frac{8e^8 + 16}{2e^{-8} + 2e^{8} + 12})^2 = 0.016004$$

Remember that the $\beta = 1$ in the 2x2 lattice case, so the susceptibility would be the same as the variance in that case. We would usually have to calculate the susceptibility with the following equation:

$$X = \frac{1}{k_b T}(< M^2 > - < M >^2) = \frac{1}{k_b T}\sigma_M^2 = 0.010853$$

Results

From the general equations in the method, the following analytical and numerical values were found:

Table 1: Analytical and numerical solutions

Type	Analytical	Numerical	MC cycles needed
$< E >$	-7.983928	-7.98437	10 000
$< M >$	3.994643	3.99483	10 000
C_V	0.128329	0.124812	100 000
$< X >$	0.016004	0.0153613	100 000

To get good results for mean energy and mean magnetic moment took very few Monte Carlo, or MC, cycles, only about 10 000. Then the values would be off only by a factor of about 10^{-3}. The susceptibility and the specific heat took more MC cycles and correct results started showing around 10^5 for susceptibility and specific heat. For 10^4 both the specific heat and susceptibility were unstable.

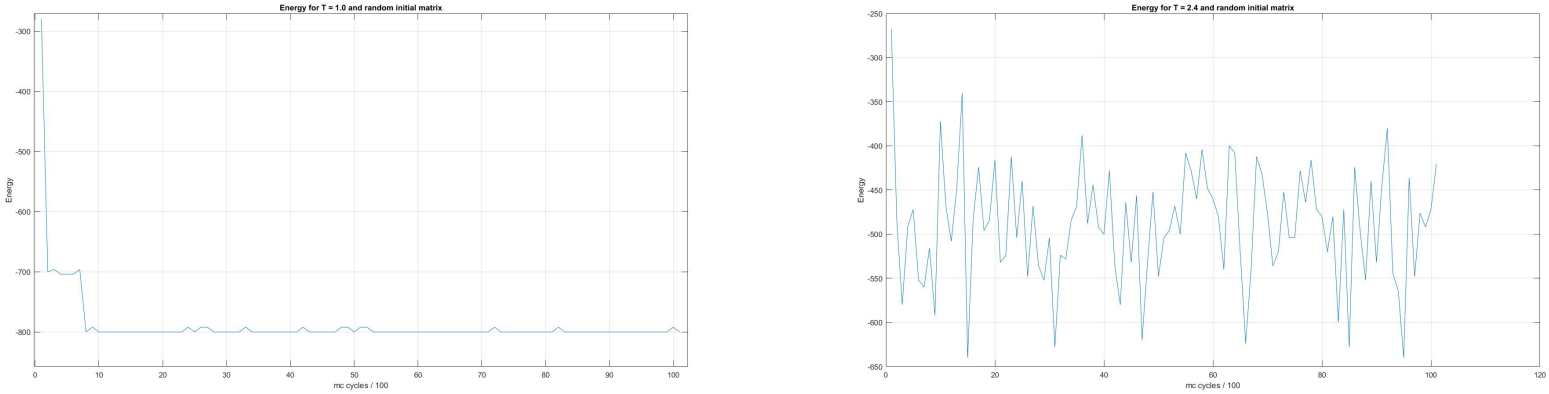


Figure 2: Energy versus Monte Carlo cycles for T = 1.0 and T = 2.4 with a random initial matrix

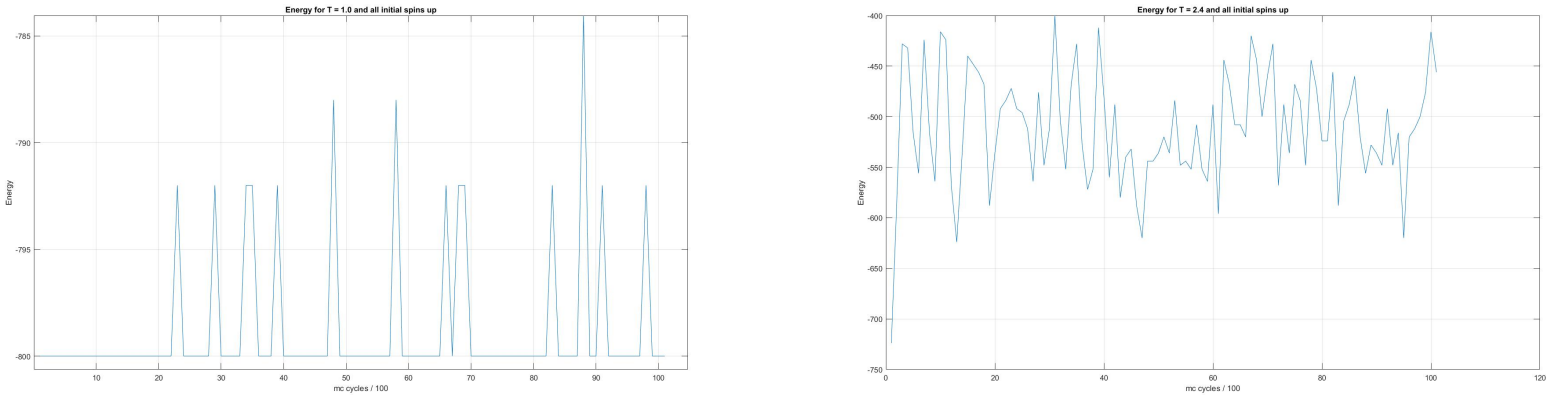
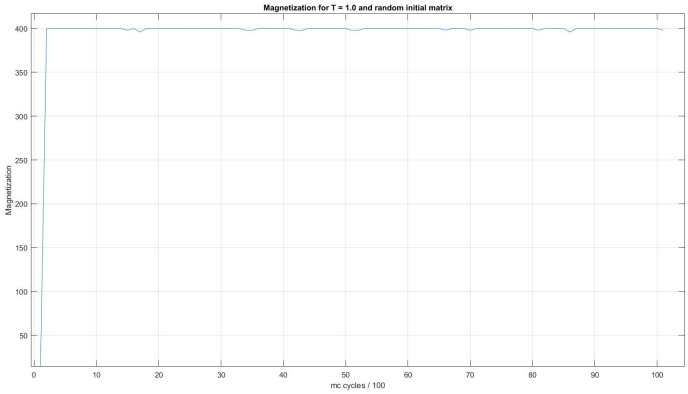


Figure 3: Energy versus Monte Carlo cycles for T = 1.0 and T = 2.4 with initial spin upwards



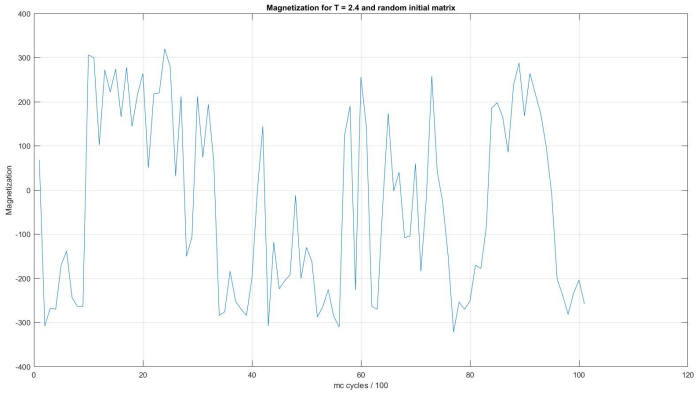
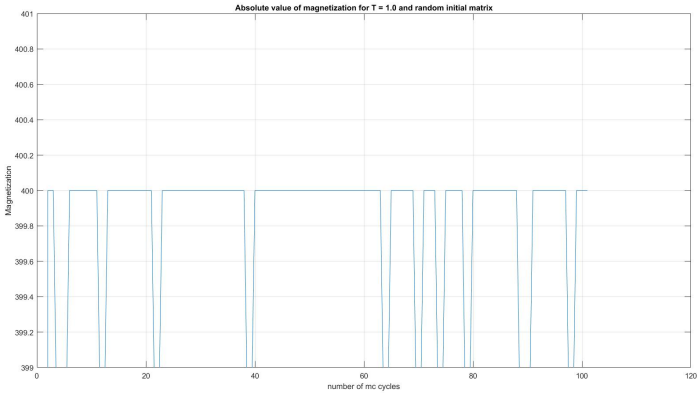


Figure 4: Magnetization versus Monte Carlo cycles for T = 1.0 and T = 2.4 with a random initial matrix



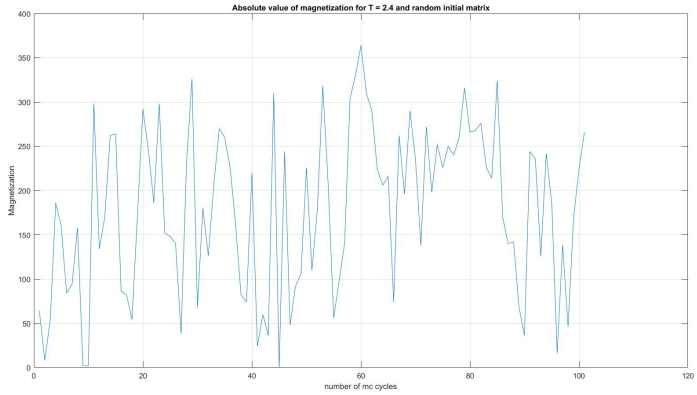
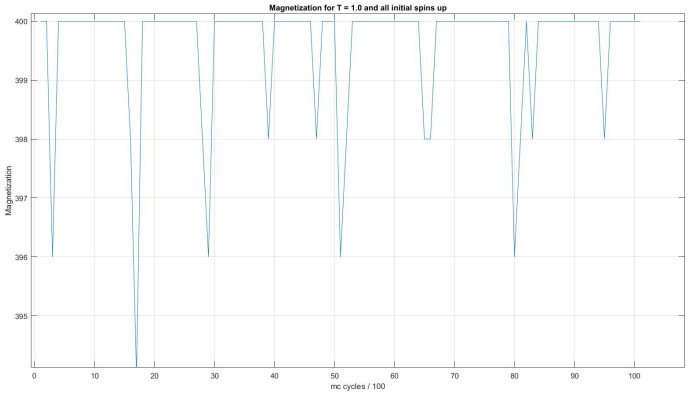


Figure 5: Absolute value of magnetization versus 10 000 Monte Carlo cycles for T = 1.0 and T = 2.4 with a random initial matrix



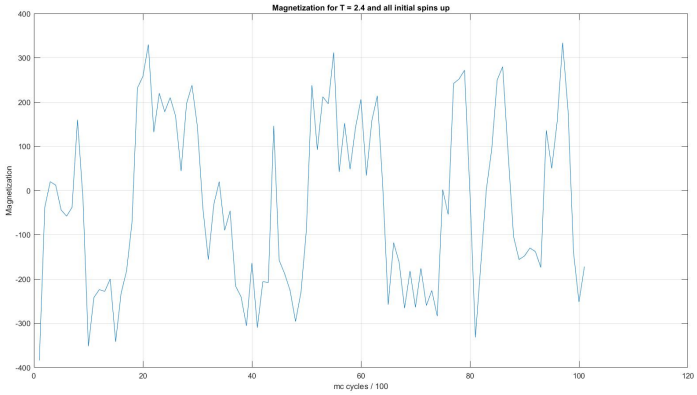
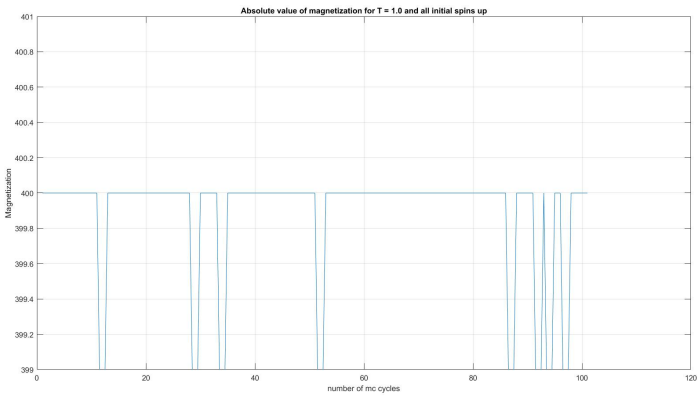


Figure 6: Magnetization versus Monte Carlo cycles for T = 1.0 and T = 2.4 with initial spin upwards



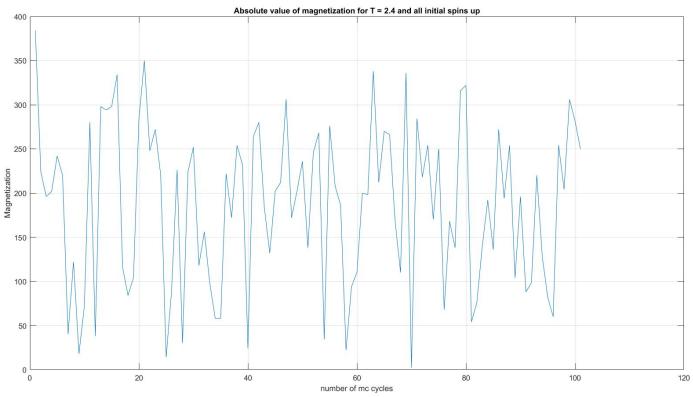


Figure 7: Absolute value of magnetization versus 10 000 Monte Carlo cycles for T = 1.0 and T = 2.4 with initial spin upwards

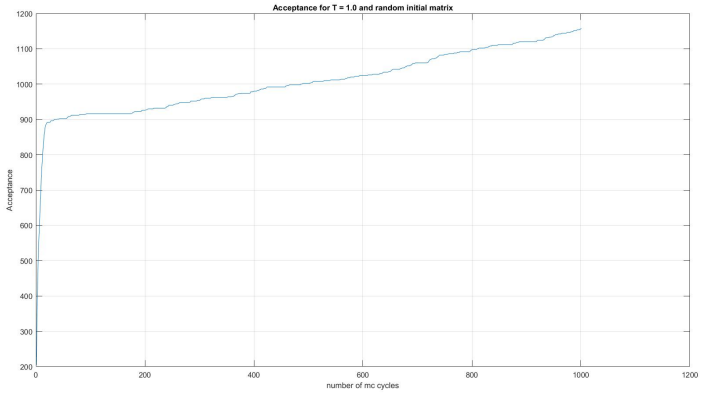
We can see from figure 2, figure 3, figure 4 and figure 6 that the mean energy and magnetization quickly approaches it's equilibrium state when the temperature equals 1. There are of coarse fluctuations after the mean energy and magnetization has reached it's equilibrium state, but the value tends to jump back to to the equilibrium state. Another observation is that the mean energy and magnetization value are more unstable if one starts with an initial matrix where all the spins are oriented upwards. The values become even more unstable when the temperature is increased to 2.4, and also the value of the equilibrium state is changed.

Table 2: EQ values for energy

Orientation	Temperature	EQ state	max MC cycles needed
Random	1.0	-790.581	600
Random	2.4	-496.494	1000
Upwards	1.0	-798.96	1
Upwards	2.4	-493.996	300

Table 3: EQ values for magnetization

Orientation	Temperature	EQ state	max MC cycles needed
Random	1.0	398.762	???
Random	2.4	165.209	???
Upwards	1.0	399.732	1
Upwards	2.4	176.087	???



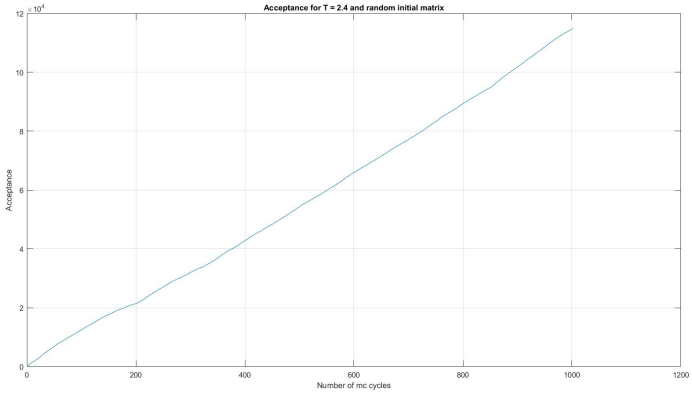
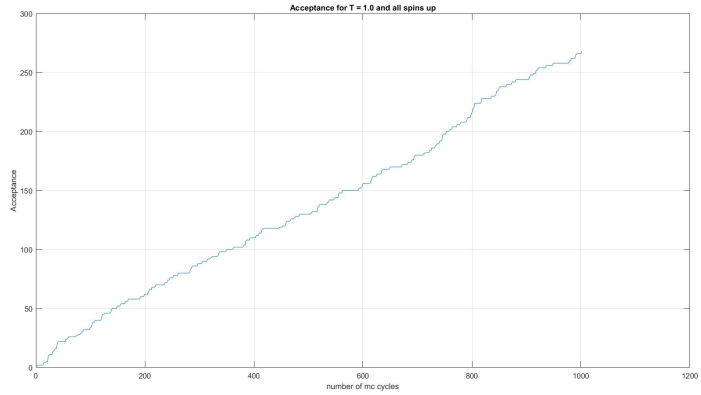


Figure 8: Acceptance versus Monte Carlo cycles for T = 1.0 and T = 2.4 with a random initial matrix



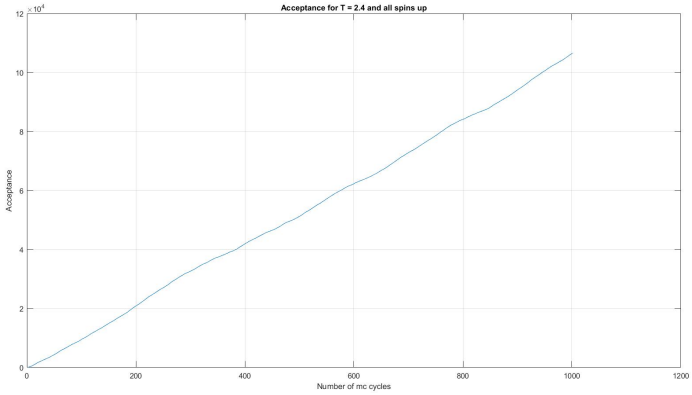
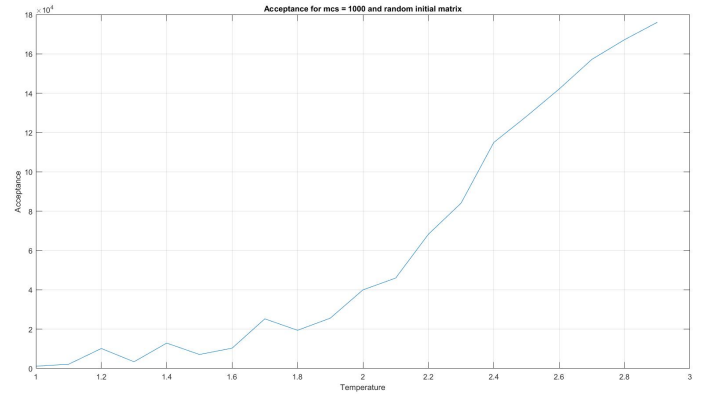


Figure 9: Acceptance versus Monte Carlo cycles for T = 1.0 and T = 2.4 with initial spin upwards



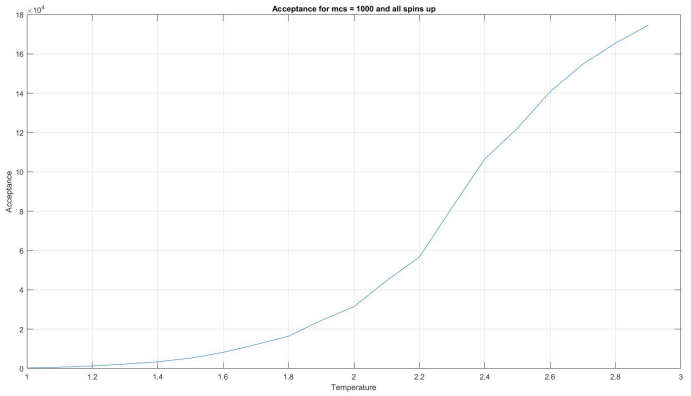


Figure 10: Acceptance versus temperature for a random initial matrix and with initial spin upwards

Acceptance is apparently also dependent on both temperature and the initial state of the spins. From figure figure 8 one can observe that with higher temperature the number of accepted values increase by a factor of 10. For $T = 1.0$, one can also observe that the acceptance spikes for few Monte Carlo cycles. If the initial spins are all positive like in figure 9, the acceptance becomes more linear. The line for

$T = 1.0$ is more squiggly than the straighter line for $T = 2.4$. The ladder does not spike for few Monte Carlo cycles in this case.

From figure 10, one can observe that the curves are not linear. The curve based on a randomly generated initial matrix is uneven at low temperatures, but smooths out when T increases. When the initial matrix only consist positive spins, the curve is smooth throughout. These two plots are plotted to a maximum temperature of 3.0, so one would have an idea of how the acceptance would evolve after $T = 2.4$.

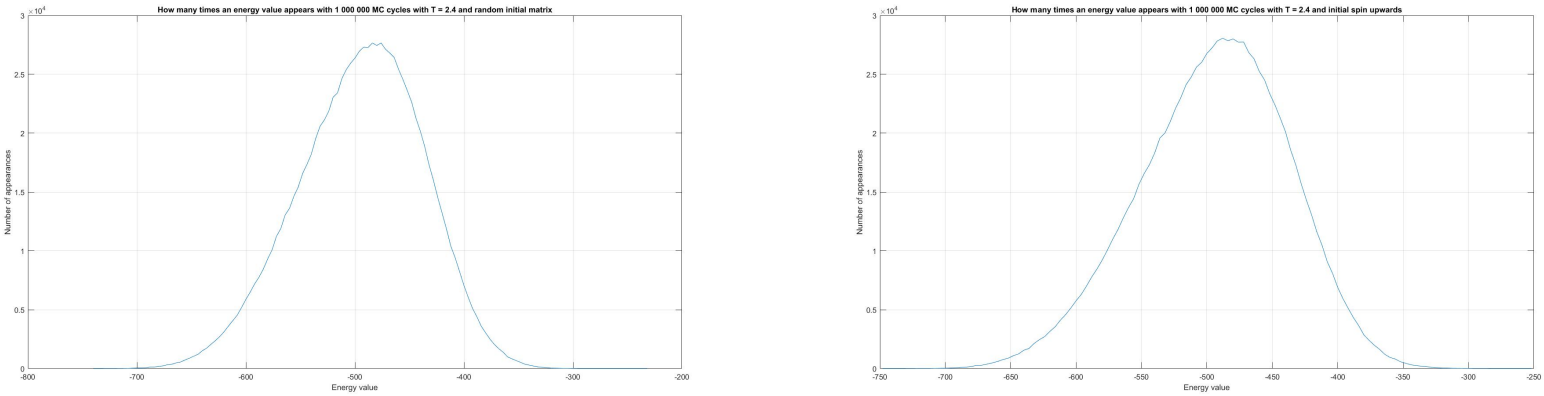


Figure 11: Number of appearances per energy value for a random initial matrix and with initial spin upwards when T = 2.4

With a randomly generated initial matrix, the variance computed in c++ becomes 3226.62. The calculated variance from the energy becomes 3226.9 for 10^6 MC cycles (calculated in MatLab script "howmanytimes.m"). This gives great confidence in the variance. For an initial matrix where all the spins point upwards, the calculated variance in c++ becomes 3236.05. The variance calculated from energy values in MatLab becomes 3236.3, again showing the stability of the variance for 10^6 MC cycles. With fewer MC cycles, the two variances calculated does not correlate.

One can observe from figure 11 that the curves are slightly skewed towards the higher energy values. The curve is bell shaped and centred around the equilibrium state for the lattice at temperature $T = 2.4$ which is -790.