Project 4

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1 Abstract

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2 Introduction

In this project we will study the Ising model in two dimensions. This is a model which is used to simulate phase transitions. The model exhibits a phase transition from a magnetic phase to a phase with zero magnetization. The temperature where this phase transition occurs is called the critical temperature, T_C. Above this temperature the average magnetization is zero. We study electrons in a lattice which is a binary system because each electron only can take two values, spin up or spin down.

The energy we get from the Ising model without an externally applied magnetic field is given by:

$$E = -J \sum_{<kl>}^{N} S_k S_l$$

where $s_k, s_l = \pm 1$ and represents classical spin values. N is the total number of spins and J is a coupling constant expressing the strenght of the interactions between neighboring spins. $< kl >$ indicates that we sum over the spins of the nearest neighbors. We apply periodic boundary conditions as well as the Metropolis algorithm. We also assume that we have a ferromagnetic ordering, so $J > 0$.

The behavior og physical quantities like the mean magnetization, the heat capacity and the susceptibility can be characterized by a power law behavior when the temperature is near T_C. This gives:

$$\begin{aligned} < M(T) > &\sim (T - T_C)^{\beta}, \\ C_v(T) &\sim |T_C - T|^{\alpha}, \\ \chi(T) &\sim |T_C - T|^{\gamma}, \end{aligned}$$

where $\beta = 1/8, \alpha = 0$ and $\gamma = 7/4$.

The correlation length is another important physical quantity which can descriped like the ones above. The correlation length, ε, defines the length scale at which the overall properties of a material start to differ from its bulk properties(Jensen, M.). We expect ε to be of the order of the lattice spacing for $T >> T_C$. As a result of more interactions between the spins as T approaches T_C the correlation length increases as we get closer to T_C. Then the divergent behavior of ε near T_C is

$$\varepsilon(T) \sim |T_C - T|^{-\nu}.$$

We will always be limited to a finite lattice and ε will be proportional with the size of the lattice. The behavior of a finite lattice can then be related to the behavior of a infinitely large lattice, so the critical temperature will scale as

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu}.$$

If we set $T = T_C$ the mean magnetization, the heat capacity and the susceptibility will be

$$\begin{aligned} < M(T) > &\sim (T - T_C)^{\beta} \to L^{-\beta/\nu}, \\ C_v(T) &\sim |T_C - T|^{\alpha} \to L^{-\alpha/\nu}, \\ \chi(T) &\sim |T_C - T|^{\gamma} \to L^{-\gamma/\nu}. \end{aligned}$$

3 Method

The calculations for the degenerated energies and for the magnetization for 16 different spin configurations is located in the appendix and theese calculations gives us the Table **??** below.

Table 1: Spinconfigurations grouped by their total energy and magnetization

# spins up	# configurations	E^2	M
4	1	-8J	4
3	4	0	2
2	4	0	0
2	2	+8J	0
1	4	0	-2
0	1	-8J	-4

We have used the values in Table **??** to calculate, the expectationvalues for the energy and the mean magnetization as well. These values have then been used to calculate the variance for the two physical quantities. The variance for the energi and the mean mean magnetization have respectively been used to calculate the heat capacity $C_v = \sigma_E^2/k_B T^2$ and the susceptibility $\chi = \sigma_M^2/k_B T$

Programming

In order to calculate the spin energies for different systems, we implement the Ising model using the Monte Carlo method. This is a mostly random method, where we perform a loop over random positions in the system grid of spins and decide whether or not we should flip spins using the Metropolis algorithm.

The most effective way to run this simulation is to loop over one random position at a time and decide if we should flip that one spin or not. Because we

can easily calculate the local energy contribution of that one spin, if we keep track of the current enery of the system before flipping, it is easy to calculate the new total energy, so we don't need to loop over the full grid each time we want to find the total energy.

In the Ising model, we know that when $N \to \infty$, the system should reach equilibrium. For our model, N is the number of Monte Carlo cycles, so we want to keep N as large as possible while still being able to run the calculations in a reasonable amount of time. This means we need to optimize our Monte Carlo loop as much as possible.

In theory, what we need to to within the MC loop is the following:

- Find the spin at a random position
- Calculate the current local energy contribution of that spin
- Calculate the new total energy of the system if the spin is flipped
- Use the Metropolis algorithm to decide if we should flip or not
- If we flip: calculate the new total energy and new total magnetization
- Update the expectation values with the (new) energy and total magnetization

Because we are looking at a 2D system, the energies actually get surprisingly easy to calculate. Because we know we only flip one spin at a time, the surrounding four spins (above, below, left and right) stay the same. The consequence of this is that the local energy contribution can only ever "flip" – if you flip the centre spin, the local energy will be $E_{new}(x, y) = -E_{old}(x, y)$). Since the local energy only ever depends on five spins, the possible local energies are also easily calculated. The only possible energies of a local part of the system are: $E(x, y) = -4J, -2J, 0, 2J, 4J$, making the only possible transition energies: $\Delta E(x, y) = 8J, 4J, 0, -4J, -8J$

We can use this knowledge to pre-calculate the probabilities of accepting a flip from one energy to another, using the Metropolis algorithm. Our requirement for flipping is:

$$r \leq e^{-\beta \Delta E} \tag{1}$$

This, again, can be simplified to say that as long as $\Delta E \leq 0$, accept the flip, to avoid having to deal with the random number at all, saving some time.

These simplifications should make our code run quite fast, in theory, fast enough that we don't need to parallelize the Monte Carlo loop itself. However, if we want to run multiple Monte Carlo loops of millions or billions of cycles, we should definitely parallelize in order to utilze our full computing power.

In this project, we parallelize using Open MPI, dividing the different Monte Carlo loops among the processors we have available, and feed the results back to the main process for analysis.

4 Results

For a 2 dimensional lattice we need 10 000 Monte Carlo cycles in order to achieve a good agreement, then the mean value of the energy is -7.9864, which is a differnce of 0.007814 from the analytical value. The values described in the sections above are represented in Table **??** we have set $J/k_BT = \beta J = 1$. The calculations for the analytical values can be found in the Appendix.

Table 2: Analytical and numerical values for T = 1.0, L = 2 and 10^7 Monte Carlo cycles

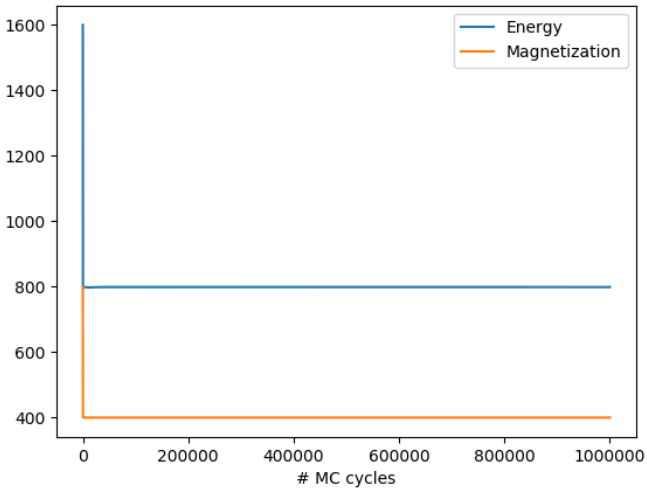
Property	Analytical	Analytical per spin	Numerical per spin
$\langle E \rangle$	-7.978586	-1.994647	-1.99594
$\langle E^2 \rangle$	63.65786	15.91447	15.9675
C_v	0.170865	0.042716	0.0324227
$\langle M(T) \rangle$	0	0	-0.0025167
$\langle \lvert M(T) \rvert \rangle$	3.991970	0.997993	0.998647
$\langle \lvert M(T) \rvert^2 \rangle$	15.962527	3.990631	3.99323
χ	0.026703	0.006676	0.00202647

We have further studied more carefull how many Monte Carlo cycles we need in order to achieve the most likley state for the mean energy and the mean magnetization in a 20 x 20 lattice. Figure **??** shows the results for two different spin matrices, one with all spins up and one random matrix. For the random spin configuration the steady state achives around 200 000 Monte Carlo cycles while for the matrix with all spins up we only need a few cycles.

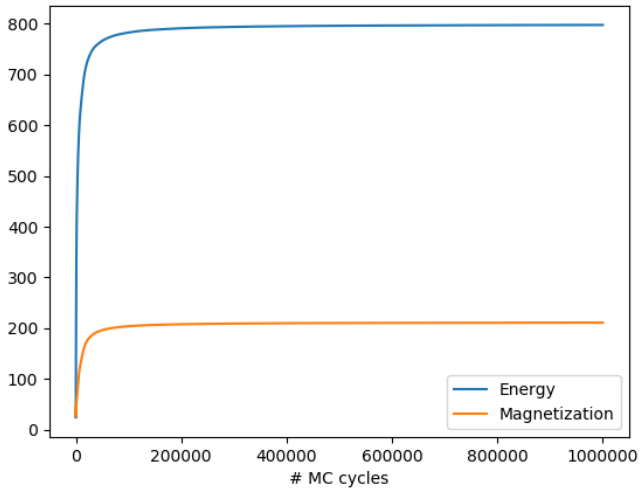
If we increase the temperature we excperience that we need several more Monte Carlo cycles to achive the steady state for the energy and the magnetization. Figure **??** shows that we would need around 1 million Monte Carlo cycles for both the random matrix and the matrix with all spins up. An estimate for the actual time it takes to reach equilibrium based on the number of Monte Carlo cycles can be made if we assume that one Monte Carlo cycle equals 1 second. The estimated equilibration times can be found in Table **??**

Figure **??** and Figure **??** show plots of the total number of accepted configurations as function of the total number of Monte Carlo cycles for respectively a start matrix with all spins up and a start matrix with random spins.

The propability distribution for the energy for T = 1.0 and T = 2.4 is shown in figure

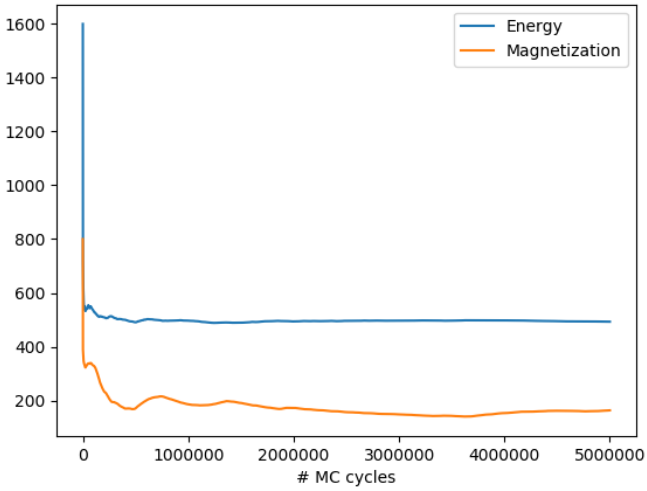


(a) Start matrix with all spins up.

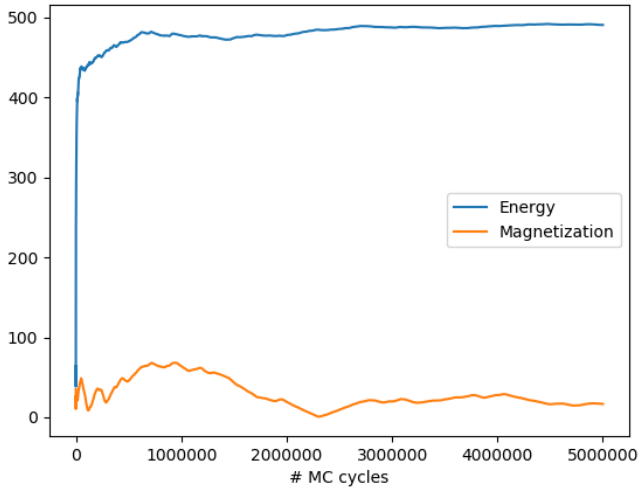


(b) Start matrix with random spins.

Figure 1: Energy and magnetization plotted against number of Monte Carlo cycles when T = 1.0.

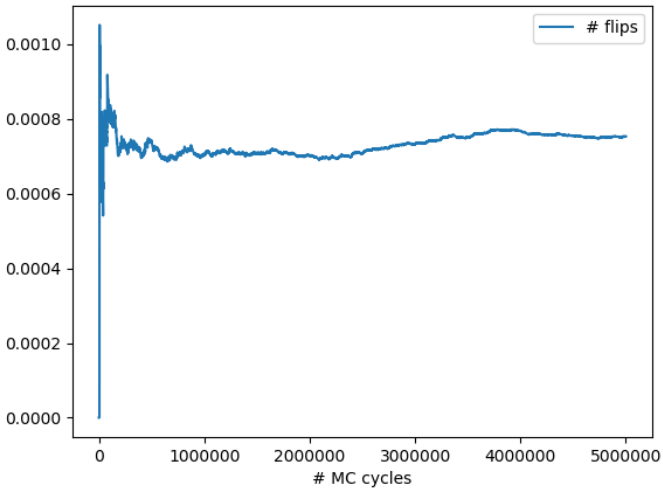


(a) Start matrix with all spins up.

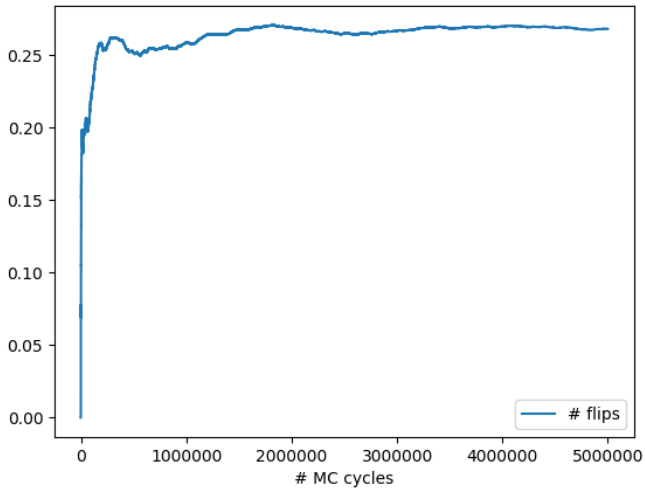


(b) Start matrix with random spins.

Figure 2: Energy and magnetization plotted against number of Monte Carlo cycles when T = 2.4.

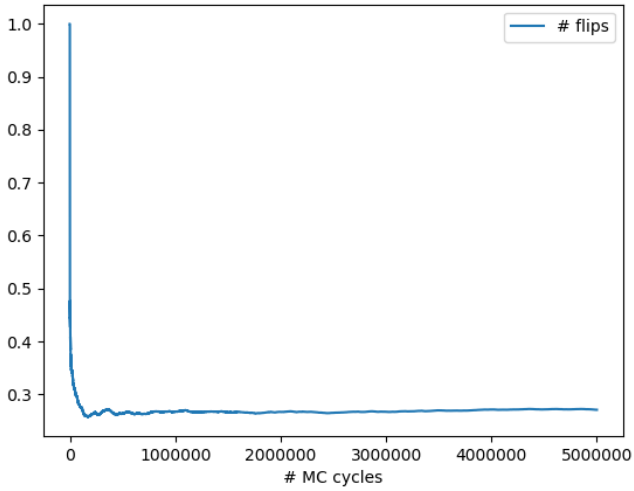


(a) T = 1.0

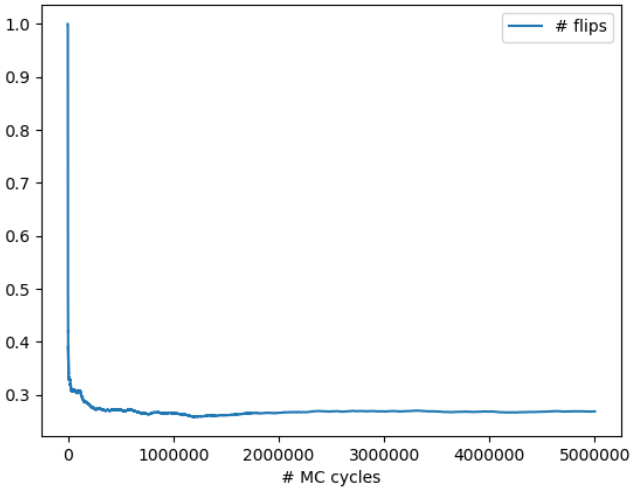


(b) T = 2.4

Figure 3: Total number of accepted spinconfiguration as a function of Monte Carlo cycles, for a start matrix with all spins up.



(a) T = 1.0



(b) T = 2.4

Figure 4: Total number of accepted spinconfiguration as a function of Monte Carlo cycles, for a start matrix with all spins up.

Table 3: Estimated equilibration times.

Matrix	Equilibration time (sec)
T = 1.0 in a random spin matrix	200 000
T = 1.0 in a matrix with all spins up	≈ 0
T = 2.4 in a random spin matrix	1 000 000
T = 2.4 in a matrix with all spins up	1 000 000

5 Discussion

The numerical value for $< E >, < E^2 >$ and C_v for a 2x2 lattice gives a godd compliance to the analytical values. However the numerical values for the magnetization and the susceptibility does not compliance well with the analytical values. The mean magnetization does vary alot more in different calculations because it depends more of how the spins flip. While the energy depends on the square of neighboring spins, the magnetization depends on the sum over all spins, this may be why we excperience different values for the mean magnetization in different calculations.

From Figure **??** and **??** we see that the energy and magnetization needs a lot less time to stabelize when all of the spins in the lattice have the same configuration and T = 1.0. When we increase the temperature the number of Monte Carlo cycles we need to get a good results also increase. For a higher temperature we can also see that the energy in the system increases. As mentioned above the magnetization is more dependent on the spin configuration in the entire matrix and therefore it will not be as stable as the energy.

We can see that the variance is incresing with temperature, that is why we get a propability distribution which is more spread out in energies when the temperature is increasing.

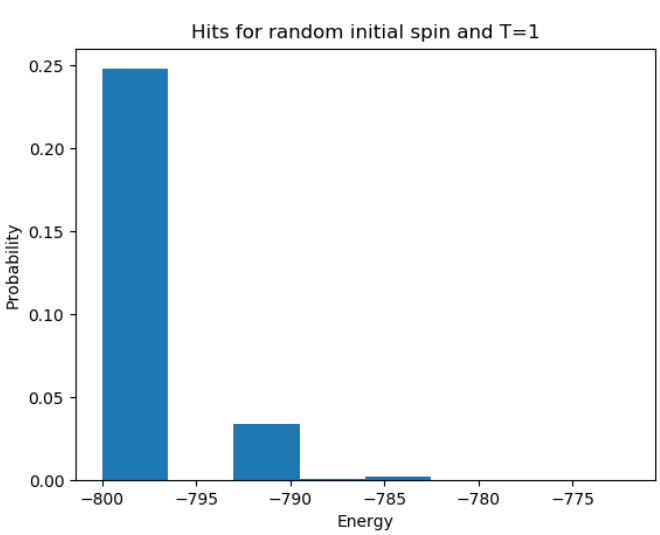
6 Conclusion

7 Appendix

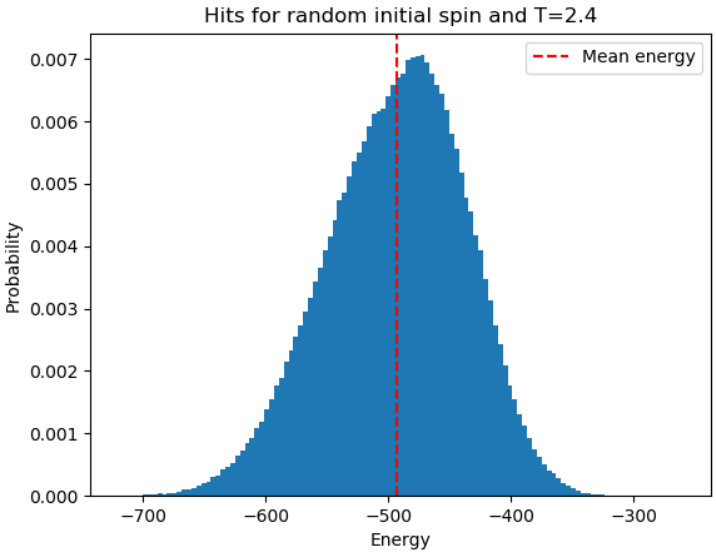
7.1 Degenerated energies and magnetization

When calculating the degenerate energies for the case of 2x2, we start with the equation $E_i = -J \sum_{\langle kl \rangle}^{2} s_k s_l$

The case for all spin up looks like this $\begin{matrix} \uparrow & \uparrow \\ \uparrow & \uparrow \end{matrix}$



(a) T = 1.0



(b) T = 2.4

Figure 5: Propability distribution for counted energies.

And the equation will be.

$$\begin{aligned} E_1 &= -J \sum_{<kl>}^{2} s_k s_l \\ &= -J((s_1 s_2 + s_1 s_3) + (s_2 s_1 + s_2 s_4) + (s_3 s_1 + s_3 s_4) + (s_4 s_3 + s_4 s_2)) \\ &= -J((1+1) + (1+1) + (1+1) + (1+1)) \\ E_1 &= -8J \end{aligned}$$

The reason why the same interaction is included several times is because of the unit cell repeating itself to infinity in both x and y derection. Therefore the s_1 will interact with s_2 and s_3 inside the unit cell, and s_2 and s_3 "outside" the unit cell.

The magnetization is defined as

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

which sums over all spins for a given configuration i. For the same spinconfiguration as above this gives:

$$M_i = \sum_{j=1}^{4} (1+1+1+1) = 4$$

7.2 The partition function

When we known the values for all the degenerate energies we can calculate the value of the partian function.

$$z = \sum_{i=1}^{2^n} e^{-\beta E_i}$$

In out case we have $n = 4$ since we have a 2x2 lattice.

$$z = \sum_{i=1}^{2^4} e^{-\beta E_i}$$
$$z = e^{-\beta E_1} + e^{-\beta E_2} + \ldots + e^{-\beta E_1 6}$$
$$z = e^{8\beta J} + 4e^{-\beta \cdot 0} + 2e^{-8\beta J} + 4e^{-\beta \cdot 0} + 4e^{-\beta \cdot 0} + 4e^{-\beta \cdot 0} + e^{8\beta J}$$
$$z = 2e^{8\beta J} + 2e^{-8\beta J} + 16$$

7.3 Expectationvalues for the energy

This gives us the ability to calculate the expectationvalue of the energy $\langle E \rangle$

$$\langle E \rangle = \sum_{i}^{2^n} \frac{E_i e^{-\beta E_i}}{z}$$

We know we have several energyvalues which is zero. If we do not write these we get

$$= \frac{-8Je^{8\beta J} + 2\left(8Je^{-8\beta J}\right) + \left(-8J\right)e^{8\beta J}}{2e^{8\beta J} + 2e^{-8\beta J} + 16}$$
$$= \frac{16J\left(e^{-8\beta J} - e^{8\beta J}\right)}{2(e^{8\beta J} + e^{-8\beta J} + 8)}$$
$$= 8J\frac{e^{-8\beta J} - e^{8\beta J}}{e^{8\beta J} + e^{-8\beta J} + 8}$$

Thus

$$\langle E \rangle^2 = \left(8J\frac{e^{-8\beta J} - e^{8\beta J}}{e^{8\beta J} + e^{-8\beta J} + 8}\right)^2$$
$$= 64J^2\frac{\left(e^{-8\beta J} - e^{8\beta J}\right)^2}{\left(e^{8\beta J} + e^{-8\beta J} + 8\right)^2}$$
$$= 64J^2\frac{e^{-16\beta J} + e^{16\beta J} + 2}{e^{16\beta J} + e^{-16\beta J} + 16e^{-8\beta J} + 16e^{8\beta J} + 66}$$

At the same time we calculate $\left\langle E^2 \right\rangle$

$$\begin{aligned}\langle E^2\rangle &= \sum_i^{2^n} \frac{E_i^2 e^{-\beta E_i}}{z} \\ &= \frac{64J^2e^{8\beta J} + 2\left(64J^2e^{-8\beta J}\right) + 64J^2e^{8\beta J}}{2e^{8\beta J} + 2e^{-8\beta J} + 16} \\ &= \frac{128J^2e^{8\beta J} + 128J^2e^{-8\beta J}}{2e^{8\beta J} + 2e^{-8\beta J} + 16} \\ &= 64J^2\frac{e^{8\beta J} + e^{-8\beta J}}{e^{8\beta J} + e^{-8\beta J} + 8}\end{aligned}$$

7.4 Expectationvalues for the magnetization

The absolute value of the mean magnetization is given by

$$\langle |M(T)|\rangle = \frac{\sum_i^{2^4} |M_i| e^{-\beta E_i}}{z}$$

and can be calculated by using the values for the energy and the magnetization from Table **??**:

$$\begin{aligned}\langle |M(T)|\rangle &= \frac{4e^{8\beta J} + 2\cdot 4 + 0\cdot 4 + 0\cdot 2 + |-2|\cdot 4 + |-4|e^{8\beta J}}{z} \\ \langle |M(T)|\rangle &= \frac{8e^{8\beta J} + 16}{2e^{8\beta J} + 2e^{-8\beta J} + 16} = \frac{4e^{8\beta J} + 8}{e^{8\beta J} + e^{-8\beta J} + 8}\end{aligned}$$

We also have that

$$\begin{aligned}\left\langle |M(T)|^2\right\rangle &= \frac{\sum_i^{2^4} |M_i^2| e^{-\beta E_i}}{z} \\ \left\langle |M(T)|^2\right\rangle &= \frac{32e^{8\beta J} + 32}{2e^{8\beta J} + 2e^{-8\beta J} + 16} = 16\frac{e^{8\beta J} + 1}{e^{8\beta J} + e^{-8\beta J} + 8}\end{aligned}$$

7.5 Heat Capacity

We the expectationvalues to calculate the variance for the energy

$$\begin{aligned}\sigma_E^2 &= \left\langle E^2\right\rangle - \langle E\rangle^2 \\ &= 64J^2\frac{e^{8\beta J} + e^{-8\beta J}}{e^{8\beta J} + e^{-8\beta J} + 8} - 64J^2\frac{e^{-16\beta J} + e^{16\beta J} + 2}{e^{16\beta J} + e^{-16\beta J} + 16e^{-8\beta J} + 16e^{8\beta J} + 66}\end{aligned}$$

When this is known we can also calculate the heat capasitace.

$$\begin{aligned}C_v &= \frac{\sigma_E^2}{k_B T^2} \\ &= \frac{64J^2}{k_B T^2}\left[\frac{e^{8\beta J} + e^{-8\beta J}}{e^{8\beta J} + e^{-8\beta J} + 8} - \frac{e^{-16\beta J} + e^{16\beta J} + 2}{e^{16\beta J} + e^{-16\beta J} + 16e^{-8\beta J} + 16e^{8\beta J} + 66}\right]\end{aligned}$$

7.6 Susceptibility

The variance for the absolute value of the mean magnetization is given by:

$$\sigma_M^2 = \left\langle |M(T)^2| \right\rangle - \left\langle |M(T)| \right\rangle^2$$

$$\sigma_M^2 = 16\frac{e^{8\beta J}+1}{e^{8\beta J}+e^{-8\beta J}+8} - 16\frac{e^{16\beta J}+4e^{8\beta J}+4}{e^{-16\beta J}+e^{-16\beta J}+16e^{-8\beta J}+16e^{8\beta J}+66}$$

We then calculate the susceptibility χ which is given by $\chi = \sigma_M^2/k_BT$, so

$$\chi = \frac{16}{k_BT}\left[\frac{e^{8\beta J}+1}{e^{8\beta J}+e^{-8\beta J}+8} - \frac{e^{16\beta J}+4e^{8\beta J}+4}{e^{-16\beta J}+e^{-16\beta J}+16e^{-8\beta J}+16e^{8\beta J}+66}\right]$$

8 Bibliography