

Project 4

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1 Abstract

The Ising model in two dimensions has been used to simulate phase transitions in a material. We have used Monte Carlo and the Metropolis algorithm and our results shows that the number of Monte Carlo cycles we need to reach equilibrium depends on the spin configuration in the start matrix.

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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.

2.1 Energy of the System

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

$$E = -J \sum_{\langle kl \rangle}^N S_k S_l$$

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. $\langle kl \rangle$ indicates that we sum over the spins of the nearest neighbors. We apply periodic boundry conditions as well as the Metropolis algorithm. We also assume that we have a ferromagnetic ordering, so $J > 0$.

2.2 Phase Transitions

The behavior of 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:

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

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

The correlation length is another important physical quantity which can be described 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 $T \gg T_C$. 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

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

3 Method

The calculations for the degenerated energies and for the magnetization for 16 different spin configurations is located in the appendix and these calculations gives us the Table 1 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 1 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 $\chi = \sigma_M^2/k_B T$

3.1 The Metropolis Algorithm

The Metropolis algorithm uses a propability distribution to obtain a sequence of random samples. In our case it is used to decide if the spins should flip or

not. If we have a uniform propability distribution function(PDF), $\omega \in [0, 1]$ this is given by:

$$\omega = \frac{P_i}{P_j} = \frac{P_{new\ state}}{P_{previous\ state}} = \frac{e^{-\beta E_i/z}}{e^{-\beta E_j/z}}$$

$$\omega = e^{-\beta(E_i - E_j)} = e^{-\beta \Delta E}$$

where ΔE is the energy difference between the new and the previous state, E_i and E_j . $\beta = 1/k_B T$ and Z is the partition function described in the Appendix(Section 7.2). If $\omega = 1$ the system will stay at the same place, there will be no change in the spin configuration. If $\omega > 1$ the system will move to a larger propability of spin configurations and if $\omega < 1$ the system move to a smaller propability.

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 diffrence of 0.007814 from the analytical value. The values described in the sections above are represented in Table 2 we have set $J/k_B T = \beta J = 1$. 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
$\langle M(T) \rangle$	3.991970	0.997993	0.998647
$\langle M(T) ^2 \rangle$	15.962527	3.990631	3.99323
χ	0.026703	0.006676	0.00202647

4.1 Number of Monte Carlo Cycles and Equilibration Times

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 1 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 achieves around 200 000 Monte Carlo cycles while for the matrix with all spins up we only need a few cycles.

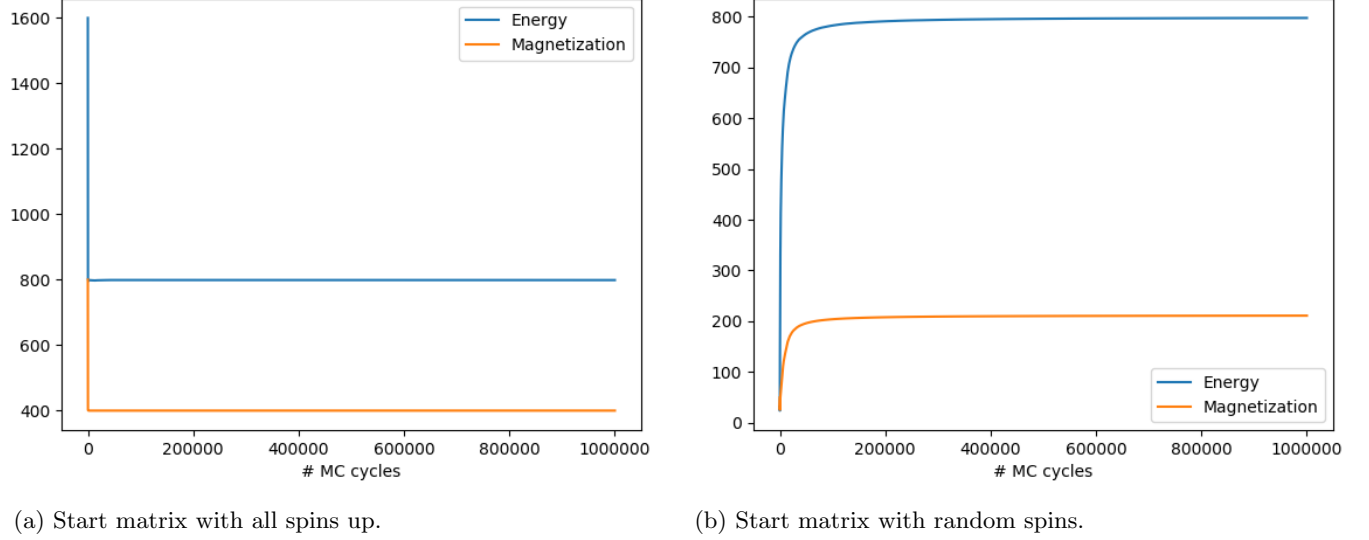
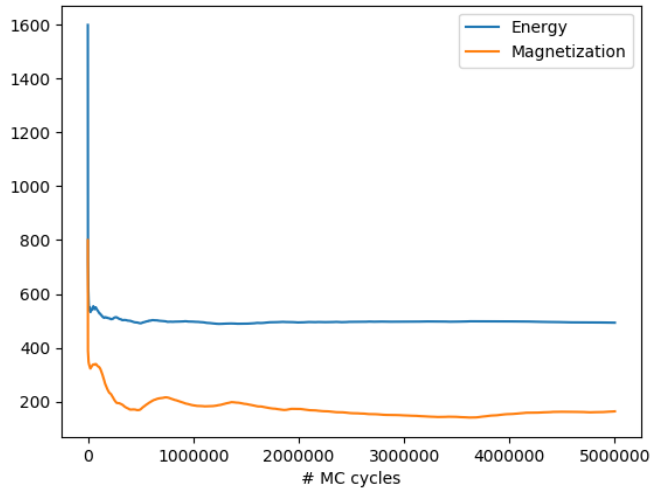
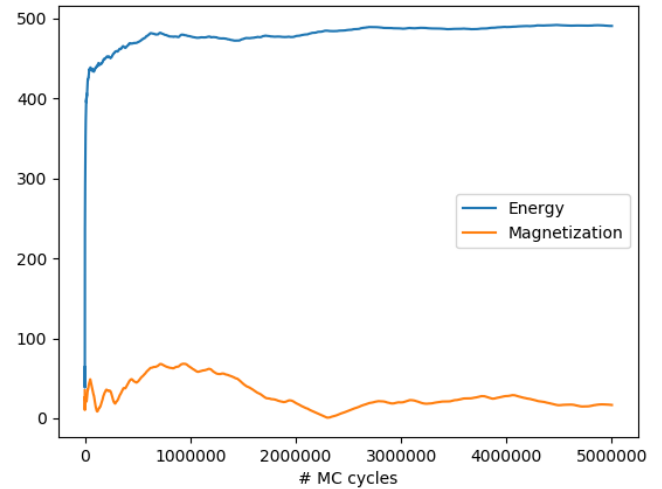


Figure 1: Energy and magnetization plotted against number of Monte Carlo cycles when $T = 1.0$.

If we increase the temperature we experience that we need several more Monte Carlo cycles to achieve the steady state for the energy and the magnetization. Figure 2 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 3



(a) Start matrix with all spins up.



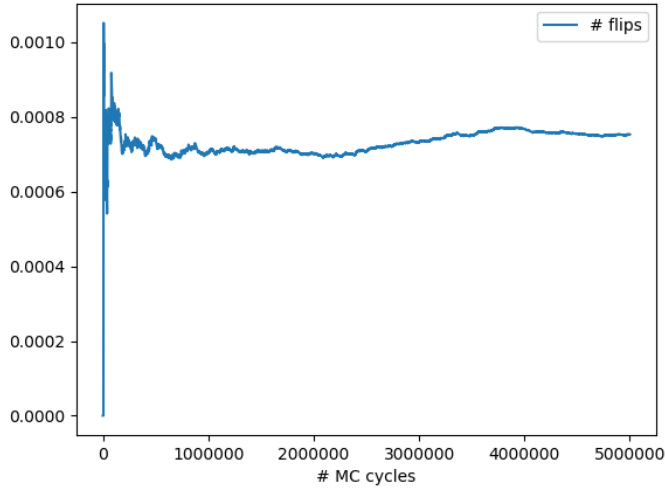
(b) Start matrix with random spins.

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

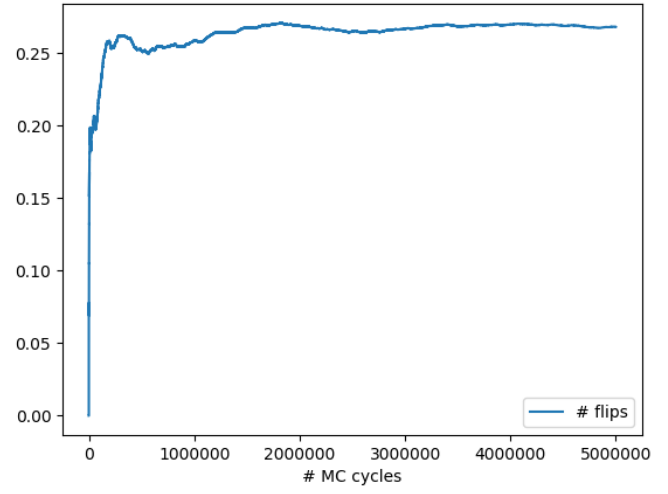
Table 3: Estimated equilibration times.

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

Figure 3 and Figure 4 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.

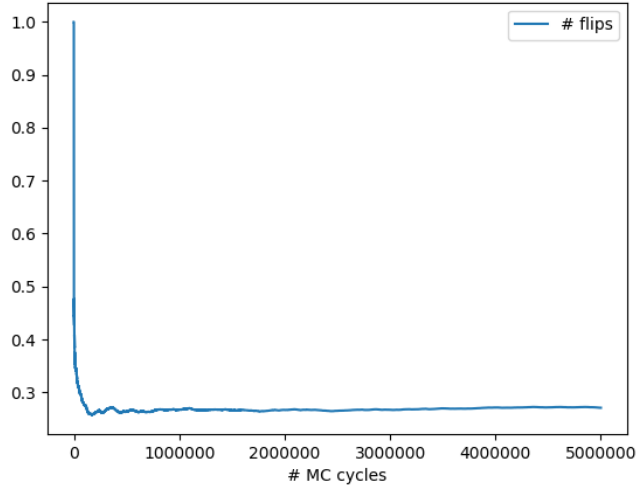


(a) $T = 1.0$

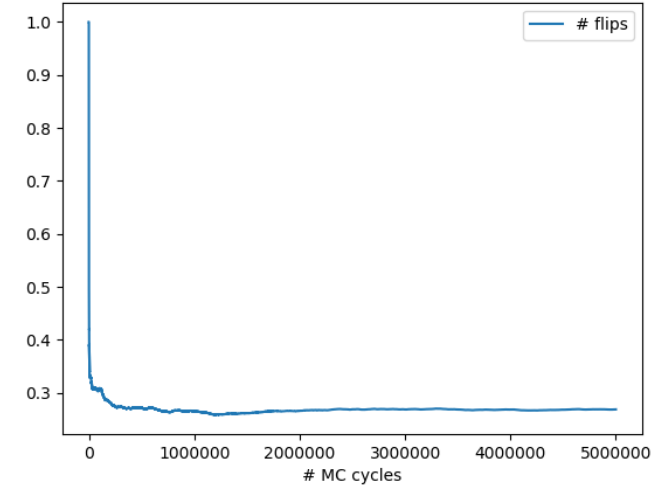


(b) $T = 2.4$

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.

4.2 Propability Distribution

The propability distribution for the energy for $T = 1.0$ and $T = 2.4$ is shown in figure 5.

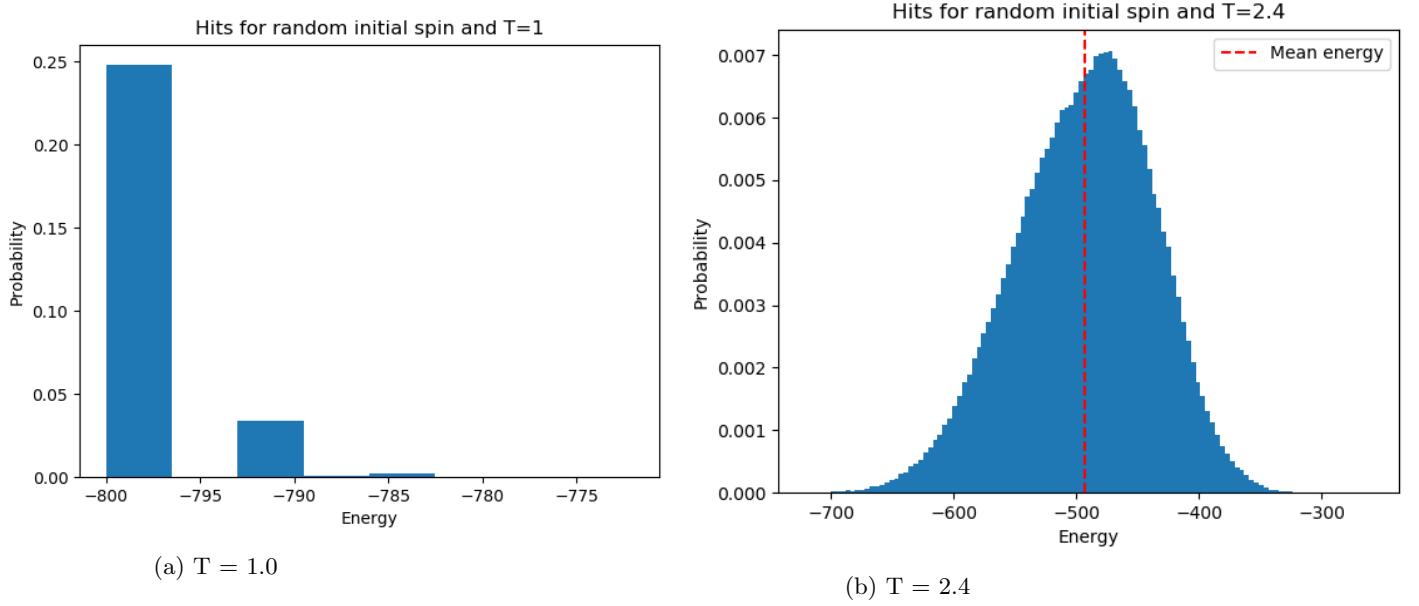


Figure 5: Probability distribution for counted energies.

4.3 Phase Transitions

5 Discussion

The numerical value for $\langle E \rangle$, $\langle E^2 \rangle$ and C_v for a 2×2 lattice gives a good 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 a lot 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 experience different values for the mean magnetization in different calculations.

From Figure 1 and 2 we see that the energy and magnetization needs a lot less time to stabilize 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 increasing with temperature, that is why we get a probability distribution which is more spread out in energies when the temperature is increasing.

6 Conclusion

We have

7 Appendix

7.1 Degenerated Energies and Magnetization

When calculating the degenerate energies for the case of 2x2, we start with the

$$\text{equation } E_i = -J \sum_{\langle kl \rangle}^2 s_k s_l$$

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

And the equation will be.

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

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 direction. 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 spin configuration as above this gives:

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

7.2 The Partition Function

When we know the values for all the degenerate energies we can calculate the value of the partition function.

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

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

$$\begin{aligned} z &= \sum_{i=1}^{2^4} e^{-\beta E_i} \\ z &= e^{-\beta E_1} + e^{-\beta E_2} + \dots + e^{-\beta E_{16}} \\ z &= e^{8\beta J} + 4e^{-\beta \cdot 0} + 2e^{-8\beta J} + 4e^{-\beta \cdot 0} + 4e^{-\beta \cdot 0} + 4e^{-\beta \cdot 0} + e^{8\beta J} \\ z &= 2e^{8\beta J} + 2e^{-8\beta J} + 16 \end{aligned}$$

7.3 Expectation values for the Energy

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

$$\langle E \rangle = \sum_i \frac{E_i e^{-\beta E_i}}{z}$$

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

$$\begin{aligned} &= \frac{-8J e^{8\beta J} + 2(8J e^{-8\beta J}) + (-8J) e^{8\beta J}}{2e^{8\beta J} + 2e^{-8\beta J} + 16} \\ &= \frac{16J (e^{-8\beta J} - e^{8\beta J})}{2(e^{8\beta J} + e^{-8\beta J} + 8)} \\ &= 8J \frac{e^{-8\beta J} - e^{8\beta J}}{e^{8\beta J} + e^{-8\beta J} + 8} \end{aligned}$$

Thus

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

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

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

7.4 Expectation values for the Magnetization

The absolute value of the mean magnetization is given by

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

and can be calculated by using the values for the energy and the magnetization from Table 1:

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

We also have that

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

7.5 Heat Capacity

We use the expectation values to calculate the variance for the energy

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

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

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

7.6 Susceptibility

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

$$\begin{aligned}\sigma_M^2 &= \langle |M(T)|^2 \rangle - \langle |M(T)| \rangle^2 \\ \sigma_M^2 &= 16 \frac{e^{8\beta J} + 1}{e^{8\beta J} + e^{-8\beta J} + 8} - 16 \frac{e^{16\beta J} + 4e^{8\beta J} + 4}{e^{-16\beta J} + e^{-16\beta J} + 16e^{-8\beta J} + 16e^{8\beta J} + 66}\end{aligned}$$

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

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

8 Bibliography