Predicting Thermodynamic Properties of the 2D Ising Model with Monte Carlo Simulations

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Abstract

Exploration of the two-dimensional Ising Model using the Monte Carlo Method has been made. The implementation of the model includes calculation of expectation values for energy, magnetization, specific heat and susceptibility as function of temperature T and spin lattice size L. In addition to this we have also performed an estimate to the critical temperature $T_C(L = \infty)$. Results show numerical calculated expectation values converging towards analytical solutions for a 2×2 lattice. Comparing expectation values for Energy $\langle E \rangle$ and magnetization $\langle |M| \rangle$ for $T = 1.0$ and $T = 2.4$, shows that fewer cycles are needed to produce accurate results when having lower temperatures and ordered starting spin configuration. When comparing systems with two temperatures shows that the acceptance rate for suggested flips for $T = 2.4$ is approximately $80 - 90$ times higher than for $T = 1.0$. A closer look at phase transitions confirms that the magnetization $M = 0$ when the temperature T reaches the critical temperature T_C. An estimate to the critical temperature gives $T_C(\infty) \approx 2.267 \pm 0.1565$, which is close to the analytical solution $T_{C,\text{exact}}(\infty) \approx 2.269$.

I Introduction

In statistical mechanics one can study how the magnetic dipole moment and energy for atomic spins varies for different temperatures. The Ising model is a mathematical model that consists of discrete atomic particles in a lattice, where each particle can be in two spin states, either +1 or -1. In two dimensions with $L \times L$ spins, the model undergoes a phase transition for a given critical temperature T_C. When the system has temperature below this particular temperature, the system has magnetic dipole moment $\langle M \rangle \neq 0$. The phase transition happens when the mean magnetization approaches zero at $T = T_C$ [1].

When having only two spins in each dimension of the lattice ($L = 2$), the system has analytical solutions for the various expectation values like energy, magnetization, specific

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heat and susceptibility. However for larger values of L, it is difficult to extract analytical solutions, and a numerical approach is therefore required.

The aim of this paper is to explore the Ising model with a numerical approach for higher L, using Monte Carlo simulations and the so-called Metropolis method. One can think of the lattice as a material with magnetic properties. When the system has temperature $T > T_C$, it no longer has magnetic dipole moment and the material lacks magnetic properties. The main goal is to estimate this particular critical temperature T_C, by choosing sufficiently large values of L and applying periodic boundary conditions to the lattice. To verify that the model has been implemented correctly we want to compare our results with analytical solutions for a 2×2 lattice.

We are also interested to see how the different expectation values for energy, magnetic dipole moment, heat capacity and suceptibility behaves when the temperature approaches T_C. Exploring how ordered and disordered starting spin configurations affect our results is also presented, and also how the number of Monte Carlo cycles MC affect the accuracy of various expectation values. We are also exploring how different temperatures affect the spin configurations in the lattice, both below and above the analytical critical temperature T_C.

All programmes of relevance to calculate expectation values for the 2 dimensional Ising model are available at https://github.com/Seedsiz/FYS4150-Project4.

II Theory and Methods

The theory section is mainly based upon Morten Hjorth-Jensen's lecture notes in the Computational Physics course (FYS4150) at the University of Oslo. The relevant themes are the Monte Carlo Method to calculate expectation values [2], parallelization [3] and the statistical physics of the Ising Model [4].

II.I The Ising Model

The Ising model describes a coupled system where only the nearest neighbours affect each other. In this report the Ising model will be applied to a two dimensional magnetic system. This will be a grid of spins, where each spin s_i can either have value 1 or -1. The total energy and magnetization is expressed as:

$$E = -J \sum_{<k,l>} s_k s_l \quad , \quad M = \sum_{i}^{n} s_i \tag{1}$$

where <k, l> indicates that we sum over nearest neighbors only and $n = L \times L$ is the total number of spins in the lattice for a given configuration.

For many atomic spins ($L > 2$), the number of configurations quickly becomes too large and we are therefore going to apply Monte Carlo Algorithm.

II.II A 2x2 Lattice

For a 2×2 lattice, the number of configurations for the spin matrix S is $2^n = 16$, where $n = L \times L = 4$. Thus we we can find the different values of energy and magnetization and their corresponding degeneracy, using eq.1. The table below shows the different spin configurations, with corresponding energy, magnetization and degeneracy.

Table 1: Energy and magnetization for the microstates

Spin ups	Degeneracy	Energy	Magnetization
4	1	-8J	4
3	4	0	2
2	4	0	0
2	2	8J	0
1	4	0	-2
0	1	-8J	-4

The analytical solutions for a 2×2 lattice is given by

$$z = 12 + 4\cosh(8J\beta), \qquad \langle E \rangle = -\frac{32J}{z}\sinh(8J\beta), \qquad \langle |M| \rangle = \frac{8}{z}\left(e^{8J\beta} + 2\right) \tag{2}$$

$$\sigma_E^2 = \frac{256J^2}{z}\left(\cosh(8J\beta) - \frac{4}{z}\sinh^2(8J\beta)\right), \qquad C_V = \frac{1}{k_B T^2}\sigma_E^2. \tag{3}$$

$$\sigma_M^2 = \frac{32}{z}\left(e^{8J\beta} + 1\right), \qquad \chi = \frac{1}{k_B T}\sigma_M^2. \tag{4}$$

where $\beta = 1/k_B T$ and J is a coupling constant. We are in this project going to measure the temperature T in units of J/k_B, and we will thoughout all calculations use $k_B = J = 1$.

The function z is the partition function which is a representation of statistical properties when the system is in thermodynamic equilibrium. The expectation value of energy $\langle E \rangle$ describes the average when weighing each energy in the spin-system, while $\langle |M| \rangle$ is the expectation value of the mean absolute value of magnetization of the system.

The heat capacity C_V describes how much heat the system needs in order to raise the temperature T. In our case we are looking at changes in magnetic dipole moment, so the susceptibility χ is a number that tells how much the system responds to a magnetic field.

These quantities will serve as benchmarks when solving the Ising Model for larger spin systems. The derivation of the analytical solutions can be found in sec.VI.

II.III Studies of phase transitions

When the temperature T of the Ising model is close to the critical temperature T_C one can relate results from a finite lattice size $L \times L$ with an infinitely large lattice. It can then be shown that the following relation for the critical temperature is valid

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu} \tag{5}$$

Here we will set both $a = \nu = 1$, and with these parameters the exact result for the critical temperature is

$$kT_C/J \approx 2.269. \tag{6}$$

These results are gathered from [5] and and will also serve as benchmarks when we use our numerical method to estimate the critical temperature T_C.

II.IV The Monte Carlo Method

For many atomic spins ($L > 2$), the number of configurations quickly becomes too large and we are therefore going to apply the Monte Carlo method. First we need to decide a total number of Monte Carlo cycles that we want to simulate over. The purpose of the method is first of all to estimate the expectation values for the different quantities presented in sec.II.II, and to study phase transitions when the system reaches temperature $T = T_C$.

For each Monte Carlo cycle we choose one random index l in our spin matrix S, and find the change in energy ΔE if we had flipped this particular spin resulting in a new configuration. Using eq.1, the change in energy can be calculated by

$$\Delta E = E_2 - E_1 = J \sum_{<k,l>} s_k^1 s_l^1 - J \sum_{<k,l>} s_k^2 s_l^2 = -J \sum_{<k,l>} s_k^2 (s_l^2 - s_l^1). \tag{7}$$

Since we are only flipping the spin with index l, all the the other neighboring spins keep their same value so that $s_k^1 = s_k^2$. In the case where $s_l^1 = +1$, we know that $s_l^2 = -1$ and

$(s_l^2 - s_l^1) = -2$ when we have flipped. Having the opposite we get $(s_l^2 - s_l^1) = 2$. We see that the sign of ΔE depends on s_l^1, and the energy difference can then be written as

$$\Delta E = 2Js_l^1 \sum_k s_k \tag{8}$$

where we now sum over the neighbouring spins with index k. When finding the change in magnetization, we consider only the flipped spin since all other spins are unchanged. The change in magnetization is $\Delta M = s_l^2 - s_l^1 = \pm 2$. If $s_l^1 = 1$, then $s_l^2 = -1$ and we get $\Delta M = -2$. For the opposite case we get $s_l^2 = +1$ and $\Delta M = 2$. The change can then be written as

$$M_2 = M_1 + 2s_l^2 \tag{9}$$

where M_2 is the new magnetization and M_1 is the previous magnetization. Going back to the energy difference we realize that since we only need to consider the 4 nearest neighbours when calculating the new energy, we get a limiting amount of configurations for the 5 spins. In fact there are only 5 possible values of energy difference ΔE. The different changes in configurations and energies are shown below in eq.10, eq.11 and eq.12.

$$E = -4J \quad \begin{array}{ccc} & \uparrow & \\ \uparrow & \uparrow & \uparrow \\ & \uparrow & \end{array} \quad \Rightarrow \quad E = 4J \quad \begin{array}{ccc} & \uparrow & \\ \uparrow & \downarrow & \uparrow \\ & \uparrow & \end{array}, \qquad E = -2J \quad \begin{array}{ccc} & \uparrow & \\ \downarrow & \uparrow & \uparrow \\ & \uparrow & \end{array} \quad \Rightarrow \quad E = 2J \quad \begin{array}{ccc} & \uparrow & \\ \downarrow & \downarrow & \uparrow \\ & \uparrow & \end{array} \tag{10}$$

$$E = 0 \quad \begin{array}{ccc} & \uparrow & \\ \downarrow & \uparrow & \uparrow \\ & \downarrow & \end{array} \quad \Rightarrow \quad E = 0 \quad \begin{array}{ccc} & \uparrow & \\ \downarrow & \downarrow & \uparrow \\ & \downarrow & \end{array}, \qquad E = 2J \quad \begin{array}{ccc} & \downarrow & \\ \downarrow & \uparrow & \uparrow \\ & \downarrow & \end{array} \quad \Rightarrow \quad E = -2J \quad \begin{array}{ccc} & \downarrow & \\ \downarrow & \downarrow & \uparrow \\ & \downarrow & \end{array} \tag{11}$$

$$E = 4J \quad \begin{array}{ccc} & \downarrow & \\ \downarrow & \uparrow & \downarrow \\ & \downarrow & \end{array} \quad \Rightarrow \quad E = -4J \quad \begin{array}{ccc} & \downarrow & \\ \downarrow & \downarrow & \downarrow \\ & \downarrow & \end{array} \tag{12}$$

As one can see the possible values of energy difference are $\Delta E = 8J, 4J, 0, -4J, -8J$. One important thing to notice is that we assumed the flipped spin to initially be $+1$. For the other case where the spin is initially -1, eq.10, eq.11 and eq.12 would be reversed, giving $\Delta E = -8J, -4J, 0, 4J, 8J$ instead.

One of our goals is to make the energy approach the minimum value after a given number of monte-carlo cycles. For a given Monte Carlo cycle we are therefore only going to flip the random spin s_l if this results in a negative energy difference ΔE. If this is the case we flip s_l and update the energy with ΔE and magnetization using eq.9.

If however $\Delta E > 0$ we investigate whether a random number $r \in [0, 1\rangle$ is smaller than the probability ratio w:

$$r \leq w = \frac{P_2}{P_1} = \frac{e^{-\beta E_2}}{e^{-\beta E_1}} = e^{-\beta \Delta E}, \quad \text{where} \quad P_s = \frac{e^{-\beta E_s}}{z}. \tag{13}$$

The quantity P_s gives the probability for finding the system in state s, P_2 and P_1 are the probabilities for finding the spin system in state 1 (before flipping) and in state 2 (after flipping). If eq.13 is satisfied, we flip s_l and update the energy and magnetization. If $r \geq w$ we are not doing anything except keeping the previous spin configuration. The procedure of accepting or not accepting a new configuration, is what is known as the metropolis method which is presented in algo.2.

The metropolis algorithm is applied $n = L \times L$ times for each Monte Carlo cycle. The main algorithm for the Monte Carlo algorithm is presented below in algo.1.

Algorithm 1 Monte Carlo Algorthm: The basic outline of the Monte Carlo algorithm for extracting expectation values for energy, magntization, heat capacity and susceptibility.

for int c=0; c < MCcycles; c++ **do** ▷ For each Monte Carlo cycle
  for int i=0; i < $L \times L$; i++ **do** ▷ For each spin-flip experiment
    Draw index l; ▷ Extract random index l from matrix S
    Find deltaE; ▷ Find change in energy ΔE if flipping index l
    Run Metropolis algorithm algo.2; ▷ Accept or not accept new configuration
  end for
  ▷ Update expectation values after each cycle
  expE += Energy ▷ $\langle E \rangle$
  expE2 += Energy×Energy ▷ $\langle E^2 \rangle$
  expM += magnetization ▷ $\langle M \rangle$
  expM2 += magnetization×magnetization ▷ $\langle M^2 \rangle$
  expMabs += abs(magnetization) ▷ $\langle |M| \rangle$
end for
ExpValues = ExpValues/MCcycles ▷ Dividing expectation values by MC cycles
Cv = $\frac{1}{T^2}(expE2 - expE \times expE)$ ▷ Calculate heat capacity C_V
$\chi = \frac{1}{T}(expM2 - expM \times expM)$ ▷ Calculate susceptibility χ

Algorithm 2 Metropolis algorithm: The basic outline of Metropolis algorithm used in Monte Carlo simulations. The method either accepts or do not accept a given configuration of the spin matrix S. If acceptance is achieved, we flip the spin with corresponding index j and update expectation values for energy E and magnetic dipole moment M.

if deltaE < 0 **then**
    Energy += deltaE ▷ Update energy
    $S_l = S_l \times (-1)$ ▷ Flip spin s_l
    magnetization += $2S_l$ ▷ Update magnetic dipole moment
else if r <= w **then** ▷ Checks if $r \in [0,1\rangle \leq w = e^{-\beta\Delta E}$
    Energy += deltaE ▷ Update energy
    S(index=j) = S(index=j)$\times(-1)$ ▷ Flip spin s_l
    magnetization += 2S(j) ▷ Update magnetic dipole moment
end if

III Results

The results from applying the Monte Carlo method to the two-dimensional Ising model are presented below. All other relevant benchmark results including the derivation of the analytical results for a 2×2 lattice are presented in the appendix (sec. VI). A study of performance and bechmarks are presented in sec.III.I. These includes runtimes for different flags and with/without parallellization in fig.1, numerical and analytical comparisons for a 2×2 lattice in fig.2, expectation values for energy and magnetization as functions of MC-cycles using both ordered and disordered starting configurations in fig.3.

In addition to this the section also shows energies as a function of fewer MC cycles, using both disordered and ordered start configuration in fig.4, and number of acceptances for suggested flips are presented in fig.5. Energy Probability distributions are also shown in fig.6 with a 20×20 lattice.

In sec.III.III a look at phase transitions is explored near the critical temperature T_C. The quantities $\langle E \rangle$, $\langle |M| \rangle$, C_V and χ are all presented in fig.7 and fig.8 as functions of temperature T and lattice size L. Different spin configurations for temperatures below and above the analytical critical temperature T_C from eq.6 are shown in fig.9. Fig.10 shows the critical temperature $T_C(L)$ as a function of L, with a estimated value of $T_C(\infty)$ presented in the same figure.

III.I Method Performance and Benchmarks

III.I.1 Runtimes with and without parallelization

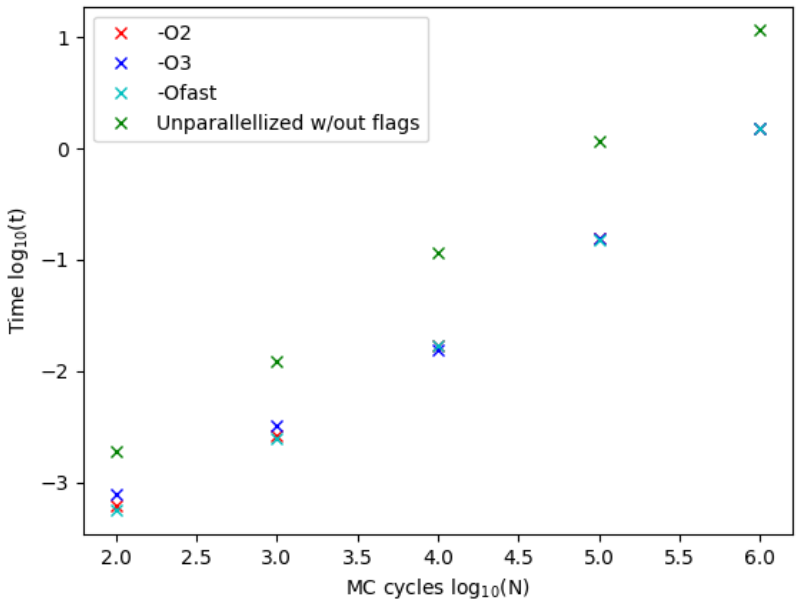
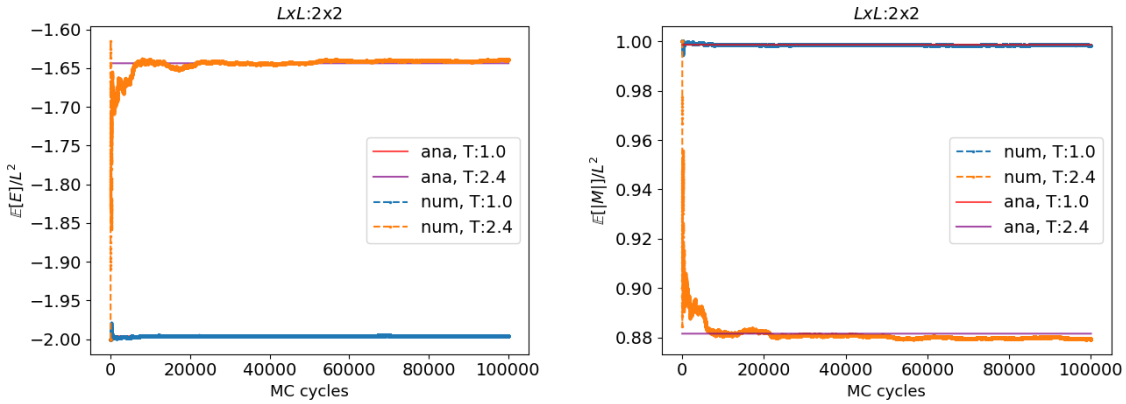


Figure 1: **Runtime as function of MC cycles**: Parallelization are performed over temperatures. The gap in runtime between temperature intervals run in parallel and sequantially increases with Monte Carlo Cycles. Up to an order of magnitude less runtime is observed with parallelized code. Parameters: Write something here SIDRA.

III.I.2 2 by 2 system: Numerical vs. Analytical solutions

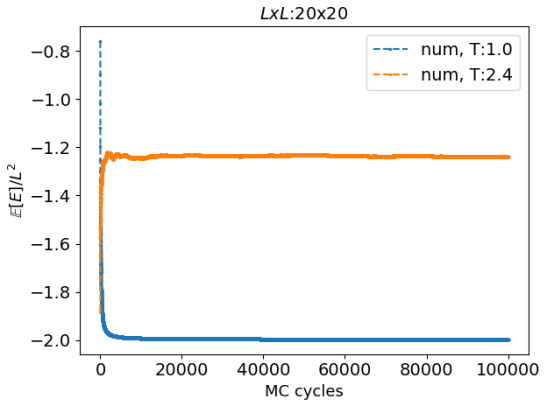


(a) $\langle E \rangle / L^2$ for 2×2 lattice

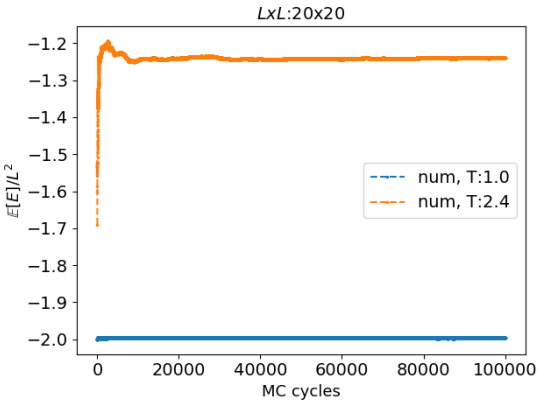
(b) $\langle |M| \rangle / L^2$ for 2×2 lattice

Figure 2: **Energy and magnetization compared to analytic solutions for $T = 1.0$ and $T = 2.4$**: Numerical expectation values approach the analytical values in both cases. At $T = 2.4$ around 20 000 cycles are needed for the numerical expectation values to converge towards a constant. At $T = 1.0$, only half as many cycles are needed before the numerical solution are stable. **a)** Comparing computed mean energy with analytic expression for $\langle E \rangle$ from eq.2 with 2×2 lattice. **b)** Comparing computed mean magnetization $\langle |M| \rangle$ with analytic expression from eq.2 with 2×2 lattice. Parameters: T = Temperature, number of Monte Carlo cycles MC: 10^5, calibration cycles: 0, number of spins in each dimension $L = 2$.

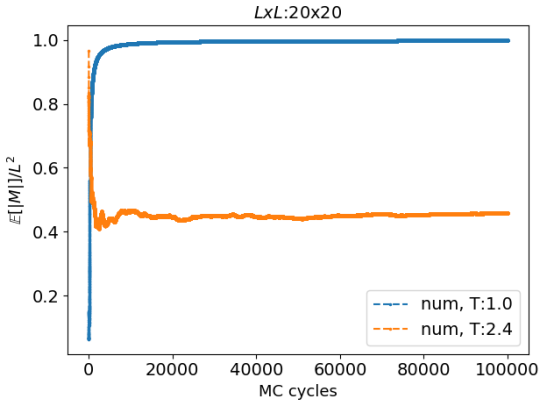
III.I.3 Disordered vs ordered start configuration



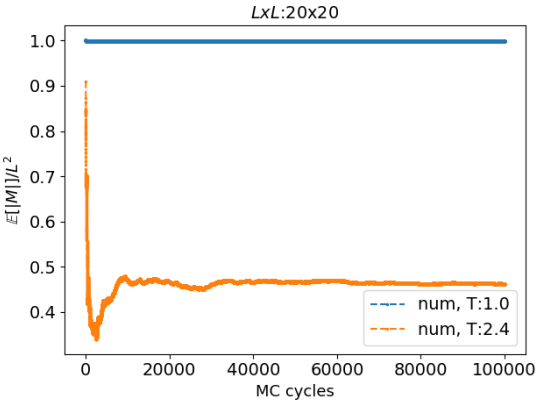
(a) $\langle E \rangle / L^2$: Disordered start



(b) $\langle E \rangle / L^2$: Ordered start

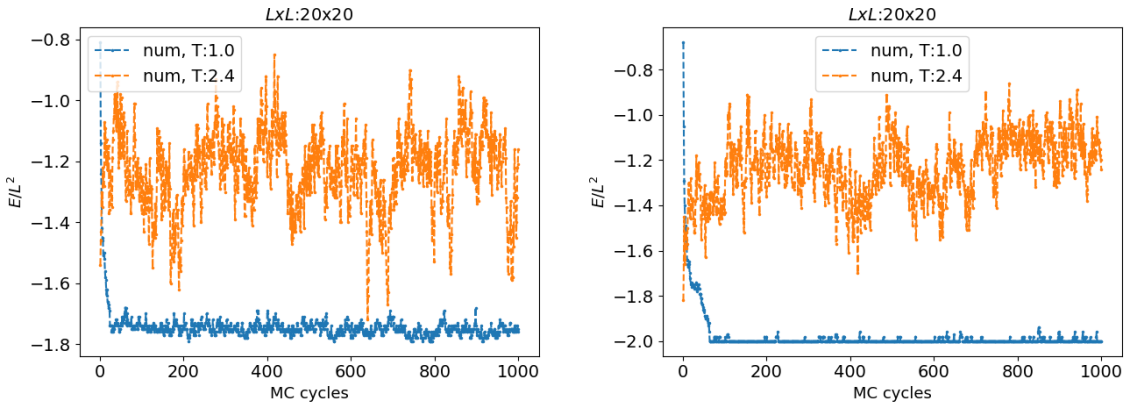


(c) $\langle |M| \rangle / L^2$: Disordered start



(d) $\langle |M| \rangle / L^2$: Ordered start

Figure 3: **Expectation values for energy and magnetization as a function of MC cycles**: **Above**: Mean energy $\langle E \rangle / L^2$ per spin. **a)** The same trend as in fig. 2 is observed. The number of cycles before convergence is larger for $T = 2.4$ (approximately 20 000), compared to lower temperatures. **b)** However, for an ordered start, one needs less cycles to obtain a near constant solution, compared to that of a disordered start. **Below**: Mean magnetization $\langle |M| \rangle / L^2$ per spin. **c)** A disordered start have around 20 000 cycles before approaching a convergent expectation value. **d)** With an ordered start, less Monte Carlo cycles are needed for low temperatures. For both $\langle E \rangle / L^2$ and $\langle |M| \rangle / L^2$, the second temperature, $T = 2.4$, begins at the spin state from the last cycle of $T = 1$. Hence, a smaller effect of an ordered start is observed for this temperature. Parameters: T: temperature, number of Monte Carlo cycles MC $= 10^5$, number of spins in each dimension $L = 20$.

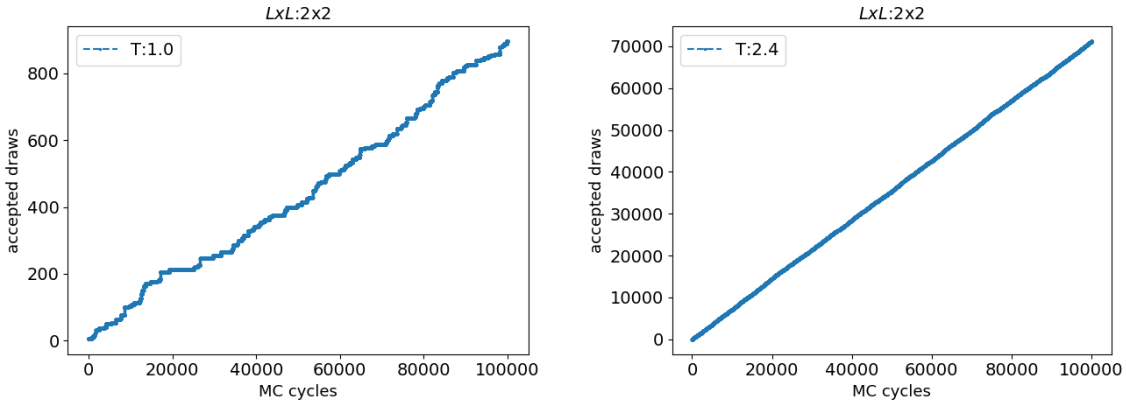


(a) E: Disordered start

(b) E: Ordered start

Figure 4: **Energies as a function of MC cycles - an explanation for poor expectation values**: Ordered starts are more precise. However, when unrealistic energy states are used in the calculation of expectation values for a steady state system, a lot more cycles is needed to get an accurate description. **a)** With a disordered starting configuration, spins are set up or down by random. At a low temperature, however, all spin up or down are more likely (an ordered system). Thus, more cycles are needed to calibrate the steady-state system. For 1000 cycles, the disordered initiation doesn't even reach it's equilibrium state (around -2.0, compared to fig 3). **b)** With an ordered start, less Monte Carlo cycles are needed for low temperatures. Here, less than 100 cycles are needed to reach an equilibrium state. However, when these points are taken into account in the calculation of expectation values, a lot more cycles are needed to get an accurate representation of the steady state. Thus a given number of calibration points are used to tune the system before adding starting calculating expectation values. Another consideration is energy fluctuation with a higher amplitude for $T = 2.4$ than $T = 1$. A consequence is that more cycles are needed in the calculation of expectation values at high T, to get accurate numerical results. The second temperature, $T = 2.4$, begins at the spin state from the last cycle of $T = 1$, thus, a less effect of an ordered start is observed for this temperature. Parameters: T: temperature, number of Monte Carlo cycles MC $= 10^5$, number of spins in each dimension $L = 20$.

III.I.4 Acceptance Rates of Suggested Flips

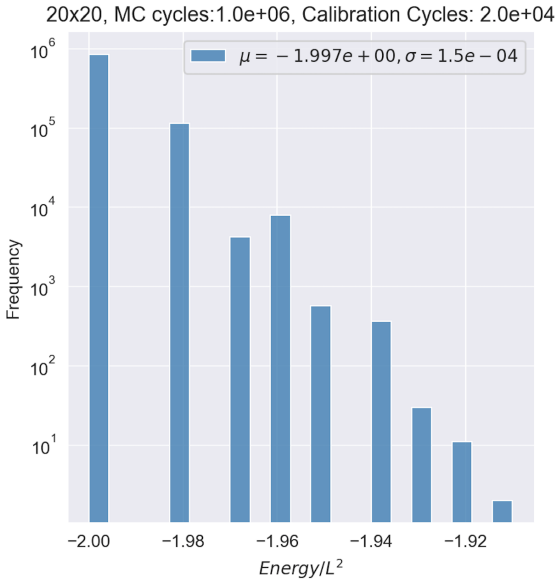


(a) Accepted configurations, $T = 1.0$

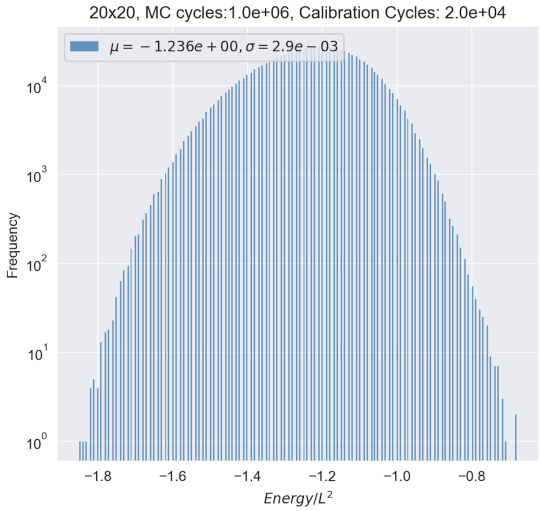
(b) Accepted configurations, $T = 2.4$

Figure 5: **Number of accepted configurations as function of Monte Carlo cycles**: With a lower temperature, less configurations are accepted, compared to a higher temperature. **a)** Total number of accepted configurations as function of MC cycles using temperature $T = 1.0$ **b)** Total number of accepted configurations as function of MC cycles using temperature $T = 2.4$. Parameters: T: temperature, number of Monte Carlo cycles MC $= 10^5$, number of spins in each dimension $L = 2$.

III.II Energy Probability Distributions for 20 by 20 grid



(a) $T = 1.0$

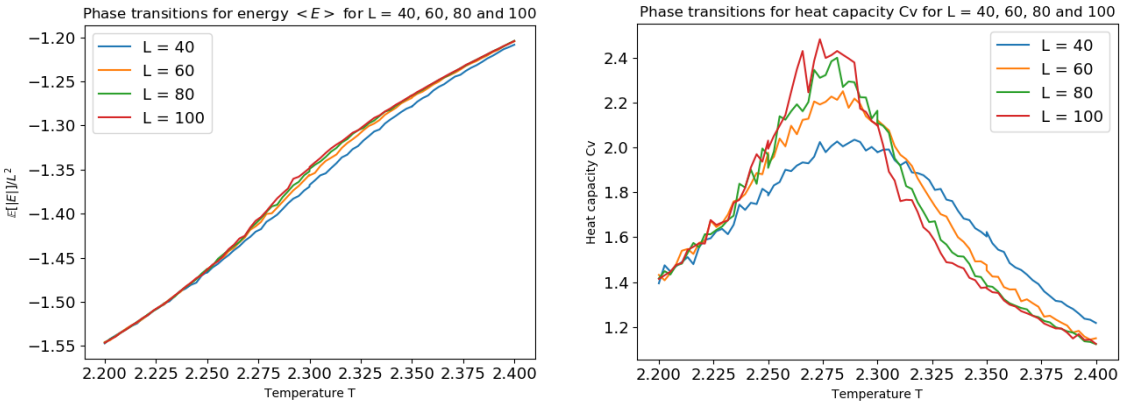


(b) $T = 2.4$

Figure 6: **Probability distribution of energies in a steady state 20-by-20 spin system**: **a)** At $T = 1$, only a few energy states are available. **b)** With $T = 2.4$, more energy states are available to the system, and the distribution are close to a Gauss curve. However, this results in a larger standard deviation in the mean value. Parameters: T: temperature, number of Monte Carlo cycles MC $= 10^6$, number of calibration cycles: 2×10^4, number of spins in each dimension $L = 2$.

III.III A Closer Look at Phase Transitions

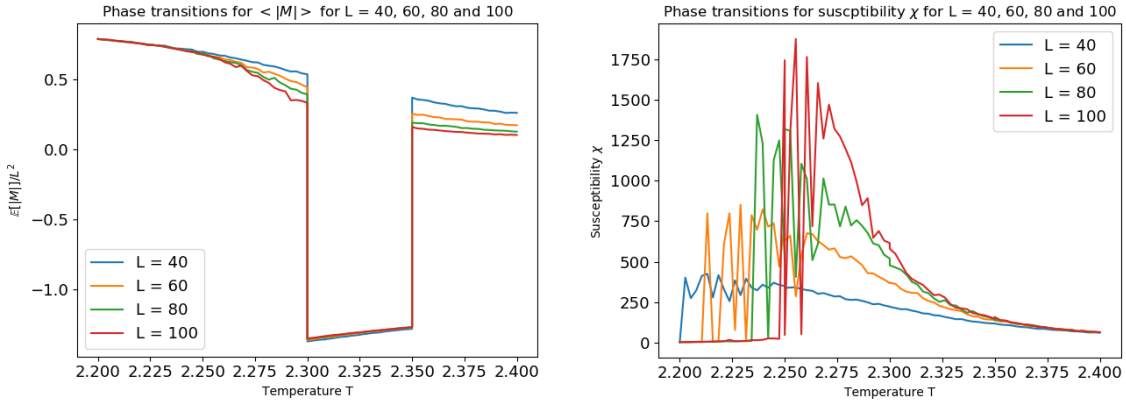
III.III.1 Energy and heath capacity



(a) $\langle E \rangle (T)/L^2$ (b) $Cv(T)$

Figure 7: **Energy $\langle E \rangle$ and heat capacity C_V as functions of temperature T**: Both expectation values are plotted close to the critical temperature T_C and shows the behaviour of phase transitions. **a)** Energy $\langle E \rangle$ as a function of temperature T and lattice size $L \times L$. The plot sees rise in energy for higher temperatures. **b)** Heat capacity C_V as a function of temperature T and lattice size $L \times L$. Somewhere between $T = 2.2$ and $T = 2.4$, we see the function diverges to a certain maximum value for different values of L. Parameters: Temperature $T \in [2.2, 2.4]$, temperature step length $\Delta T = 0.0025$, number of Monte Carlo cycles MC $= 10^6$, number of calibration cycles: 2×10^4, number of spins in each dimension $L = 40, 60, 80, 100$.

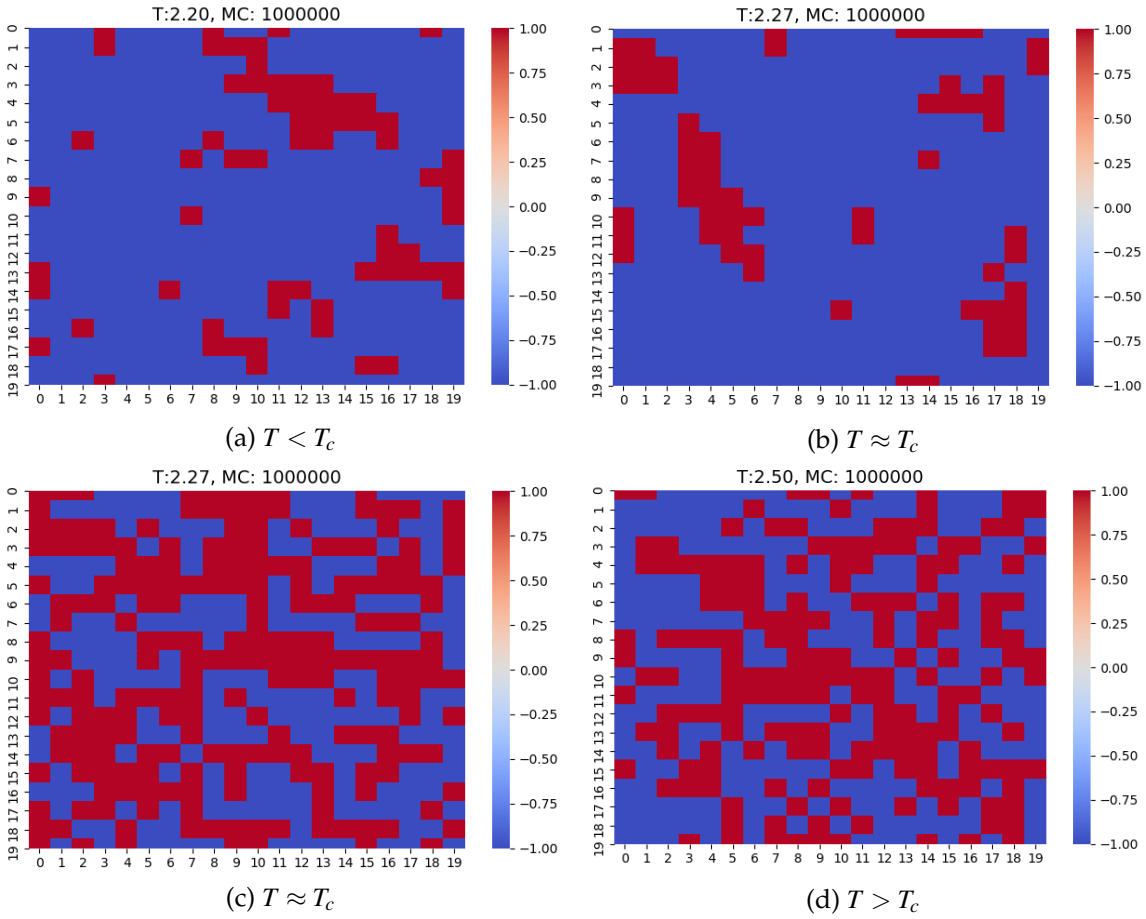
III.III.2 Magnetic Moment and Susceptibility



(a) $\langle |M| \rangle (T)/L^2$ (b) $\chi(T)$

Figure 8: **Magnetization $\langle |M| \rangle$ and susceptibility χ as functions of temperature T and lattice size $L \times L$**: Both expectation values are plotted close to the critical temperature T_C and shows the behaviour of phase transitions. **a)** Mean magnetization $\langle |M| \rangle$ as a function of temperature T and lattice size $L \times L$. **b)** Susceptibility χ as a function of temperature T and lattice size $L \times L$. Somewhere between $T = 2.2$ and $T = 2.4$, we see χ diverges to a certain maximum value for different values of L. Parameters: Temperature $T \in [2.2, 2.4]$, temperature step length $\Delta T = 0.0025$, number of Monte Carlo cycles MC $= 10^6$, number of calibration cycles: 2×10^4, number of spins in each dimension $L = 40, 60, 80, 100$.

III.III.3 Spin configurations



(a) $T < T_c$ (b) $T \approx T_c$

(c) $T \approx T_c$ (d) $T > T_c$

Figure 9: **Spin configurations for a 20 by 20 grid at scaled temperatures**: Below the critical temperature $T_c = 2.269$, a majority of spins are flipped in one direction. Either up or down. For **a)** and **b)** most are flipped down. **c)** Near the critical temperature, a phase transition occurs. Here, the spin system goes from ordered to chaotic in nature. **d)** The unordered configuration is kept for $T > T_c$. Parameters: T: temperature, number of Monte Carlo cycles MC:10^6, calibration cycles: 2×10^4, number of spins in each dimension $L = 20$.

III.III.4 Critical temperature $T_C(L)$

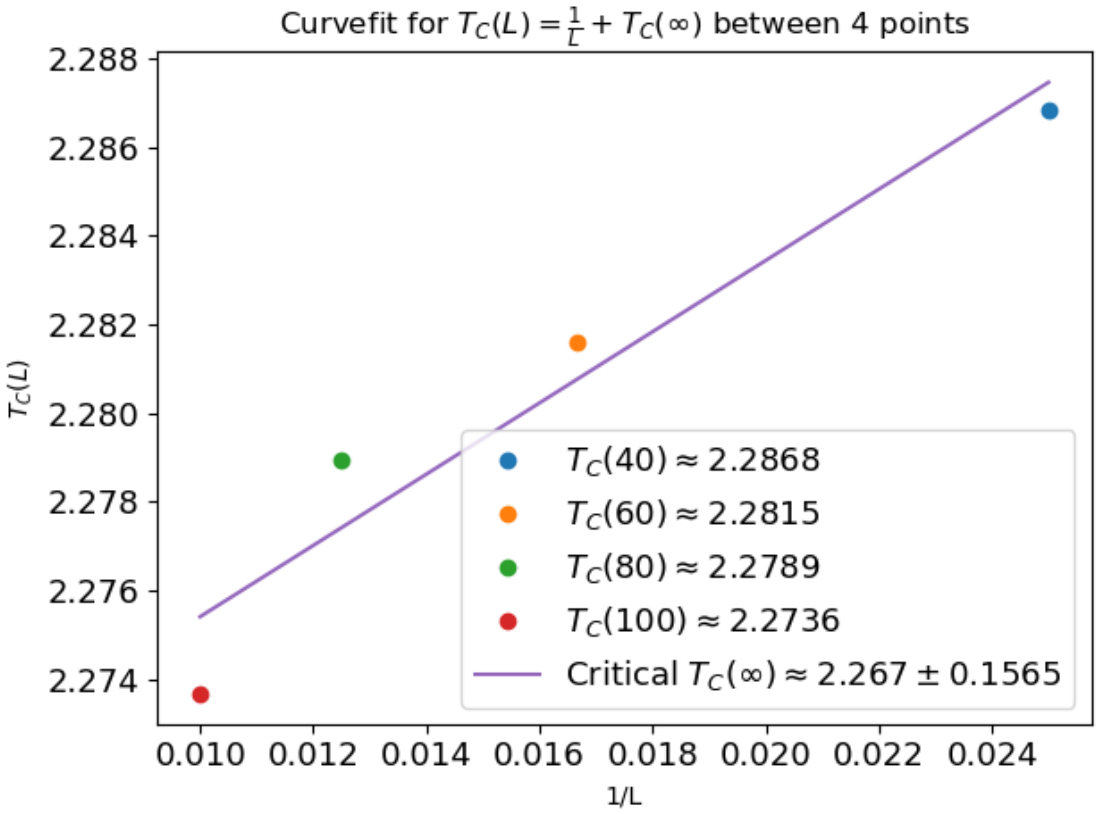


Figure 10: **Critical temperature $T_C(L)$ as function of $1/L$**: The linear function has been achieved by fitting a curve between critical temperatures that corresponds to the peaks in fig.7b for $L = 40, 60, 80, 100$. Each dot in this figure represents these temperatures, and a curve has been drawn between these points to find the behavior of the function $T_C(L)$. The critical temperature $T_C(\infty)$ is then given by the value of the function, when the curve crosses the vertical axis. This constant term was found to be $T_C(\infty) \approx 2.267 \pm 0.1565$. Parameters: Number of spins in each dimension $L = 2$, number of Monte Carlo cycles MC $= 10^6$, number of calibration cycles: 2×10^4.

IV Discussion

As mentioned in the introduction of this paper, the motivation for the numerical approach to the two-dimensional Ising model is to investigate the magnetic properties of a given material with temperature T. Since the number of spin configurations increases drastically for higher L, having numerical tools is both crucial and very useful. The results presented in sec.III are discussed in the context of this motivation.

The different runtimes in fig.1 shows that CPU times increases linearly as expected. It is also no surprise that runtimes is significantly reduced when using parallellization with all four cores of the computer. Comparing numerical and analytical results for energy and mean magnetization in fig.2, sees the numerical results move towards equilibrium after a significant amount of Monte Carlo cycles. Having analytical solutions for a 2by2 lattice, we expected this to happen. This also shows that the Ising Model has been implemented to satisfy analytical soultions, as it should.

The behaviour of energy and magnetization varies for disordered and ordered starting configuration. In fig.3b and 3d we see that for a ordered system with lower temperatures ($T = 1.0$), fewer Monte Carlo cycles are needed in order to achieve accurate results for expectation values. This is something we would expect since lower temperatures leads to a more ordered spin system with lower entropy. In contrast we see the opposite in fig.3a and fig.3c with disordered start system, where more Monte Carlo cycles are needed for lower temperatures to reach equilibrium. The number of Monte Carlo cycles also affects the accuracy of the expectation values, and in fig.4 we see how lower cycles give poor results.

The implementation of the metropolis method in algo.2 suggests that we get more accepted spin flips with higher temperatures. This is because higher temperatures leads to a system with higher entropy, and the number of flips pointing up or down are almost random. Fig.5 agrees with this, where we see that for higher temperatures ($T = 2.4$), the acceptance rate increases, while for lower temperatures ($T = 1.0$) we see that the acceptance rate of suggested flips is drastically reduced.

When studying the system close to the critical temperature T_C, we see from fig.9 that the spin system undergoes a phase transition. For $T < T_C$ most of the spins are flipped down, but for $T \geq T_C$ the entropy increases drastically and the number of spins pointing up or down are mostly random. This also confirms why the mean magnetization becomes zero at T_C, since the spins are more or less equally distributed. Looking at eq.1 we can easily see that this is indeed the case.

Due to the fact that the Monte Carlo algorithm needs a finite number of cycles before it produces accurate results for the various expectation values, we found this to be around

2×10^4 callibration cycles. Fig.6a and fig.6b shows the probability distributions of energies for a 20by20 spin system, when neglecting the first 2×10^4 callibration cycles. For $T = 1.0$ we see that there are only a few energy states available with energy $E/L^2 = -2.00$ being the state that occurs most often. For higher temperatures ($T = 2.4$), the number of energy states for the system increases and one can see that the distribution has almost the same shape as a Gauss curve. This is expected since the system has higher entropy and the acceptance rate for suggested flips is higher, which results in a larger number of different energies for each cycle.

Another look at phase transition is shown in fig.7b and fig.8b where the heat capacity and susceptibility diverges for $L = 40, 60, 80, 100$ somewhere between $T = 2.2$ and $T = 2.4$, which is expected. When extracting the critical temperature $T_C(L)$ which corresponds to the peaks of the various values of L, fig.10 shows the behaviour of $T_C(L)$ as function of $1/L$. Due to the relation between finite and infinite lattice sizes from eq.5, the estimated $T_C(\infty)$ was found to be $T_C(\infty) \approx 2.267 \pm 0.1565$. With the given uncertainty, this result agrees quite well with the analytical result found in eq.6, with $T_{C,\text{exact}}(\infty) \approx 2.269$.

V Conclusion

We have now explored the two-dimensional Ising Model using the Monte Carlo method. The implementation satisfies the analytical solutions for a 2×2 lattice. Results show that lower temperatures requires fewer monte carlo cycles to reach equilibrium when having ordered starting spin configuration, which was expected. Having larger acceptance rate for suggested flips with higher temperature is also in agreement with the implementation of metropolis algorithm algo.2.

When exploring phase transitions, we see that the number of spins pointing up or down are almost equally distributed when the temperature of the system is close to the critical temperature T_C. This confirms why the system no longer has mean magnetization when T_C is reached, and the material lacks magnetic properties. An estimate of the critical temperature for an infinitely large lattice produced a result very close to the analytical result in eq.6, which is in agreement with [5]. This also strengthens our implementation of the two-dimensional Ising Model.

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VI Appendix

VI.I Derivation of analytical quantities for 2×2 lattice

The partition function and expectation value of energy for a 2×2 lattice is given by

$$z = \sum_i^{16} e^{-\beta E_i}, \qquad \langle E \rangle = -\frac{1}{z}\frac{\partial z}{\partial \beta} \tag{14}$$

and by using tab.1 we find that

$$z = 12 + 2\left(e^{8J\beta} + e^{-8J\beta}\right) = 12 + 4\cosh(8J\beta) \tag{15}$$

The quantity $\langle E \rangle$ can then be found

$$\langle E \rangle = -\frac{1}{z}\frac{\partial z}{\partial \beta} = -\frac{32J}{z}\sinh(8J\beta) \tag{16}$$

The expectation values of the mean absolute value $\langle |M| \rangle$ and non-absolute value $\langle M \rangle$ of magnetic moment, can be found by

$$\langle |M| \rangle = \sum_i^{16} |M_i| e^{-\beta E_i} = \frac{1}{z}\left(4e^{8J\beta} + 4e^{8J\beta} + 4e^0 + 4e^0\right) = \frac{8}{z}\left(e^{8J\beta} + 2\right) \tag{17}$$

$$\langle M \rangle = \sum_i^{16} M_i e^{-\beta E_i} = \frac{1}{z}\left(4e^{8J\beta} - 4e^{8J\beta} + 8e^0 - 8e^0\right) = 0. \tag{18}$$

The heat capacity C_V is given by

$$C_V = \frac{1}{k_B T^2}\sigma_E^2, \quad \text{where} \quad \sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2 \tag{19}$$

and by first calculating $\langle E^2 \rangle$

$$\langle E^2 \rangle = \frac{1}{z}\sum_{i=1}^{16} E_i^2 e^{-\beta E_i} = \frac{1}{z}\left(2 \cdot (-8J)^2 e^{8J\beta} + 2 \cdot (-8J)^2 e^{-8J\beta}\right) = \frac{256J^2}{z}\cosh(8J\beta), \tag{20}$$

we find the variance and thereby the heat capacity

$$\sigma_E^2 = \frac{256J^2}{z}\left(\cosh(8J\beta) - \frac{4}{z}\sinh^2(8J\beta)\right), \quad \Rightarrow \quad C_V = \frac{1}{k_B T^2}\sigma_E^2. \tag{21}$$

The susceptibility χ is given by

$$\chi = \frac{1}{k_B T}\sigma_M^2, \quad \text{where} \quad \sigma_M^2 = \langle M^2 \rangle - \langle M \rangle^2 \tag{22}$$

We have that $\langle M \rangle = 0$ so then we get

$$\sigma_M^2 = \frac{1}{z}\sum_{i=1}^{16} M_i^2 e^{-\beta E_i} = \frac{1}{z}\left(8e^{8J\beta} + 8e^{8J\beta} + 32\right) = \frac{32}{z}\left(e^{8J\beta} + 1\right), \quad \Rightarrow \quad \chi = \frac{1}{k_B T}\sigma_M^2 \tag{23}$$