Project 4: Modelling Phase Transitions in Magnetic Systems

Hedvig Borgen Reiersrud, Kamilla Ida Julie Heida Sulebakk og Andrea Jensen Marthinussen
(Dated: November 29, 2020)

I. INTRODUCTION

Understanding the properties of a magnet is a fundamental part of research. A magnetic field is generated when charged objects are accelerated. An acceleration can be due to an object having the quantum mechanical feature, spin. Due to all elementary particles, except the Higgs boson, have spin, a material containing free elementary particles, they will generate a magnetic field. When a material generates a magnetic field caused by its particles having spin, it is called a ferromagnet. The spin of the electrons in atoms is the main source of ferromagnetism. It is fascinating to simulate how the magnet generates magnetic fields and behave at different temperatures.

The aim of the project is to simulate a phase transition of a magnetic material. If the spins are aligned, the material has a maximum value of *magnetization*. In contrast, when the spins are fully unaligned the magnetization is zero. This is reached at the Curie temperature, or so-called critical temperature. The Curie temperature is generally very high for the most popular ferromagnets including the metals iron, cobalt and nickel.

The Ising model is a broadly used model. It can be used to simulate brain neurons, model motions of atoms in a gas and magnetism. In this report we will focus on its ferromagnetic application, which initially was the motivation for the model. We will simulate a ferromagnet by confining the particles with spin in a square lattice, where the particles can only interfere with its neighbouring lattice points. Though the model is very simplified, as the system is in actuality enormously complicated, it will still generate applicable results. By using the Ising model we can analyze the different dependencies that affect the critical temperature.

In order to solve the Ising model numerically, we will use the Metropolis algorithm. The algorithm uses Monte Carlo cycles in order to simulate the estimations of the Ising model [4]. The algorithm initializes a matrix with the particles' spins ordered randomly. The simulation is stopped when a criteria is met. In our case the result is a ferromagnetic structure, where the spins are coordinated in the same direction. We will also arrive at a probability distribution, which is a very exciting quantity to investigate. The algorithm can also be used in other to solve other cases, as is preforms a numerical integration which is applicable in many situations.

The Ising model uses randomized initial values of energies and magnetization in addition to a random choosing of which spins to flip. Therefore one would need to utilize a random number generator in order to set the initial values. A computer cannot give us non-deterministic random numbers. Though, if a random number generator have a sufficient period length, it will not be a significant issue. Here, we will use the Mersenne Twister random number generator. It is by far the most used randomizer in computer science, due to its large period length.

II. THEORY

The Ising model

The Ising model is a model describing ferromagnets in statistical physics. The model uses discrete variables that represents magnetization, or so-called magnetic dipole moments, of atomic spins. Magnetization is the total strength of a system which produces a magnetic field. In addition, spin is a quantum mechanical feature which is characterized by either spin pointing up, $\uparrow = 1$, or spin pointing down, $\downarrow = -1$. The spins are positioned in a lattice, which let the spin of a particle to interfere only with its neighbouring particles. Each particle with spin will generate its own magnetic field. In reality, modelling a phase transition is a very complicated process. However, using the Ising model will greatly simplify the process. Though the model is not thoroughly accurate, it will still give us valuable information on physical properties, such as the critical temperature.

With no external magnetic field, the energy of the simplest form of the Ising model from ref. [1] is,

$$E = -J \sum_{\langle k,l \rangle}^{N} s_k s_l. \tag{1}$$

Where $\langle k, l \rangle$ demonstrates that we will only sum over nearest neighbouring particles. s_k and s_l have the value ± 1, and represents the spins of the lattice points k and l. N denotes the total number of lattice points. J is the coupling constant, signifying the strength of the interaction between neighbouring spins. Since J is only a constant, we can calculate the energy with the coupling constant as a unit. J varies for different materials. Since we ignore the value of J, our simulations are applicable to any magnetized material.

The magnetization, M, is the sum of each particle's spin. Therefore,

$$M = | \sum_{i}^{N} s_i |, \tag{2}$$

where s_i the spin of the lattice point i. In figure 1 two 2-d lattices are presented with different spins. From equation 2 the aligned spins have a higher magnitude of magnetization.

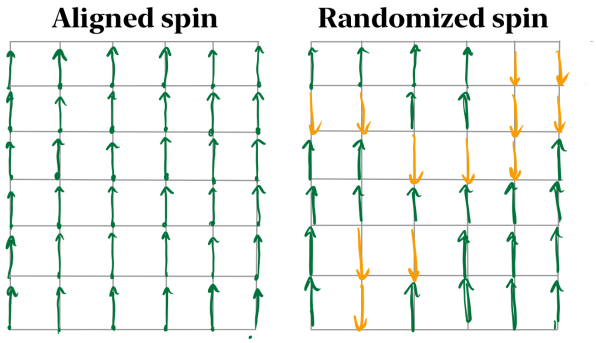

Figure 1. A schematic of a two dimensional lattice structure $L \times L$ where the lattice points' spins are aligned and randomized. The absolute value of the magnetization and energy is higher for the aligned spins.

Statistical mechanics

The partition function is a dimensionless value describing the statistical assets of a system at equilibrium. That is the system will not have a net flow of matter or energy. This results in the temperature being uniform. The partition function reads,

$$Z = \sum_i^N e^{-\beta E_i}. \tag{3}$$

β is a constant equal to $\frac{1}{k_B T}$, where k_B is the Boltzmann's constant and T the temperature. E_i is the energy state of each of the $i \in \{1, N\}$ (in steps of 1) accessible states. $e^{-\beta E_i}$ is the so-called Boltzmann factor.

The partition function plays the role of normalizing the probabilities of observing a state i. The probability is,

$$P_i = \frac{1}{Z} e^{-\beta E_i}. \tag{4}$$

It is apparent that it is most likely to observe the lowest energy states. The relationship between probabilities of measuringn the energy states E_i and E_j is,

$$\frac{P_i}{P_j} = e^{(E_i - E_j)\beta}. \tag{5}$$

From equation 1, the change of energies, $\Delta E_{i,j} = E_i - E_j$, can be written as,

$$\Delta E_{i,j} = 2S_{i,j}(S_{i+1,j} + S_{i-1,j} + S_{i,j+1} + S_{i,j-1}), \tag{6}$$

when ignoring the coupling constant J.

Furthermore, we can use the partition function in order to find expressions of the expectation values of obtaining different physical properties, such as the magnetization $\langle M \rangle$ and energy $\langle E \rangle$.

$$\langle M \rangle = \frac{1}{Z} \sum_i^N M_i e^{-\beta E_i} \tag{7}$$

$$\langle E \rangle = \frac{1}{Z} \sum_i^N E_i e^{-\beta E_i} \tag{8}$$

Additionally, we can express the expectation values of the squared magnetization and energy in the same way. This let us calculate the standard deviation of the energies and magnetization. The heat capacity at constant volume, C_V, is proportional to the squared standard deviation of energy, σ_E. It reads,

$$C_V = \frac{\beta}{T}(\langle E^2 \rangle - \langle E \rangle^2) = \frac{\beta}{T}\sigma_E^2. \tag{9}$$

The size proportional to the squared standard deviation of magnetization, σ_M, is the magnetic susceptibility, χ.

$$\chi = \beta(\langle M^2 \rangle - \langle M \rangle^2) = \beta \sigma_M^2. \tag{10}$$

Phase transitions

The critical temperature, T_C, is defined as the temperature in which a system can be right between two states, e.g solid and liquid state. The critical temperature is therefore the temperature in which the phase transition will appear. At T_C, the system is unstable, meaning a small change of spins, will result in a large change of the system, as the system is no longer right between two states. From figure 2, the different oriented flips are shown as black and white respectively. For increasing temperature, the model becomes more and more disordered. Therefore the highest rate of change of the observables will be at T_C.

From ref. [1] we have that the magnetization for temperature less than the critical temperature is,

$$\langle M(T) \rangle \propto (T - T_C)^\beta. \tag{11}$$

Where $\beta = \frac{1}{8}$ is the critical exponent, meaning the exponent where thermodynamic quantities are near a continuous phase transition. The heat capacity and susceptibility have a similar relation.

$$C_V(T) \propto \mid T - T_C \mid^\alpha, \tag{12}$$

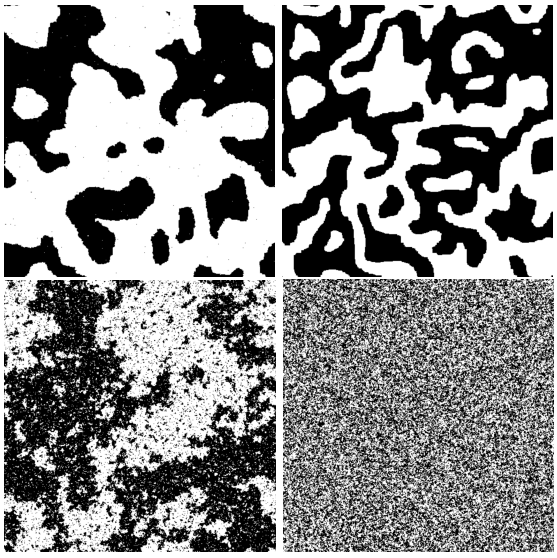

Figure 2. The figure displays a 512x512 Ising lattice, for $T = 0.0, T = 1.0, T = 2.269$ and $T = 4.0$ respectively. Up and down spins are white and black pixels. Ref. [5].

$$\chi(T) \propto \mid T - T_C \mid^{\gamma} . \tag{13}$$

Where the critical exponents are set to $\gamma = 7/4$ and $\alpha = 0$.

The correlation length ξ, which is the order of the lattice spacing for $T_C \ll T$, is another relevant quantity. The spins will be more coordinated as the temperature approaches the critical temperature, resulting in a higher magnetization. In addition, the correlation length will increase. The divergent behaviour of the correlation length near T_C is given by,

$$\xi(T) \propto \mid T - T_C \mid^{-\nu} . \tag{14}$$

Where ν is the critical exponent for the correlation length. The correlation length can be shown to be proportional to the lattice size L, for a finite L. The critical temperature will be scaled as,

$$T_C - \lim_{L\to\infty} T_C = aL^{-1/\nu}. \tag{15}$$

Where a is a constant.

Using equation 15 and setting $T = T_C$, we arrive at the following relations,

$$\langle M \rangle \propto L^{-\beta/\nu}, \tag{16}$$

$$C_V(T) \propto L^{\alpha/\nu}, \tag{17}$$

$$\chi(T) \propto L^{\gamma/\nu}. \tag{18}$$

Analytic results

Lars Onsager was the first to solve the Ising model analytically in two dimensions. From ref. [1] Onsager's analytical solution of the critical temperature is presented. It states,

$$\frac{k_B T_C}{J} = \frac{2}{\ln(1+\sqrt{2})} \approx 2.269. \tag{19}$$

The analytical value is obtain when setting ν equal to 1. From figure 2 and ref.[5], it is apparent that the spin become disordered at $T = 2.269 \approx T_C$. For temperatures higher than T_C, the spin configuration become more an more chaotic.

Moreover, by using equations 3, 7 and 8, in addition to using the same method to find the expectation values of the squared magnetization and energy, we arrive at the analytical results which are deviated in Appendix A. They read,

$$Z = 12 + 4\cosh(8\mathrm{J}\beta), \tag{20}$$

$$\langle E \rangle = -8J\frac{\sinh(8J\beta)}{3+\cosh(8J\beta)} \tag{21}$$

$$\langle M \rangle = 2\frac{2+e^{8J\beta}}{3+\cosh(8J\beta)} \tag{22}$$

$$\langle E^2 \rangle = 64J^2\frac{\cos 8J\beta}{3+\cosh(8J\beta)} \tag{23}$$

$$\langle M^2 \rangle = 8\frac{1+e^{8J\beta}}{3+\cosh(8J\beta)} \tag{24}$$

The analytical values of heat capacity and susceptibility are easily obtained by equations 9 and 10. These are also deviated analytically in the appendix.

These results are for the lattice size of 2×2 with periodic boundary conditions (PBCs). PBCs are a set of boundary conditions which will generate a system which approximates for an infinite boundary condition. In equation 15 one would need to calculate for $T_C(L = \infty)$. It goes without saying that a computer cannot represent infinity, so we will approximate the infinite value with the PBCs.

III. ALGORITHM

The Metropolis algorithm

In this project we will use the Metropolis algorithm in order to simulate the Ising model to achieve numerical

values of the different physical entities. Intuitively we would assume that in order to find the probability distribution, one would need to utilize the partition function in equation 3. However, this is a very costly computational operation, as one would need to iterate over every possible state. Instead we will use an algorithm which uses repeated random sampling in order to obtain numerical results of the probability distributions. The algorithm uses only ratios between probabilities, such that the partition function and the probability function in equations 3 and 4 are irrelevant to obtain the approximation of the probability distribution.

For our specific case the algorithm reads,

Define sampling points N
Define matrix size $L \times L$
Randomize values of $s_{i,j}$ for the i, j element in the matrix, 1 or -1
Set $\langle E\rangle, \langle E^2\rangle, \langle M\rangle, \langle M^2\rangle = 0$
for $n \in \{1, N\}$ **do**
  i, j randomly chosen in $\{0, L\}$
  Metropolis sampling
  $r \in \{0, 1\}$
  if $\Delta E < 0$ **then**
    $E = E + \Delta E$
    $s_{i,j} = -s_{i,j}$
    $M = M + 2s_{i,j}$
  end if
  if $r < e^{-\beta \Delta E}$ **then**
    $E = E + \Delta E$
    $s_{i,j} = -s_{i,j}$
    $M = M + 2s_{i,j}$
  end if
  $\langle E\rangle = \langle E\rangle + E$
  $\langle E^2\rangle = \langle E^2\rangle + E^2$
  $\langle M\rangle = \langle M\rangle + \mid M \mid$
  $\langle M^2\rangle = \langle M^2\rangle + M^2$
  $\langle E\rangle = \langle E\rangle / N$
  $\langle E^2\rangle = \langle E^2\rangle / N$
  $\langle M\rangle = \langle M\rangle / N$
  $\langle M^2\rangle = \langle M^2\rangle / N$
end for

Normally, instead of looping over N, one loop over total number of spins (L^2). However, we found that in order to decrease the number of FLOPs[2] and thus having a lower run-time, it would be sufficient to only loop over N which is the number of Monte Carlo cycles (MCCs). (????????)

When the for-loop have accepted L^2 values of randomized spin, it is called a Monte Carlo cycle (MCC). The Monte Carlo implementation of the algorithm chooses which spins we will choose to flip in a randomized matter. However, in order to optimize the algorithm, we will choose to loop over total number of cycles, N, and sample the system each time a configuration is accepted.

Computers cannot truly choose a randomized number, through a random number generator (RNG). The randomized number is called a random seed state. Though seeming random, the randomized numbers are in actuality deterministic when given an initial random seed. In our program we will use the Mersenne Twister random number generator. The RNG has a period of $2^{1997} - 1$, meaning the RNG is *random* for programs which generate random numbers for a lower period than than $2^{1997} - 1$. The maximum matrix size we will simulate for is $L \times L = 100 \times 100$ with a number of 10^6 MCCs. This results in a period of 10^{10}. Since the Mersenne RNG is $\gg 5 \cdot 10^{10}$, it will be more than sufficient to randomize the spins and indices i and j for our largest number of sampling points and matrix size.

IV. METHOD

Initial spin	Final spin	Initial E	Final E	ΔE
↑ ↑ ↑ ↑ ↑	↑ ↑ ↓ ↑ ↑	-4J	4J	8J
↓ ↑ ↑ ↑ ↑	↓ ↑ ↓ ↑ ↑	-2J	2J	4J
↓ ↓ ↑ ↑ ↑	↓ ↓ ↓ ↑ ↑	0J	0J	0J
↓ ↓ ↑ ↓ ↑	↓ ↓ ↓ ↓ ↑	2J	-2J	-4J
↓ ↓ ↑ ↓ ↓	↓ ↓ ↓ ↓ ↓	4J	-4J	-8J

Table I. The table displays the different spin combinations of neighbouring lattice points and in its initial and final state, when the lattice points are only allowed to interfere with its neighbouring lattice points. The change of spins are calculated through equation 6. There are only 5 different ΔEs for a two dimensional system.

Testing

We start by initializing lattice and write a code implementing the general Metropolis algorithm for the lattice size of 2×2 at temperature $T = 1$. The analytical values of the expectation values, from equations 21, 22, 23, and 24, can then be tested against the numerically calculated ones. If they match up, we can assume that the algorithm holds for a higher number of lattice points.

By using equation 19 we can compare our numerical result to the analytical for the critical temperature. We ex-

pect that an increasing lattice size, will generate numerical critical temperatures which will become more and more coordinated with the analytic results. We would expect that an increasing lattice size, would produce more accurate results of the critical temperature.

Initial state

Initially, a two dimensional lattice structure containing $L \times L$ spin-1/2's is defined either as an highly ordered matrix where all spins are "up" or as a matrix where each spin is randomly by the Mersenne Twister RNG, and chosen to be up or down (1 or -1). Thereafter, the total energy of the system is calculated by 1, while the total magnetization of the system is calculated by 2. These initial values we name E_0 and M_0.

Boundary conditions

Nonetheless, as we intend to simulate an infinite two dimensional grid, all lattice points need to have four neighbours. As the size of the matrix configuration must be finite, this is not realistically the case. The highest lattice size we will simulate is 100×100. However, by defining an indexing array simulating periodic boundary conditions as follows,

$$I = [L-1, 0, 1, ..., L-1, 0],$$

the problem for the outer-most elements only having two neighbours is avoided. In the loops where matrix elements are utilized, instead of indexing the matrix itself, by the indices i and j, we send the iterative index to the indexing array and use the indexing array as the index argument for the matrix. (skrive bedre)
In reality, a lattice size of 100×100 is minor compared to 'normal' magnets containing many moles (10^{23}) of particles. This is not solvable numerically, as one would need to loop over $> 10^{23}$ states. However, by using the boundary conditions above, one would expect to approximate a larger system.

Efficiency

The efficiency increases when we utilize the benefit of the Metropolis algorithm. That is the fact that we never have to calculate the partition function, only the energy differences, ΔE.

All the spins are either represented as $+1$ or -1, with ΔE given by equation 6, the only ΔE's possible for a two dimensional Ising model is shown in table I. As a result, the accessible change of energy states are $\Delta E = -8\text{J}, -4\text{J}, 0\text{J}, 4\text{J}, 8\text{J}$. Thus, it is irrelevant to calculate equation 6 for each value of the spins for j and i. By using only these 5 possible ΔEs will increase the efficiently to a great extent as the values can be calculated outside the loop to decrease the number of FLOPs (ref. [2]). As a consequence, we only need to calculate the five achievable change of energies. This will decrease the run-time substantially.

Additionally, we can avoid running calling the exponential function L^2 times in the MCCs in order to calculate the probability distribution. This by only calculating for ΔE inside the cycle. After the MCC have accepted L^2 states, we can then go on and taking the result of ΔE as the exponent in order to obtain the probability distribution.

Equilibrium

When we initialize the lattice, we assign to each lattice point randomly. This initial configuration will likely not be an equilibrium state. We expect that the system will approach equilibrium as the number of MCCs increase. We say that the system has reached equilibrium when the energy is constant in time. When the system has reached equilibrium, the number of MCCs is called the Burn-In period.

Units

We want to scale the temperature in such a way that the axis of the plots of quantities which depend on T are easily readable. We achieve this by setting the Boltzmann constant $k_B = 1$ and thus measuring T in units of energy. In addition to making the plots becoming more readable, scaling the quantities appropriately also helps us avoid under- and overflow.

Furthermore, the coupling constant J is generally quite large, and vary for different materials. To minimize numerical error, we will also set this constant to 1Joule [J]. This also let us generalize the simulation to different materials.

Parallelization

Though having maximized the efficiency considerably, the numerical operation is still costly for our largest matrix size $L^2 = 100 \times 100$ and number of sampling points $N = 10^6$. Therefore we need to use parallelization of our computation in order to decrease the run-time. Parallelization enables the simulation to run parallel on different processors ref. [3]. The final results are the values we wish to develop in this project.

In our case we will use MPI in order to parallelize our MCCs in the C++ program language. This will increase the run-time substantially.

Obtaining numerical values of the critical temperature

In order to discuss the reliability of our results, we will compare the numerically obtained values of the critical temperature for different lattice sizes with the analytical T_C in equation 19.

We can obtain numerical values of the critical temperature in a myriad of different approaches. Here we will both use equation 15 and by using the traits of the phase transitions. We expect the physical entities to be unstable near T_C, meaning the highest slope rate, will be at T_C when the entities are plotted as a function of temperature.

V. RESULTS

The 2 × 2 lattice size

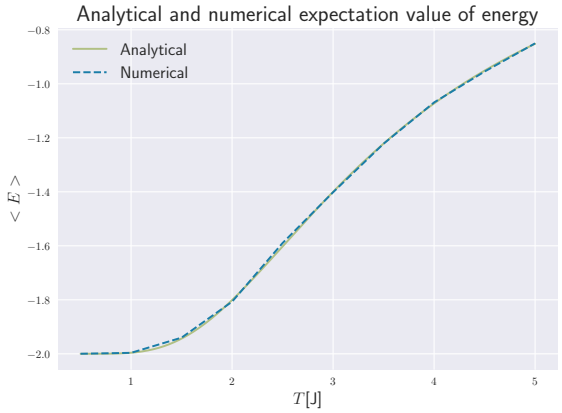

Figure 3. The figure shows the agreement between the numerical and analytical expectation energy as function of T for a 2×2 lattice with MCC = 10 000.

The figures 3 and 4 display the analytical and numerical expectation value of energy and magnetic moment as functions of T. We see that the numerical value to a large degree matches the analytical.

The figures 5 and 6 show the analytical and numerical value for the specific heat capacity and magnetic moment as function of temperature.

From table II it is shown that the differences of the analytical and numerical values vary. Since $T = 1$ the variance $\sigma_E^2 = C_V$ and $\sigma_M^2 = \chi$.

The figures 7 and 8 display the analytical and numerical C_V and χ as functions of MCCs. The analytical values stay constant for different MCCs. The numerical values however, are not constant.. Nevertheless, when the numbers of MCCs increases, the numerical values seem to stabilize, close to the analytical values.

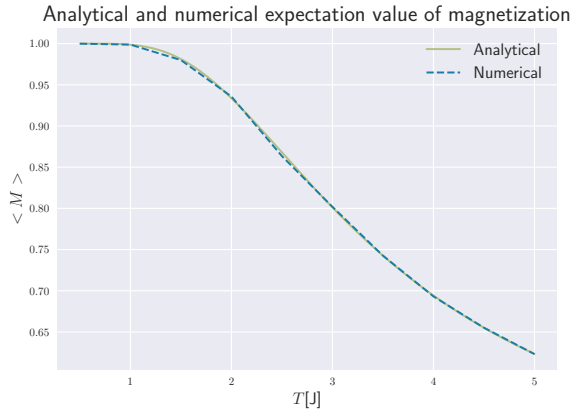

Figure 4. The figure shows the agreement between the numerical and analytical magnetic moment as function of T for a 2×2 lattice with MCC = 10 000.

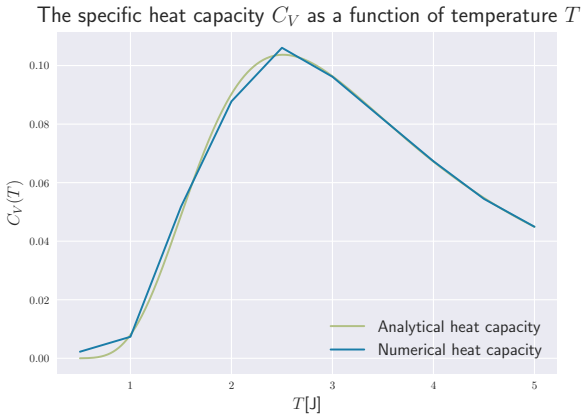

Figure 5. The figure shows the agreement between the numerical and analytical specific heat capacity as function of T for a 2×2 lattice with MCC = 10 000.

The 20 × 20 lattice size

From figure 9, the expectation value of the energy as function of MCCs is shown. The expectation values seem more at more constant for increased values of MCCs. For more than 10^4 number of MCCs, the expectation value stays more or less constant. Additionally, T = 2.4 gives higher expectation value than for T = 1.

From figure 10, the expectation value of the magnetization of function of MCCs is shown, in a similar matter than in figure 9. Also, the Burn-In period happens at MCCs $\approx 10^4$.

The figure 11 shows that for $T = 2.4$J have a higher rate of accepted number of spins. From the figure, it seems that the number of accepted spins for $T = 1$J stay constant at 0. However, this is due to the number of flips at $T = 2.4\text{J} \gg T = 1\text{J}$ with an increasing number of MCCs.

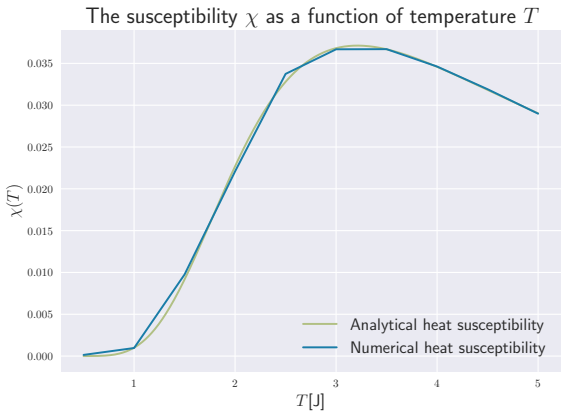

Figure 6. The figure shows the agreement between the numerical and analytical magnetic susceptibility as function of T for a 2×2 lattice with MCC = 10 000.

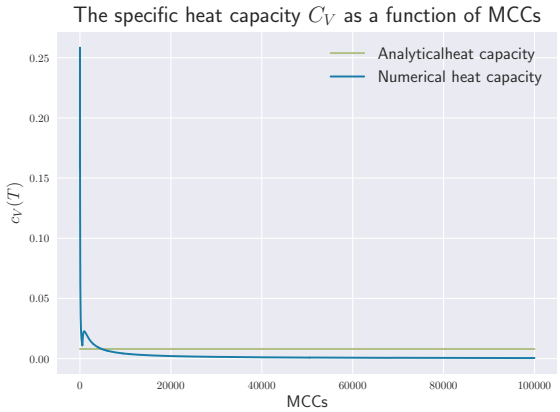

Figure 7. The figure shows the specific heat capacity C_V for T = 1, as a function of number of MCCs compared with analytical value, for $L = 2$

	Analytical	Numerical	Differences
$\langle E \rangle$	-1.99598	1.99600	$2.00 \cdot 10^{-5}$
$\langle E^2 \rangle$	3.99197	3.98200	$9.97 \cdot 10^{-3}$
$\langle \lvert M \rvert \rangle$	0.998661	0.998645	$1.60 \cdot 10^{-5}$
$\langle M^2 \rangle$	0.99833	0.99832	$1.00 \cdot 10^{-5}$
χ	0.0010027	0.0010282	$8.01 \cdot 10^{-5}$
C_V	0.0080206	0.0079840	$3.66 \cdot 10^{-3}$

Table II. Table of analytical and numerical calculated observables, and their differences. These values are for the number of MCCs = 100, 000, lattice size $L = 2$ and temperature $T = 1$.

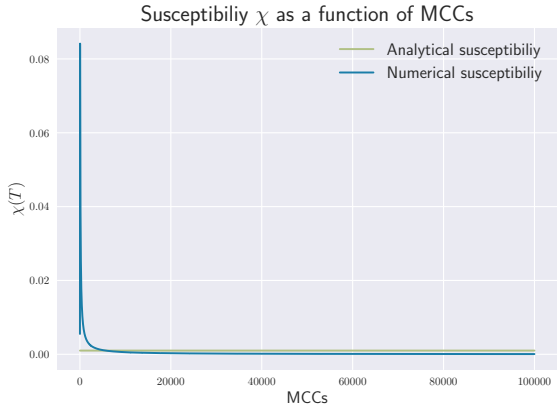

Figure 8. The figure shows the susceptibility χ for T = 1, as a function of number of MCCs compared with analytical value, for $L = 2$

From figure 12, the number of accepted flips with temperatures varying from 0J to 5J. The highest rate of change is obtained at ≈ 2.27J. This value is quite compiling with the analytical result from equation 19.

Figure 13 and 14 shows the normalized probability of measuring different energies in the system. We see that for T = 2.4, the probability takes a Gaussian distribution form. In comparison, for T = 1, the system seems to stabilize around -800 J. (Dette må skrives om)

Lattice size larger that 20 × 20

Need to add a table of the obtained values of T_C for different L.

VI. DISCUSSION

The 2 × 2 lattice size

The agreement between the numerical and analytical values is quite satisfying in figures 3, 4, 5 6. The agreement also holds for higher temperatures Thus, we can say that the tests have succeeded and that our algorithm will hold for a larger number of lattice size.

From figure 7 and 8 we see that we need approximately 500 MCCs, for T = 1, in order to achieve a good agreement between the numerical and analytical values for the specific heat capacity and susceptibility. There is, however, a small difference between the numerical and analytical values, as the numerical values for both the specific heat capacity and susceptibility tends to stabilize just under the analytical curve. This might be due to small numerical errors, but will most probably not affect larger calculations to a great extent, as the difference between the numerical . In other words, when testing the numerically calculated observables against the analytical for $L \times L = 2 \times 2$, we observe that they to a large degree match up. We can therefore assume that the algorithm holds for a higher number of lattice points.

From table II, the analytical and numerical values of the different physical entities are somewhat complying

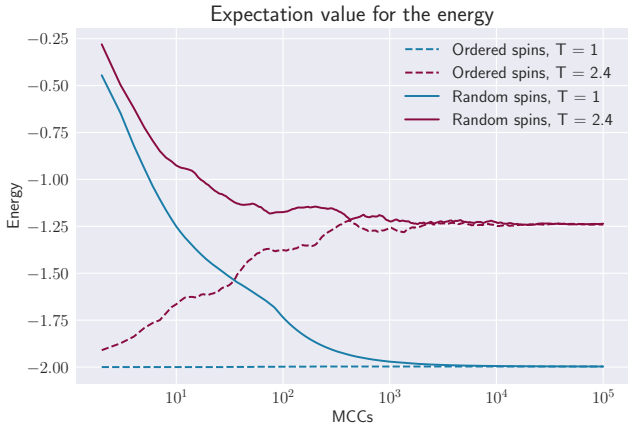

Figure 9. The figure displays the expectation value of the energy as function of MCCs.

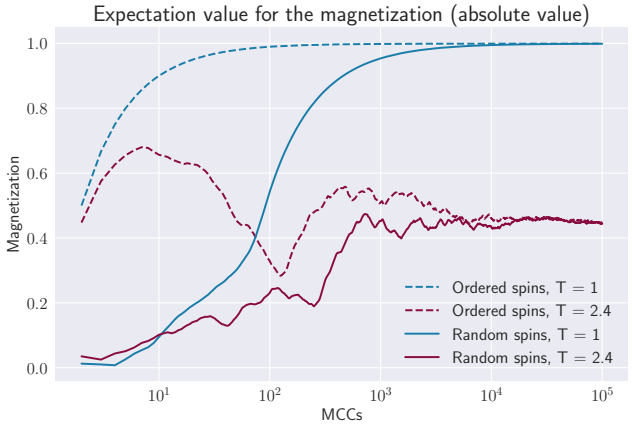

Figure 10. The figure displays the expectation value of the magnetization as function of MCCs.

with the analytical values in the case of the number of MCCs $= 100,000$ and $L = 2$. However...

The 20 × 20 lattice size

Figures 9 and 10 show the expectation value of energy and magnetic moment for ordered- and random spins for $T = 1$J and $T = 2.4$J. It is apparent that the system reaches an equilibrium situation for both temperatures at MCCs $\approx 10^4(10^5$ nå?). Moreover, we see from figure 11 that we have a more chaotic state for T = 2.4. In other words the number of accepted flips increases with temperature, T, indicating that the system gets more and more disordered. Having that the critical temperature $T_C \approx 2.27$ (from figure 12), is in alignment with our expectations, as the system goes through phase transition. However, we only have 3 digits in this calculation, so one would expect that the numerical and analytical values of T_C calculated here are not in total

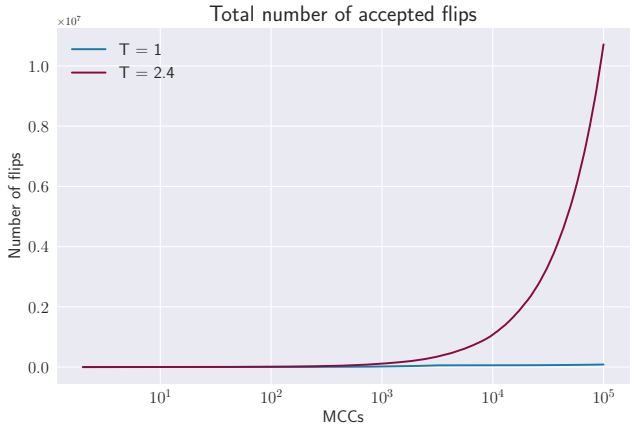

Figure 11. The figure displays the number of accepted flips of spin elements of the lattice as function of Monte Carlo cycles for $T = 1.0$ J and $T = 2.4$ J.

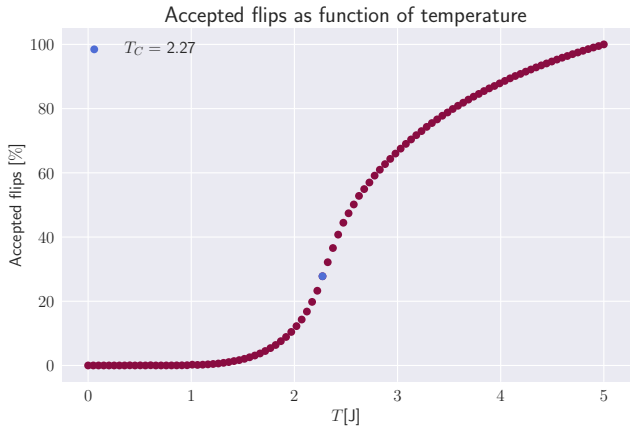

Figure 12. The figure displays the number of accepted flips of spin elements of the lattice as function of temperature. We see that at $T \approx 2.27$ J, the graph has the highest rate of change. This is for L = 20 and MCCs = 100,000.

compliance since we have rounded up the numerical value. In addition, the number of steps is quite small, and the number of points in the steepest part of the graph is insufficient. Nonetheless, the obtained T_C indicates that our algorithm produces results with high precision, which is fulfilling.

When computing the probability $P(E)$ for the 20 × 20 system with $T = 1.0$ and $T = 2.4$ we see that the probability of finding the system in a state with $E \approx 800J$ is close to 1 when $T = 1$ and that the probability of measuring different energy states is Gaussian with mean equal to -500 for $T = 2.4$. This corresponds with theory, since equation 4 indicates that the lowest temperature level (the scaled $T = 1$) will be in the lowest energy state. For $T = 2.4$ however, the system ...

Having that the variance in energy σ_E^2 is equal to ??, we see that the probability distribution for $T = 2.4$ is in

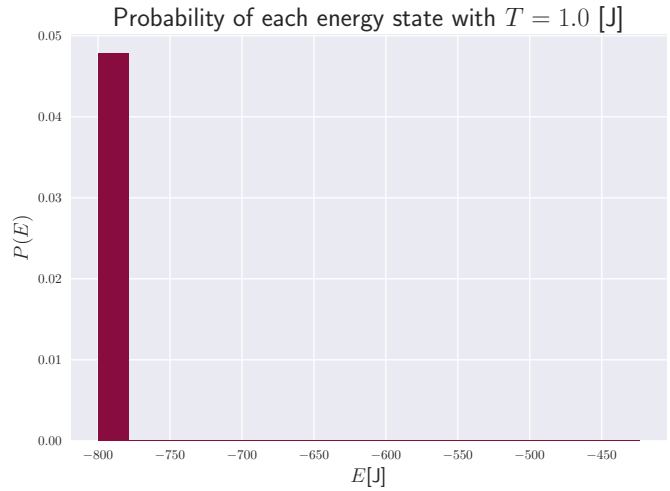

Figure 13. The figure displays the normalized probability P(E) for L = 20 with T = 1.

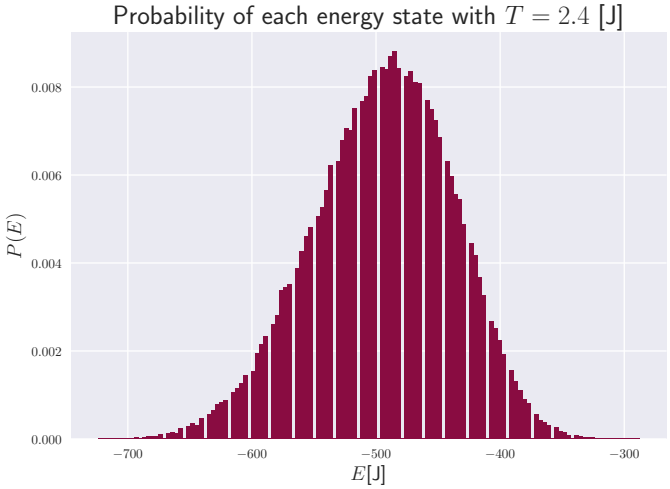

Figure 14. The figure displays the normalized probability $P(E)$ for L = 20 with T = 1.

alignment with our expectations. (Skrive mer om dette)

Lattice size larger that 20 × 20

In the last part of this project we wanted to study the behavior of the Ising model in two dimensions close to the critical temperature as function of the lattice size $L \times L$. When calculating the expectation values for $\langle E \rangle$, $\langle M \rangle$, C_V and χ as function of T for $L = 40$, $L = 60$, $L = 80$ and $L = 100$ for T $\in \{2.0, 2.3\}$ with a step in temperature $\Delta T = 0.05$, we parallelized the code using MPI. Using parallelization, reduced the CPU-time to a great extent.

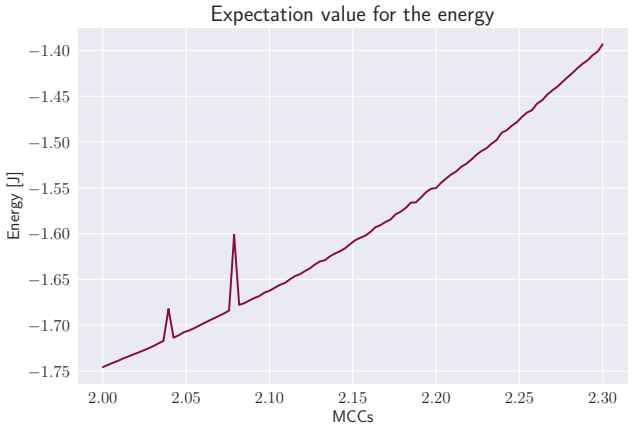

Figure 15. The figure displays the expectation value of the energy as function of temperature for MCC = 1 000 000.

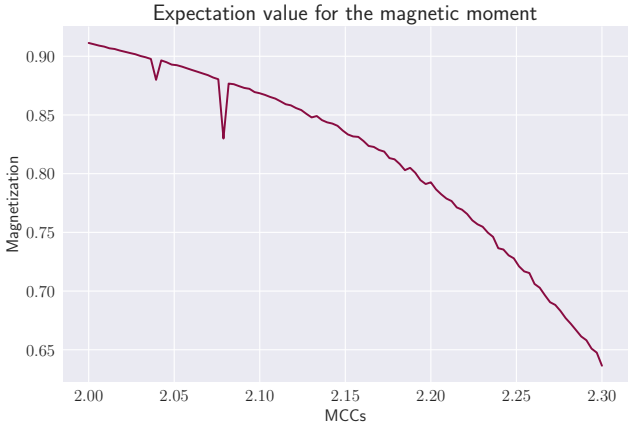

Figure 16. The figure displays the expectation value of the magnetization (magnetic moment) as function of temperature for MCC = 1,000,000.

Different values of T_C. Need to add table in results. The obtained values of T_C in table... is in agreement with what we would expect, as the difference between the numerical and analytical value of T_C decreases with the the increasing MCCs.

VII. CONCLUSION

We have utilized the Ising model in two dimension, for different lattice sizes, $L \times L$, in order to study a phase transition from a magnetic phase to a phase with zero magnetization (eller motsatt?). Together with the Metropolis algorithm, the Ising model has allowed us to calculate the mean energy E, magnetization M, the specific heat C_V and the susceptibility χ as function of temperature T. We have found that the numerical calculated values to a large degree agreed with the values theoretically predicted. This agreement held for a

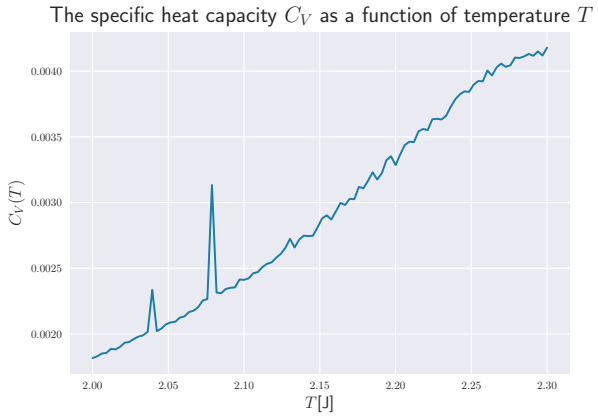

Figure 17. The figure displays the specific heat capacity as function of temperature for MCC = 1,000,000.

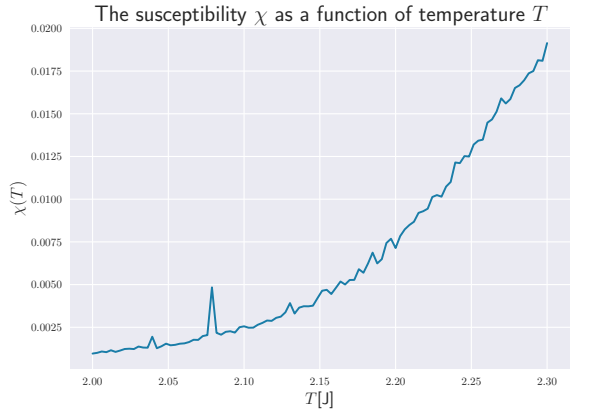

Figure 18. The figure displays the magnetic susceptibility as function of temperature for MCC = 1,000,000.

number of Monte Carlo cycles larger than 500 (dette må sjekkes). When turning up the lattice size to 20×20, we found that the number of Monte Carlo cycles needed in order to reach the most likely state were 10^4 for random spin orientation with $T = 1$ and both ordered and random spin orientation for $T = 2.4$. After this burning period, the system had reached its equilibrium situation. However, for ordered spin orientation with $T = 1$, the system were in its equilibrium state to begin with. Additionally, when studying the the total number of accepted configurations as function of the total number of Monte Carlo cycles, we found that accepted configurations increased as the temperature increased. For the 20×20 lattice, with 1 000 000 Monte Carlo cycles we observed that a phase transition took place at $T = -2.27$.

Furthermore when computing the probability $P(E)$ for the 20×20 lattice with $T = 2.4$, we found that the energy distribution had a Gaussian form, as predicted. For a lower temperature, $T = 1$, all particles is located in the lowest energy state, with $E = -800J$. As a result, the variance in energy for $T = 2.4$ is to a high extent larger than the variance in energy for $T = 1$.

GITHUB

All data, code and plots are available at our GitHub page: https://github.com/hedvigborgen/fys3150. Follow the README.md file in order to run the codes.

REFERENCES

- [1] Project 4 - FYS3150 (2020), M. H. Jensen, https://github.com/CompPhysics/ComputationalPhysics/blob/master/doc/Projects/2020/Project4/pdf/Project4.pdf

- [2]Project 1 - Solving the one dimensional Poisson Equation (2020), K. Sulebakk, A. Marthinussen, H. Reiersrud. https://github.com/hedvigborgen/fys3150/blob/master/project1/FYS3150___Project_1.pdf

- [3] Parallel Algorithms (date unknown), G. E. Blelloch and B. M. Maggs, Carnegie Mellon University, https://www.cs.cmu.edu/~guyb/papers/BM04.pdf

- [4] "Monte Carlo Methods in Statistical Physics"(1999), Newman M. E. J., Barkema G. T., Clarendon Press.

- [5] Ising lattice simulation (Oct. 2015) https://www.ibiblio.org/e-notes/Perc/ising.htm

VIII. ACKNOWLEDGEMENTS

Thanks to all the very helpful group teachers for investigating some very intricate problems in our code.

IX. APPENDIX

Appendix A: Deviation of the analytical results for L = 2 × 2

In order to obtain the analytical results for 2×2 number of lattice points, we will use the configurations presented in figure 19. The magnetization and energies are

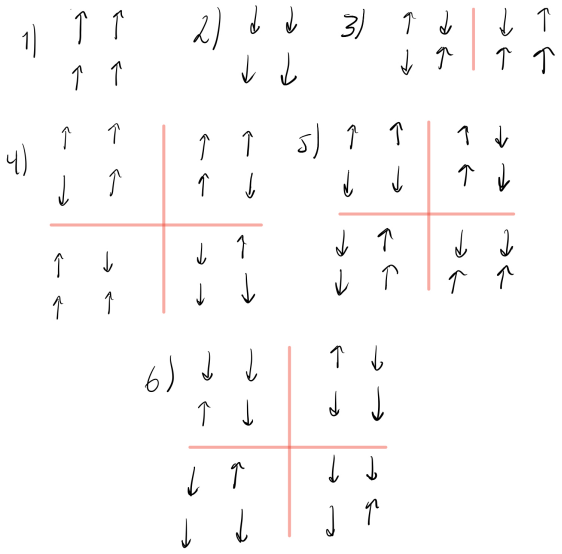

Figure 19. The spin configuration for a 2 × 2 lattice size. 1) and 2) have degeneracy 1, 3) two-fold degeneracy and 4), 5) and 6) have a four-fold degeneracy.

obtained by equations 2 and 1. We start by using equation 3 in order to calculate the analytical value of the partition function. It reads,

$$\sum_{i}^{L\times L} e^{E_i\beta} = e^{8J\beta} + 4e^{0} + 4e^{0} + 4e^{0} + 2e^{-8J\beta} + e^{8J\beta} = 12 + 2e^{8J\beta} + 2e^{-8J\beta} = 12 + 4\cosh(8J\beta).$$

For the expectation value of magnetization, we will use equations 2 and 7. It yields,

$$\langle M\rangle = \frac{1}{Z}\sum_{i}^{L\times L} M_i e^{E_i\beta} = \frac{1}{Z}(4e^{8J\beta} + 4\cdot 2e^{0} + 4\cdot 2e^{0} + 4e^{-8J\beta}) = \frac{16 + 4e^{8J\beta} + 4e^{8J\beta}}{12 + 4\cosh(8J\beta)} = 2\frac{2 + e^{8J\beta}}{3 + \cosh(8J\beta)}.$$

In addition, the expectation value for the squared magnetization is expressed in the same way as in equation 7 by switching out M_i by M_i^2. This results in,

$$\langle M^2\rangle = \sum_{i}^{L\times L} \frac{M_i^2 e^{-E_i\beta}}{Z} = \frac{1}{Z}(4^2e^{8J\beta} + 4^2\cdot 2e^{0} + 4^2e^{-8J\beta}) = 8\frac{1 + e^{8J\beta}}{3 + \cosh(8J\beta)}.$$

We calculate the analytical expectation value of energy by equation 8.

$$\langle E\rangle = \sum_{i}^{L\times L} \frac{E_i e^{-E_i\beta}}{Z} = \frac{1}{Z}(-8\cdot 2e^{8J\beta} + 8\cdot 2e^{-8J\beta}) = -16J/4\frac{e^{8J} - e^{-8J}}{3 + \cosh(8J\beta)} = -8J\frac{\sinh(8J\beta)}{3 + \cosh(8J\beta)}.$$

We arrive at the squared expectation value of the energy in the same matter as for squared magnetization.

$$\langle E^2\rangle = \sum_{i}^{L\times L} \frac{E_i^2 e^{-E_i\beta}}{Z} = \frac{1}{Z}((-8)^2\cdot 2e^{8J\beta} + 8^2\cdot 2e^{-8J\beta}) = \frac{64J^2}{4}\frac{e^{8J} + e^{-8J}}{3 + \cosh(8J\beta)} = 64J^2\frac{\cosh 8J\beta}{3 + \cosh(8J\beta)}$$

As for the heat capacity C_V and susceptibility χ we use equations 9 and 10 and the results above to achieve the analytical results.

$$C_V = \frac{\beta}{T}(\langle E^2\rangle - \langle E\rangle^2) = \frac{\beta}{T}(64J^2\frac{\cosh(8J\beta)}{3 + \cosh(8J\beta)} - (-8J)^2(\frac{\sinh(8J\beta)}{3 + \cosh(8J\beta)})^2) = \frac{64J^2}{\beta}\frac{3\cosh(8J\beta) + \cosh^2(8J\beta) - \sinh(8J\beta)}{(3 + \cosh(8J\beta))^2} = \frac{64J^2}{\beta}\frac{3\cosh(8J\beta) + 1}{(3 + \cosh(8J\beta))^2}$$

$$\chi = \beta(\langle M^2 \rangle - \langle M \rangle^2) =$$
$$\beta\Big[8\frac{1+e^{8J\beta}}{3+\cosh(8J\beta)} - \Big(2\frac{2+e^{8J\beta}}{3+\cosh(8J\beta)}\Big)^2\Big] =$$
$$4\beta\Big[\frac{2(1+e^{8J\beta})(3+\cosh(8J\beta)) - (2+e^{8J\beta})^2}{(3+\cosh(8J\beta))^2}\Big] =$$
$$4\beta\frac{3+2e^{8J\beta}+\cosh(8J\beta)}{(3+\cosh(8J\beta))^2}$$