The study of phase transitions by use of the 2D Ising model

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This article aims to study phase transitions in the two-dimensional Ising model. The analytical mathematical framework is demonstrated on a 2×2 lattice system with periodic boundary conditions before a combined C++ and Python program is written with the purpose of performing numerical analysis for greater $L\times L$ systems. The exponential term of the Boltzmann distribution is calculated in advance in order to increase the efficiency of the numerical analyses. The program uses a Monte Carlo approach with the Metropolis algorithm, and is verified using the exact analytical results from the 2×2 system and then applied to $L\in\{20,40,60,80,100\}$ lattices. The numerical analysis determines the number of Monte Carlo cycles required before the system reaches its equilibrium, and returns the mean energy $\langle E\rangle$, the mean magnetisation $\langle M\rangle$, the specific heat capacity C_V and the susceptibility χ as functions of temperature. The final part of the numerical analysis is determining the critical temperature, T_C, of the system.

Certain issues is encountered regarding the variance in energy and magnetisation for larger $L\times L$ lattices causing in inaccuracies in the studies of particularly the specific heat capacity and the susceptibility, and resulting in a less than optimal analysis of the critical temperature. These issues and possible causes are discussed.

I. INTRODUCTION

We want to study phase transitions in a magnetic system using the Ising model in two dimensions. We will study different $L\times L$ lattices at given temperatures T. The Ising model shows a phase transition from a magnetic phase to a non-magnetic phase (zero magnetisation). The lattice used in the Ising model is a binary system, in that each individual object in the system can only take two values. In this report we will use that the objects in the system is either spin up or spin down, with corresponding values of +1 or -1 respectively. This is an highly popular model, as it gives a fairly good understanding of phase transitions, and is therefore interesting to study. When simulating the system, we will be using Monte Carlo simulations with the Metropolis algorithm. This algorithm is a method for obtaining random numbers from a probability distribution which is difficult to directly sample from.

We want to write a code containing both analytical expressions and a numerical analysis. We want to investigate how long it takes before the system reaches equilibrium, know as the the "burn in time" (or equilibration time) by counting the number of Monte Carlo simulations needed to reach the equilibrium state, in order to figure out when to start the evaluation of expectation values in the analysis. Further on, we will perform calculations on lattices of different sizes for a temperature range, and plot the mean energy $\langle E\rangle$, mean magnetisation $\langle M\rangle$, specific heat capacity C_V and susceptibility χ as functions of temperature, in order to see indication of a phase transition in the system. Lastly, we calculate the critical temperature and compare with the exact value from Lars Onsager.

II. METHOD

2D Ising model

The energy, without an externally applied magnetic field, of the Ising model for a two dimensional lattice, is expressed as,

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

where $s_k=\pm1$, N is the total number of spins and J is a constant expressing the strength of the interaction between neighboring spins. We only want to sum over the nearest neighboring spins, and only count each spin once, this is what we mean by $\langle kl\rangle$ in the sum in expression (1). From this point we use dimensionless quantities where J and the Boltzmann constant k_b is equal to 1 and the temperature is given in units of kT/J. We will use the Metropolis algorithm only and periodic boundary conditions.

A. Benchmark calculations

We want to find analytical expressions for a few quantities in order to compute benchmark calculations for our numerical calculations. We find in the literature that the analytical expression for the partition function is

$$Z=\sum_i e^{-\beta E_i}, \tag{2}$$

where β is $1/k_bT$, but becomes $1/T$ with our dimensionless units, and i is the number of spin configurations.

We also want to find the analytical expressions for the expectation values for the mean energy $\langle E \rangle$, the mean absolute value of the magnetic moment $\langle |M| \rangle$ (which we will refer to as the mean magnetisation), the susceptibility χ and the specific heat C_V as functions of T. All these expressions and calculations are found in the appendix (section V).

B. 2×2 lattice

We start of assuming we have a 2×2 lattice, i.e. two spins in each dimension L=2. From the literature we have that

$$\Delta E = 2s_k^1 \sum_{\langle j \rangle}^{N} s_j, \tag{3}$$

$$M_2 = M_1 + 2s_k^2, \tag{4}$$

where the numeral indices in M_1, M_2, s_k^1 and s_k^2 indicates the spin state before and after a possible spin flip. There are only five possible values for this energy difference ΔE for the 2D Ising model. This is independent of L and we therefore want to determine these so that we later can encode the energy differences in the Boltzmann distribution more efficiently. We start with the Boltzmann distribution given as,

$$P_i(\beta) = \frac{e^{-\beta E_i}}{Z}, \tag{5}$$

from the literature, where Z is the partition function presented in Eq.(2).

We then show how we determine the five values of ΔE, by looking at a spin flip. As the spin has binary values

$$s_k^\mu \to s_k^\nu = -s_k^\mu, \tag{6}$$

where the upper indices indicate the state of the spin before and after a flip. Using equations (1) and (3) we find that the expression for ΔE is

$$\begin{aligned} \Delta E &\equiv E_\nu - E_\mu, \\ \Delta E &= -\Big(\sum_{\langle kj \rangle} s_k^\nu s_j^\nu - \sum_{\langle kj \rangle} s_k^\mu s_j^\mu \Big), \\ \Delta E &= -\sum_{\langle kj \rangle} s_j^\mu (s_k^\nu - s_k^\mu). \end{aligned} \tag{7}$$

We know that $s_k^\nu = -s_k^\mu$, so we get that $s_k^\nu - s_k^\mu = -2s_k^\mu$, and we can generalize Eq.(7) and get

$$\Delta E = 2s_k^\mu \sum_{\langle kj \rangle} s_j^\mu, \tag{8}$$

where we find that $\sum s_j^\mu$ can only be 4,2,0,-2 and -4, depending on how many of the spins are up or down, and since we multiply this by $2s_k^\mu$ we get that

$$\Delta E \in \{8, 4, 0, -4, -8\}, \tag{9}$$

where the s_k^μ only decides the sign since it is either +1 or -1.

C. Exponential term in Boltzmann distribution

Now that we have the five possible values for ΔE, in order to make the code more efficient by avoiding calculating the exponential term in the Boltzmann distribution each time we update the energy, we want to find a way to calculate this in advance so that we later can retrieve them from a list. We can look at the ratio between $P(E_\nu)/P(E_\mu)$,

$$\begin{aligned} P(\Delta E) &= \frac{P(E_\nu)}{P(E_\mu)}, \\ &= \frac{e^{-E_\nu \beta}/Z}{e^{-E_\mu \beta}/Z}, \\ &= e^{-E_\nu \beta} e^{E_\mu \beta}, \\ &= e^{-\Delta E \beta}, \end{aligned} \tag{10}$$

and inserting the five known values for ΔE from expression (9), so we get that the exponential terms calculated in advance for the energy difference in the Boltzmann distribution is

$$e^{-\Delta E \beta} \in \{e^{8\beta}, e^{4\beta}, e^0, e^{-4\beta}, e^{-8\beta}\}. \tag{11}$$

D. Periodic boundary conditions

We also need to implement periodic boundary conditions. As previously mentioned, when we calculate the energy we only want to sum over the nearest neighboring spins, and only count the interaction between two spin particles once, i.e when we calculate the energy for say the first spin, we only need to look at the spin to the right and below. Thus, when we get to the spins in the right column, we say that the spin to the right is the same as the first spin in that same row. When we look at spins in the bottom row, we say that the spin below is the same as the top spin in that same column. Generally, these spins can be expressed as,

$$\text{Spin to the right of the lattice :} \quad s_{L,j} = s_{0,j}, \tag{12}$$

$$\text{Spin below the lattice :} \quad s_{i,L} = s_{i,0}, \tag{13}$$

where $i = 0, 1, 2, ...$ is the column number, $j = 0, 1, 2, ...$ is the row number and L is the number of elements in each row and column.

There are a number of ways to implement such boundary conditions, the simplest would be to use if tests. However, this is a very inefficient method, computationally speaking. Another way to implement the periodic boundary conditions is to use an index array. By flattening the lattice matrix the indices goes from 0 to L, so we get an index array looking like

$$\text{Index array} = [L, 0, 1, 2, ..., L-2, L-1, L, 0].$$

Looping through this array is much faster than looping through x- and y-direction and using if tests to check for boundaries.

E. Numerical analysis - Monte Carlo

Now that we have presented and computed all the analytical expressions and boundary conditions we also want to perform a numerical analysis. We want to perform Monte Carlo simulations on a lattice initially ordered or disordered, meaning that either all the spins are initially pointing up or they are randomly designated as +1 or -1, and figure out how many Monte Carlo simulations we need in order to reach the most likely state, that is how many simulations we need before the system reaches an equilibrium state.

We want to compute the mean energy, mean magnetisation, the specific heat capacity and the susceptibility as functions of T using periodic boundary conditions for $L = 2$ in the x and y directions. This we want to do in order to compare the results with the analytical expressions presented in the appendix (section V).

F. The Metropolis Algorithm

The Metropolis algorithm calculate the change in energy and magnetisation by randomly flipping spins. The algorithm will either accept a proposed spin flip or not. The criterion for a spin flip to be accepted is either that the change in energy is smaller than zero, $\Delta E < 0$, or that a random number, N_{random}, between 0 and 1 is smaller than the exponential term in the Boltzmann distribution, $N_{random} < e^{-\beta\Delta E}$. If either of these are true, then the spin will get an opposite sign and the change in magnetisation will be calculated by use of Eq.(4). If the situation is otherwise, the spin flip will not be accepted and the change in energy will be zero.

After we have looked at a 2×2 lattice with $T = 1.0$, we want to evaluate a larger lattice system. First we will study a system with $L = 20$, with temperatures $T = 1.0$ and $T = 2.4$, initiated both randomly and ordered. We investigate the number of Monte Carlo cycles needed in order to reach equilibrium by studying and plotting the mean energy and magnetisation. To determine the "burn in time" needed to reach equilibrium, we first compute the energies of the system for a large number of Monte Carlo cycles, $N = 10^6$. We determine the standard deviation of the energies by evaluating only the values computed after the system reaches a lower energy than the median energy. We then determine the time the system reaches equilibrium to be when the system reaches an energy within 1σ of the median energy.

G. Probability distribution

Finding the probability of an energy state in the system numerically is fairly straight forward. The number of times a given energy appears during the Monte Carlo cycles is summed up, and then divided by the total number of Monte Carlo cycles

$$P(E_i) = \frac{\sum_{n=1}^{N_{MC}} \delta_{l(n)i}}{N_{MC}}, \tag{14}$$

where N_{MC} is the total number of Monte Carlo cycles and $l(n)$ is the state-number of the lattice after Monte Carlo cycle n. In other words, if the probability calculated is that of the energy state E_5, then the Kronecker-delta will only contribute to the sum if the energy state after n cycles is $E_5 \Rightarrow l(n) = 5$.

The expectation value for energy is then determined numerically using

$$\langle E \rangle = \sum_i E_i P(E_i). \tag{15}$$

H. Numerical studies of phase transitions

We can study phase transitions by looking at physical quantities near the critical temperature T_C. The spins become more and more correlated as T approaches T_C, so the correlation length ξ, which is always proportional to the size of the finite lattice we are limited to, increases as we get closer to T_C. Through finite size scaling relations, we can relate the behavior of the finite lattices with results from an infinitely large lattice. We can then express the critical temperature as

$$T_C(L = \infty) = T_C(L) - aL^{-1/\nu}, \tag{16}$$

where a is a constant which we choose to be 1 and we set $\nu = 1$ in order to make an estimation of T_C when $L \to \infty$.

We will build on the methods already described and first study the behaviour of the Ising model around the critical temperature for lattices of sizes (40×40), (60×60), (80×80) and (100×100). The temperature range evaluated will be $T \in [2.1, 2.4]$ with

a step size of $\Delta T = 0.005$. The burn in time used for these calculations is found by determining the burn in time of a lattice with $L = 100$ and $T = 2.4$, and assuming this to be the largest bunr in time of all the cases. The number of cycles is found to be $2 \cdot 10^5$ and is applied to all the cases. After these calculations have been performed, we want to plot $\langle E \rangle$, $\langle |M| \rangle$, C_V and χ as functions of temperature. This we want to do in order to see if we can observe any indication of a phase transition. These calculations are expected to require some time so ideally, we should parallelize the code to improve efficiency, however we choose not to do so in this report.

At last, we will look at lattices of different dimensions, $L = 40$, 60, 80 and 100, compare the results we obtain by use of Eq.(16) and $\nu = 1$ with the exact result for T_C after Lars Onsager, which is

$$\frac{kT_C}{J} = \frac{2}{\ln(1+\sqrt{2})} \approx 2.269. \tag{17}$$

III. RESULTS

	$\langle E \rangle$	$\langle M \rangle$	C_V	χ
Analytical	-7.98392	3.99464	0.12833	15.97322
Numerical	-7.98376	3.99458	0.12966	15.96887

TABLE I. Numerical and analytical calculations of $\langle E \rangle$, $\langle M \rangle$, C_V and χ for a lattice of size (2×2) with $T = 1.0$.

The numerical calculation of the mean energy $\langle E \rangle$, mean magnetisation $\langle M \rangle$, specific heat capacity C_V and susceptibility χ for a 2×2 lattice with $T = 1.0$ is presented in table I. Approximately 10^5 number of Monte Carlo simulations are required before the numerical calculations match the analytical results.

Next, we evaluate a lattice of size (20×20) for various temperatures and initial states.

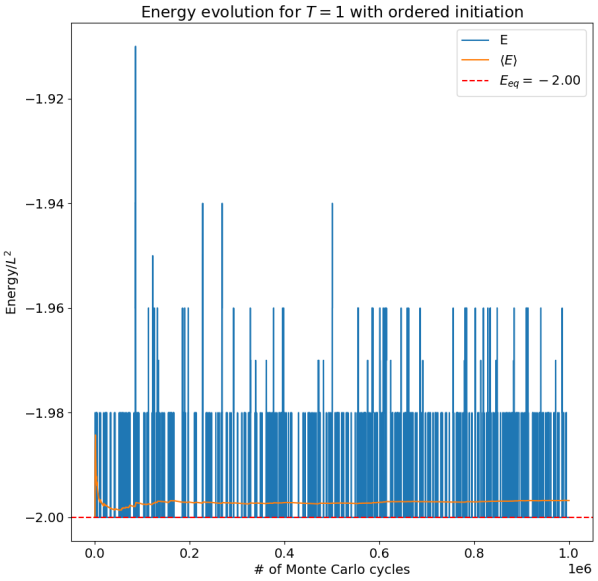

FIG. 1. Mean energy per spin for $L = 20, T = 1$ and an ordered initial state, as a function of Monte Carlo cycles performed.

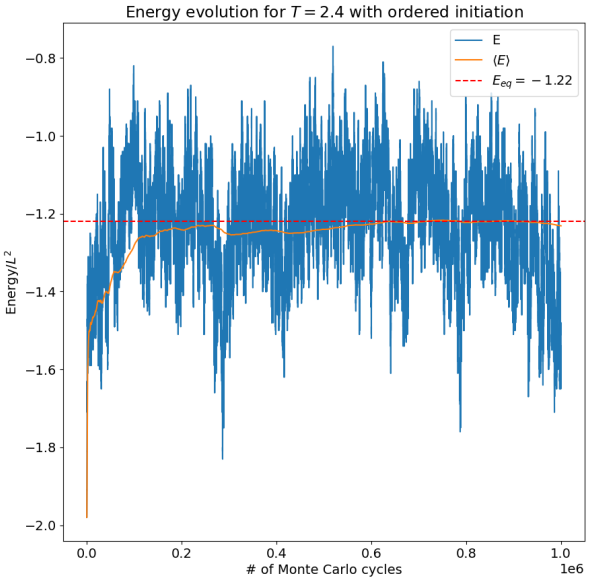

FIG. 2. Mean energy per spin for $L = 20, T = 2.4$ and an ordered initial state, as a function of Monte Carlo cycles performed.

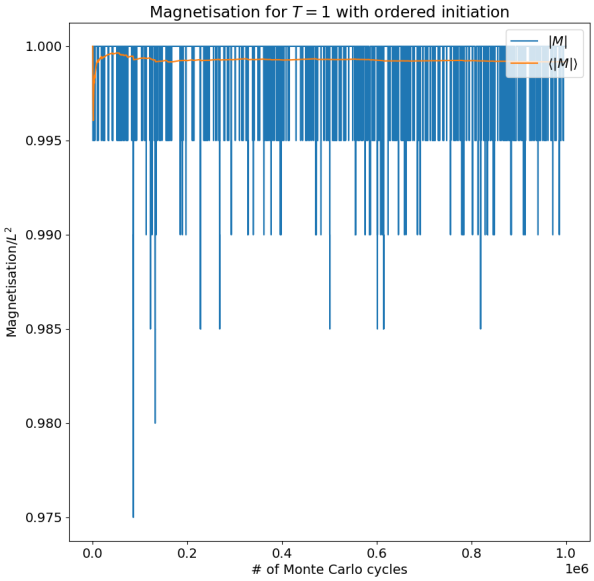

FIG. 3. Mean absolute magnetisation, $\langle|M|\rangle$ per spin for $L = 20, T = 1$ and an ordered initial state, as a function of Monte Carlo cycles performed.

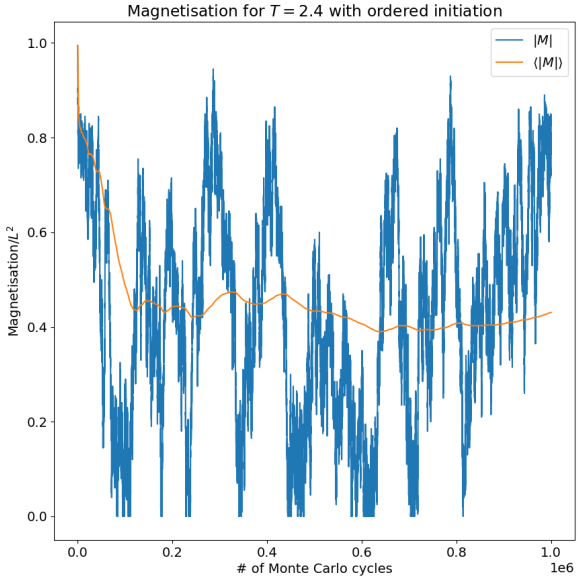

FIG. 4. Mean absolute magnetisation, $\langle|M|\rangle$ per spin for $L = 20, T = 2.4$ and an ordered initial state, as a function of Monte Carlo cycles performed.

In figures 1, 2, 3 and 4 we plot the mean energy and mean absolute magnetisation for a (20×20) lattice with $T = 1$ and $T = 2.4$, initialized with the spins ordered. The equilibrium energy per spin is -2.00 when $T = 1.0$ and -1.22 when $T = 2.4$.

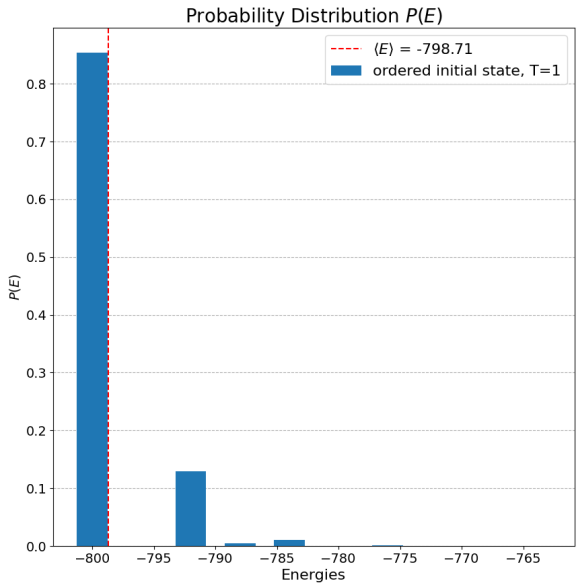

FIG. 5. Probability distribution for the energy for $L = 20, T = 1$ and an ordered initial state, as a function of Monte Carlo cycles performed.

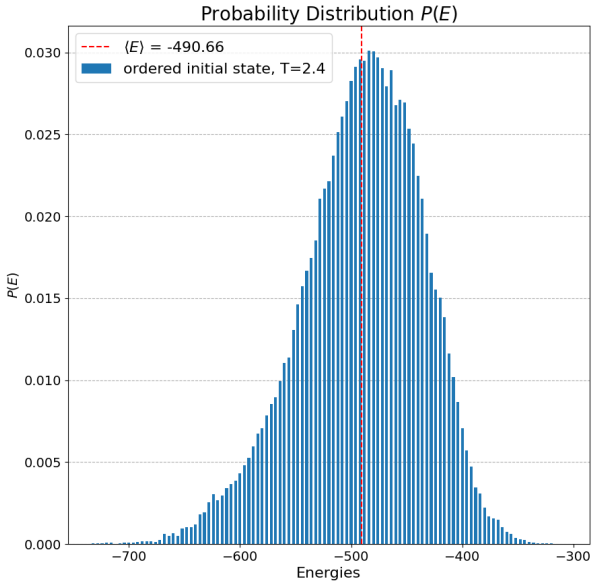

FIG. 6. Probability distribution for the energy for $L = 20, T = 2.4$ and an ordered initial state, as a function of Monte Carlo cycles performed.

In figures 5 and 6 we plot the probability distribution

of the energies for a (20×20) lattice with $T = 1.0$ and $T = 2.4$, initialized with the spins ordered.

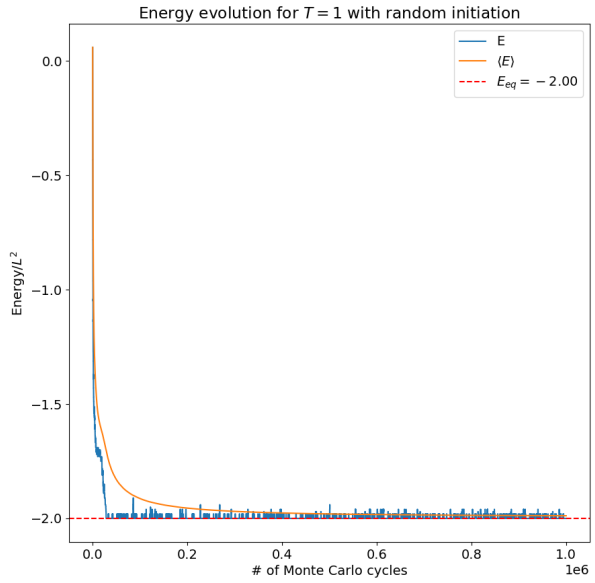

FIG. 7. Mean energy per spin for $L = 20, T = 1.0$ and a random initial state, as a function of Monte Carlo cycles performed.

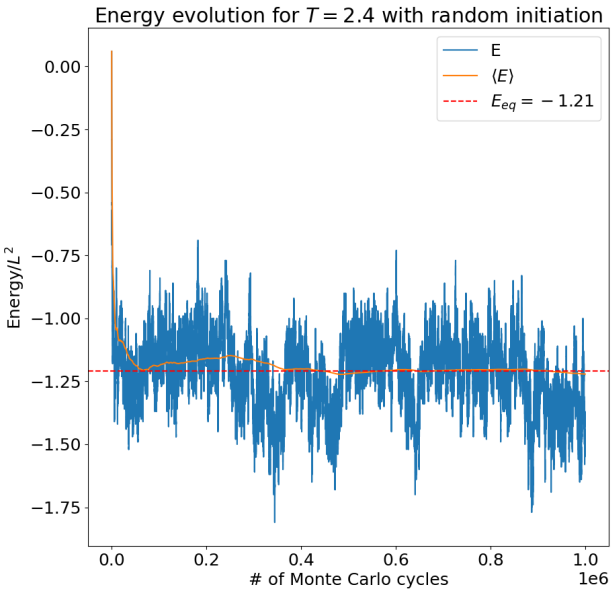

FIG. 8. Mean energy per spin for $L = 20, T = 2.4$ and a random initial state, as a function of Monte Carlo cycles performed.

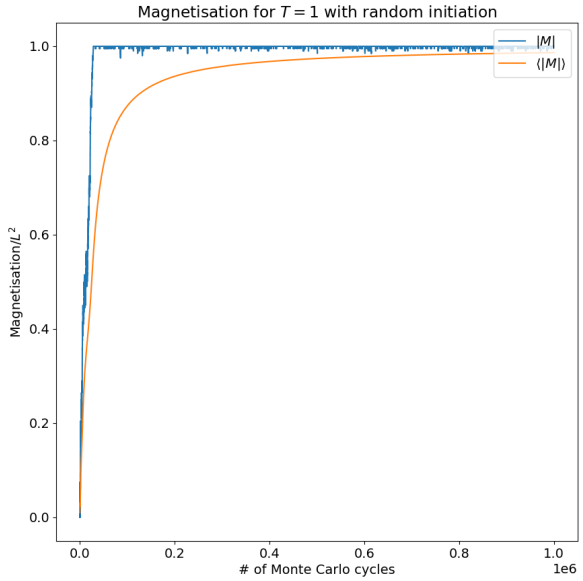

FIG. 9. Mean absolute magnetisation, $\langle |M| \rangle$ per spin for $L = 20, T = 1.0$ and a random initial state, as a function of Monte Carlo cycles performed.

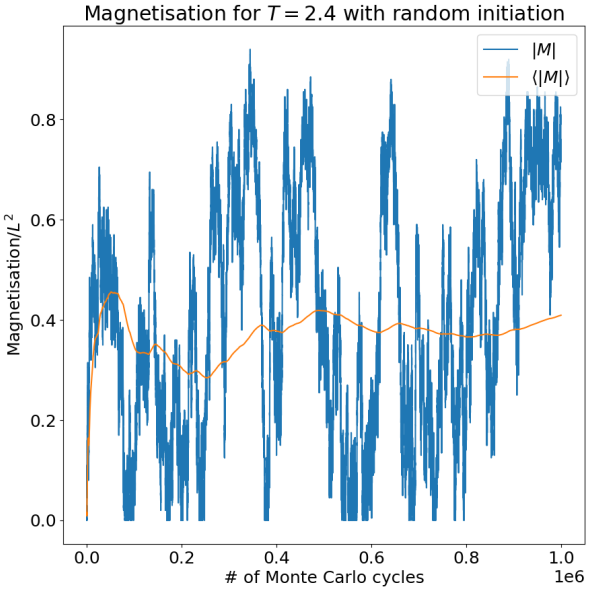

FIG. 10. Mean absolute magnetisation, $\langle |M| \rangle$ per spin for $L = 20, T = 2.4$ and a random initial state, as a function of Monte Carlo cycles performed.

In figures 7, 8, 9 and 10 we plot the mean energy and mean magnetisation for a (20×20) lattice with $T = 1$ and $T = 2.4$, initialized with the spins randomly oriented.

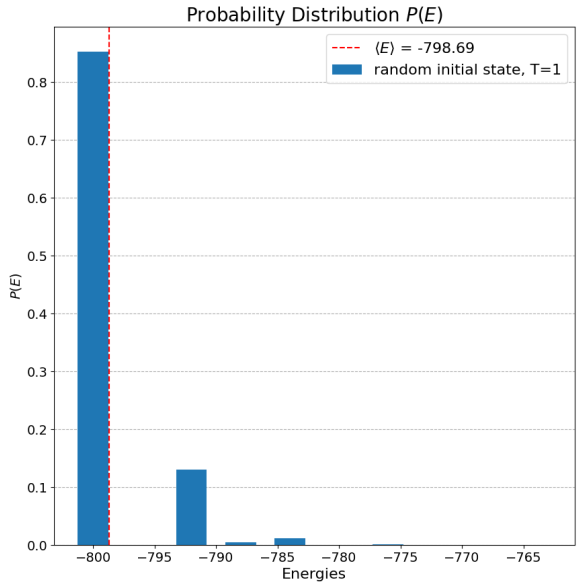

FIG. 11. Shows the probability distribution $P(E)$ for $L = 20$, $T = 1$ with a disordered initial state and a burn in period of 28 332 MC cycles. The expectation value $\langle E \rangle$ is found to be $-798.69J$.

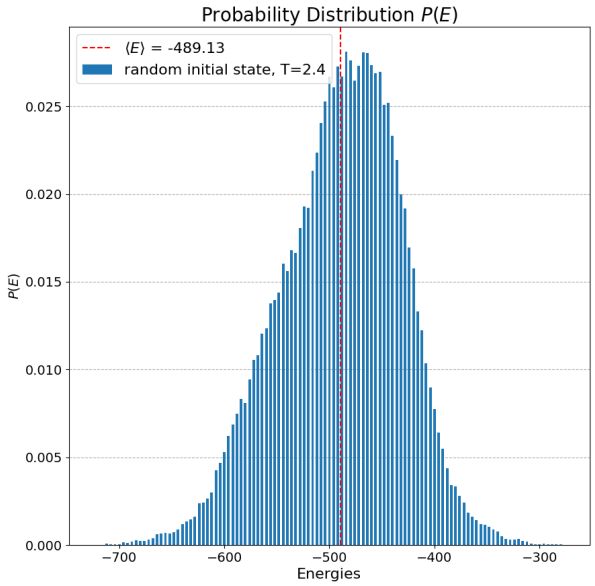

FIG. 12. Shows the probability distribution $P(E)$ for $L = 20$, $T = 2.4$ with a disordered initial state and a burn in period of 5483 MC cycles. The expectation value $\langle E \rangle$ is found to be $-489.13J$

In figures 11 and 12 we plot the the probability distribution of the energies for a (20×20) lattice with $T = 1.0$ and $T = 2.4$, initialized with the spins randomly oriented.

	Random	Ordered
$T = 1$	3.3	3.3
$T = 2.4$	57.6	54.3

TABLE II. The standard deviations of the energies calculated for a lattice of size (20×20)

The standard deviations of the energy of a system in equilibrium are computed for all variations mentioned in the (20×20) lattice. We present the result in table II.

	Random	Ordered
$T = 1$	28332	0
$T = 2.4$	5483	20402

TABLE III. Burn in times for the variations of the (20×20) lattice

The burn in times computed using the method described in the methods section for the variations of the (20×20) are presented table III.

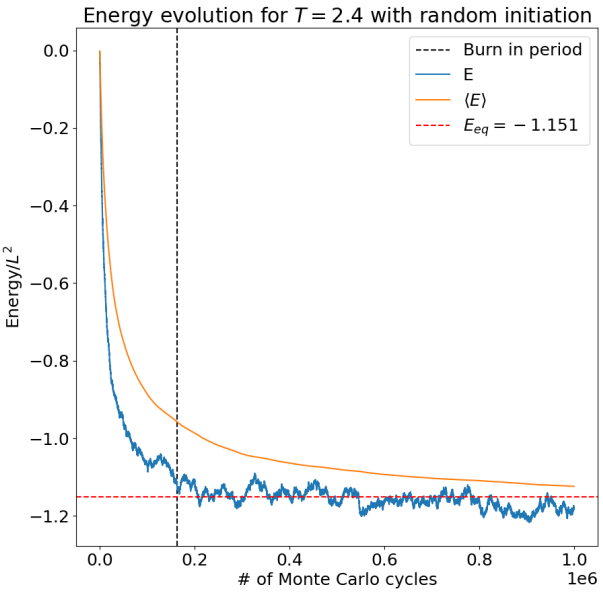

FIG. 13. Energy per spin evolution, and illustration of burn in period.

Figure 13 presents energy per spin values computed for a (100×100) lattice and $T = 2.4$. The burn in time needed for the system to reach equilibrium is determined to be $\sim 2 \cdot 10^5$ Monte Carlo cycles.

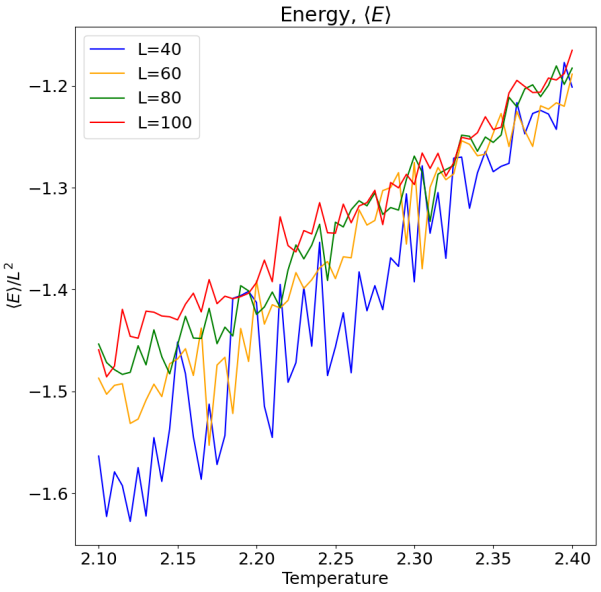

FIG. 14. Mean energy per spin for various lattice sizes as a function of temperature.

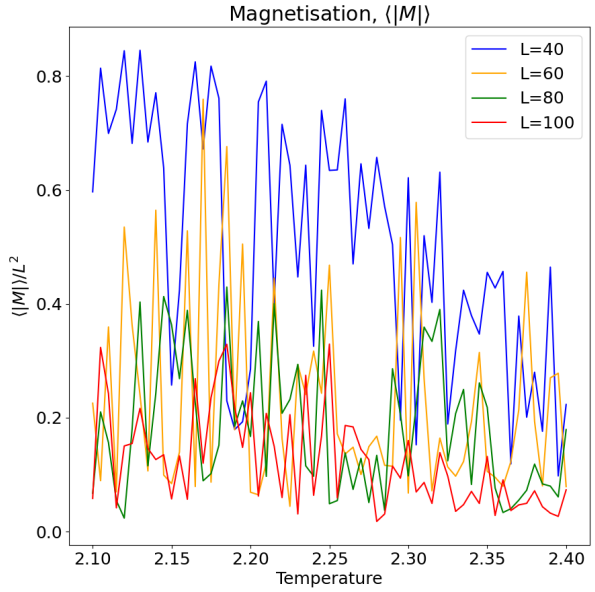

FIG. 15. Mean magnetisation, $\langle |M| \rangle$ per spin for various lattice sizes as a function of temperature.

Figures 14 and 15 presents the computed mean energy and mean magnetisation for lattice sizes (40×40), (60×60) and (80×80) and (100×100) in the temperature range $T \in [2.1, 2.4]$ with a step size of $\Delta T = 0.005$. We used a burn in time of $n = 2 \cdot 10^5$ and ran the system for $5 \cdot 10^5$ Monte Carlo cycles.

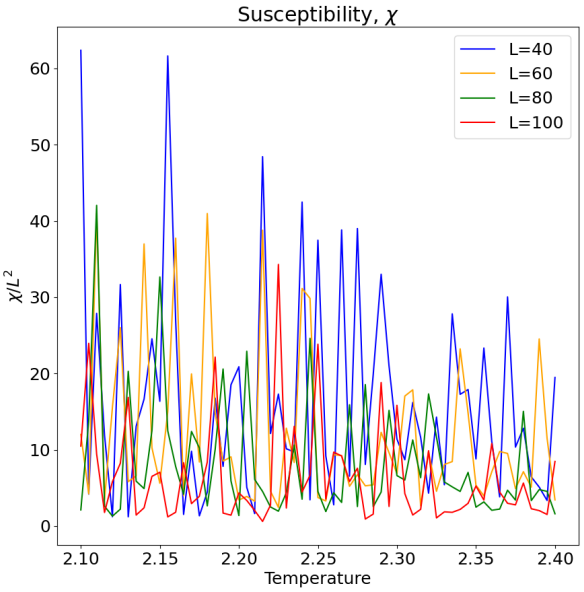

FIG. 16. Susceptibility per spin for various lattice sizes as a function of temperature.

The susceptibility is computed using Eq.(20) and plotted in figure 16 for various lattice sizes and temperatures.

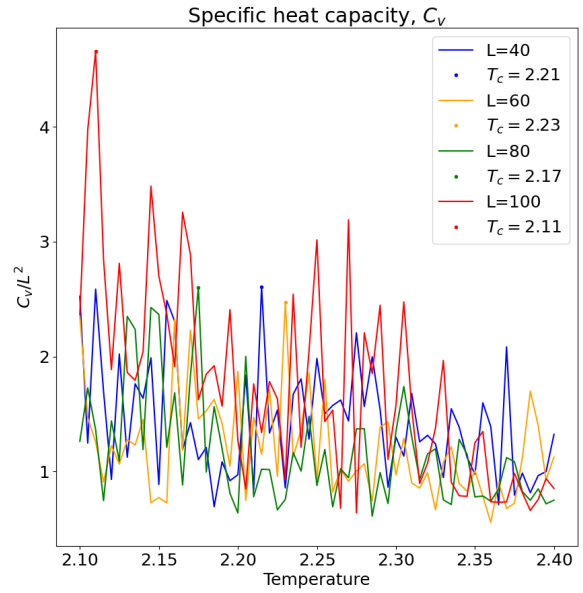

FIG. 17. Heat capacity per spin for various lattice sizes as a function of temperature.

The specific heat capacity is computed using Eq.(21) and

presented in figure 17 for various lattice sizes and temperatures.

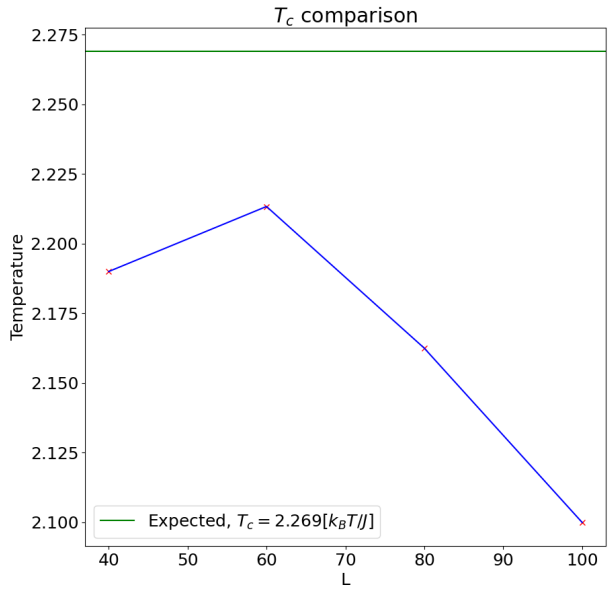

FIG. 18. Estimated critical temperature for a lattice of size $L \to \infty$

The critical temperature for each lattice size is determined to be where the specific heat capacity in figure 17, is at its maximum. Using these temperatures we estimate the critical temperature for the model in the limit $L \to \infty$ using the relation (16).

IV. DISCUSSION AND CONCLUSION

When looking at the numerical calculations of the mean energy $\langle E \rangle$, mean magnetisation $\langle M \rangle$, specific heat capacity C_V and susceptibility χ for a lattice with $L = 2$ and $T = 1.0$, we observe that they correspond well with the analytical calculations when the number of Monte Carlo cycles reaches around 10^5, indicating that the algorithm works.

In figure 1 where we present the mean energy for a $L = 20$, initially ordered lattice with $T = 1.0$, we observe that the system starts in equilibrium. The number of Monte Carlo cycles needed for this lattice to reach equilibrium is found to be 0 and is consistent with the observation. The system starting in equilibrium is a consequence of the lattice initially being ordered, which is also the lowest possible energy state, and that a temperature as low as $T = 1$ has a very low equilibrium energy. When comparing this plot with figure 2, we observe that the equilibrium energy is no longer the minimal energy of the system. This indicates that the equilibrium energy increases with temperature. We also observe the same regarding the equilibrium energy in figure 7 and 8.

In table II we see that the energy computed with $T = 1$ has a very small standard deviation compared to the results from the $T = 2.4$ computations. Figures 5 and 11 illustrates the reason for this; there is no possible states lower than the equilibrium values. The standard deviations of the energy for $T = 2.4$ are significantly larger, but consistent with expectations drawn from figures 6 and 12. Figure 13 illustrates how the burn in time is determined.

The mean energies in figure 14 indicate a trend of higher equilibrium energies for higher temperatures for all the lattice sizes evaluated. The mean energies as a function of temperature are on an expected order of magnitude, but the variance is significantly larger than expected. The mean absolute magnetisation in figure 15 show similar characteristics, but the variations seem to be more significant. The variation as a function of temperature in the mean energy and mean magnetisation will have consequences for the following computations of the susceptibility and specific heat capacity, as they depend on the two former. Figures 16 and 17 has the correct orders of magnitude, but has none of the other characteristics expected. A phase transition is characterized by the diverging of the susceptibility and heat capacity around the critical temperature and we expected an apex to form around this temperature. Because of this lack of an apex characterizing the critical temperature, the estimated values show no sign of containing a signal. The only reason the estimated critical temperature for $L \to \infty$ in figure 18 is even close to the expected temperature is because we evaluate such a small range of temperatures around the expected value.

Seeing as the algorithm produces values on the expected order of magnitude we suspect the error to be located somewhere in the implementation of the algorithm. It was attempted to up the number of Monte Carlo cycles as well as the burn in times, but these attempts were not successful in improving the results and indicates an inherent problem with the implementation of the algorithm. In addition to correct the errors, it would be useful to explore a more efficient way of performing the computations. One possibility would be to parallelise the implementation of the algorithm.

In conclusion, the results of C_V and χ is useless in indicating a temperature corresponding to phase transitions in the lattices evaluated using the Metropolis algorithm. The apparent consistency of the energies up to 10^6 Monte Carlo cycles for one lattice size and one temperature makes it difficult to understand the significant variance as a function of temperature for the mean energy and mean absolute magnetisation.

V. APPENDIX

Following, the analytical expressions and calculations of the mean energy $\langle M \rangle$, the mean absolute value of the magnetic moment $\langle M \rangle$ (mean magnetisation), the susceptibility χ and the specific heat C_V as functions of T are presented. The calculations are performed by use of the values presented in table IV.

$N_\uparrow$	d	E	M	$\lvert M \rvert$
4	1	-8	4	4
3	4	0	2	2
2	4	0	0	0
2	2	8	0	0
1	4	0	-2	2
0	1	-8	-4	4

TABLE IV. An overview over possible spin combinations in a 2×2 lattice. N is the number of spins up, d is the degree of degeneracy, E is the energy, M is the magnetisation and $|M|$ is the absolute value of the magnetisation for each of the possible states

where N is the number of spins up, d is the number of possible ways to get this configuration of spins at the same energy level (degree of degeneracy), E is the energy calculated by use of Eq.(1), M is the mean magnetisation and $|M|$ is the absolute value of the mean magnetisation for each state.

The analytical expression for the partition function Z is presented in Eq.(2), and the Boltzmann distribution is presented in Eq.(5). We have that the mean energy and mean magnetisation is

$$\langle E \rangle = \sum_i E_i P_i(\beta) = \frac{1}{Z} \sum_i E_i e^{-\beta E_i}, \tag{18}$$

$$\langle M \rangle = \sum_i M_i P_i(\beta) = \frac{1}{Z} \sum_i M_i e^{-\beta E_i}, \tag{19}$$

that the susceptibility χ is

$$\chi = \frac{1}{T}\big(\langle M^2 \rangle - \langle M \rangle^2\big), \tag{20}$$

and that the specific heat capacity C_V is

$$C_V = \frac{1}{T^2}\big(\langle E^2 \rangle - \langle E \rangle^2\big). \tag{21}$$

By use of the values in Table 1, we get that

$$\begin{aligned} Z &= 1e^{8\beta} + 4e^0 + 4e^0 + 2e^{-8\beta} + 4e^0 + 1e^{8\beta} \\ &= 12 + 2e^{8\beta} + 2e^{-8\beta}, \end{aligned} \tag{22}$$

$$\langle M \rangle = \frac{1}{Z}\big(4e^{8\beta} + 8 - 8 - 4e^{8\beta}\big) = 0, \tag{23}$$

$$\begin{aligned} \langle |M| \rangle &= \frac{1}{Z}\big(4e^{8\beta} + 8 + 8 + 4e^{8\beta}\big) \\ &= \frac{1}{Z}\big(8e^{8\beta} + 16\big), \end{aligned} \tag{24}$$

$$\begin{aligned} \langle M^2 \rangle &= \frac{1}{Z}\big(16e^{8\beta} + 16 + 16 + 16e^{8\beta}\big) \\ &= \frac{32}{Z}\big(e^{8\beta} + 1\big), \end{aligned} \tag{25}$$

$$\begin{aligned} \langle E \rangle &= \frac{1}{Z}\big(-8e^{8\beta} + 16e^{-8\beta} - 8e^{8\beta}\big) \\ &= \frac{16}{Z}\big(e^{-8\beta} - e^{8\beta}\big), \\ &= \frac{-32}{Z}\sinh\big(8\beta\big), \end{aligned} \tag{26}$$

$$\begin{aligned} \langle E^2 \rangle &= \frac{1}{Z}\big(64e^{8\beta} + 128e^{-8\beta} + 64e^{8\beta}\big) \\ &= \frac{128}{Z}\big(e^{8\beta} + e^{-8\beta}\big), \\ &= \frac{256}{Z}\cosh\big(8\beta\big), \end{aligned} \tag{27}$$

which is benchmark calculations we need in order to calculate Eq.(20) and Eq.(21). We get sinh and cosh in the expressions for $\langle E \rangle$ and $\langle E^2 \rangle$ since we generally have that

$$\sinh(x) = \frac{e^x - e^{-x}}{2}, \tag{28}$$

$$\cosh(x) = \frac{e^x + e^{-x}}{2}. \tag{29}$$

The specific heat capacity C_V and the susceptibility χ is

$$C_V = \frac{256}{ZT^2}\Big(\cosh(8\beta) - \frac{4\sinh^2(8\beta)}{Z}\Big), \tag{30}$$

$$\chi = \frac{32e^{8\beta} + 32}{ZT}. \tag{31}$$