Exploring the 2D Ising model using Markov Chain Monte Carlo approach

Lars Opgård & Sunniva Kiste Bergan
(Dated: February 6, 2023)

We investigate the phase transition of the two-dimensional Ising model using the Markov Chain Monte Carlo (MCMC) method to sample expectation values for energy, magnetization, heat capacity, and susceptibility. We used a 2×2 lattice of spin configurations to compare the results from the MCMC cycles (eq. 28) with the analytical values (eq. 29), and found that they fit quite well with a relative error of less than 1%. We investigated the burn-in time (figure 2), and the probability function for the energy of the Ising model (figure 3), by using a 20×20 square lattice. Finally, the phase transition was found at the peak formed by the sampled heat capacity and susceptibility as a function of temperature for a given lattice size (figure 4). Using the critical temperatures $T_c(L)$ for a given lattice size, we could find an approximation for the critical temperature $T_c(L = \infty)$ for an infinite two-dimensional lattice. This was found from the intercept of the linear regression between the critical temperature $T_c(L)$ and the inverse of the lattice size L^{-1} (eq. 26). The critical temperatures we found for the lattice sizes (of lengths 40, 60, 80, 100) is $T_c(40) = 2.303J/k_B$, $T_c(60) = 2.304J/k_B$, $T_c(80) = 2.293J/k_B$ and $T_c(100) = 2.295J/k_B$. This gave us the approximate critical temperature $T_c(L = \infty) = 2.288$, which compared to the critical temperature Lars Onsager found $T_c(L = \infty) = 2.269$, gives a relative error of 0.8%.

https://github.com/sunnikbe/comfys/tree/main/Project4

I. INTRODUCTION

The Ising model[1] is a model for ferromagnetism in statistical mechanics. The model is based on a lattice of spins with discrete variables representing the magnetic dipole moment. The spins can point either up (+1) or down(−1), and each spin interacts with its nearest neighbor. The model have been used in numerous studies, where the most studied case is the ferromagnetic zero-field model on a d-dimensional lattice[3]. Studying the Ising model on a 2-dimensional lattice provides some insight into the phase transition, which can be observed at some critical temperature $T = T_c$, separating two distinct phases[1].

In the following section (section II), the Ising model and our numerical approach will be explained in more detail. Namely, the Markov Chain Monte Carlo (MCMC) method will be explained in subsection II A. Section III will present our results along with their meaning and importance before a conclusion is presented in section IV.

II. METHOD

As previously stated, the Ising model we will study consists of two-dimensional square lattices of spins. Each spin is given by $s_i = +1$ or $s_i = -1$. A lattice containing N spins will have a length L, giving the relation $N = L^2$.

[1] Or Lenz-Ising model after physicists Ernst Ising and Wilhelm Lenz.

To refer to the spin state of our entire system we will use the notation of vector $\mathbf{s}$, given by

$$\mathbf{s} = (s_1, s_2, ..., s_N). \tag{1}$$

The total energy of the system is given by

$$E(\mathbf{s}) = -J \sum_{\langle \mathrm{kl} \rangle}^{N} s_\mathrm{k} s_\mathrm{l}, \tag{2}$$

where J is a coupling constant expressing the strength of the interaction between each neighbouring pairs of spins[4]. In this report we will give the energy in units of J, that means that we can also give the temperature in units of J/k_B. $\langle \mathrm{kl} \rangle$ means that the sum goes over these neighbouring spins. The energy per spin is given by

$$\epsilon(\mathbf{s}) = \frac{E(\mathbf{s})}{N}. \tag{3}$$

We will use periodic boundary conditions on our lattice, meaning that all the spins will have four neighbours. With the absence of an external magnetic field the total magnetization of the system is given by

$$M(\mathbf{s}) = \sum_{i}^{N} s_i. \tag{4}$$

In the same way as we have the energy per spin (ϵ), the magnetization per spin will be given by

$$m(\mathbf{s}) = \frac{M(\mathbf{s})}{N}. \tag{5}$$

When studying the Ising model of a two-dimensional lattice, its useful to have a probability distribution

$$p(\mathbf{s}; T) = \frac{1}{Z} e^{-\beta E(\mathbf{s})}. \tag{6}$$

Here, the probability (p) will be given by the Boltzmann distribution for a given temperature T. β is the inverse temperature $\beta = 1/kT$ and Z is the partition function for the possible states of a mechanical system in thermal equilibrium

$$Z = \sum_{\text{all possible } \mathbf{s}} e^{-\beta E(\mathbf{s})}. \tag{7}$$

As we will calculate the total energy of our system using spins, which are unitless, we will use J as our energy unit.

Assuming a 2×2 lattice with periodic boundary conditions, all possible states can be listed as follows in table II.

Number of spins in state +1	Total energy	Total magnetization	Degeneracy
4	-8J	4	1
3	0	2	4
2	0	0	4
2	8J	0	2
1	0	-2	4
0	-8J	-4	1

TABLE I. Total energy, magnetization and degeneracy for a two-dimensional Ising model with a 2×2 lattice with periodic boundary conditions.

In order to test our numerical results, we want to find some analytical expressions for the 2×2 lattice using periodic boundary conditions. These include an expression for the partition function, some expectation values, the specific heat capacity C_V and the susceptibility χ of the system.

The partition function is given by equation 7. This can be rewritten using equation 2

$$Z_N = \sum_{s_1=\pm1} \cdots \sum_{s_N=\pm1} e^{\beta J \sum_{\langle \mathrm{kl}\rangle}^{N} s_\mathrm{k} s_\mathrm{l}}, \tag{8}$$

which is equal to

$$Z_N = \sum_{\text{all } \mathbf{s}} \prod_{\langle \mathrm{kl}\rangle}^{N} e^{\beta J s_k s_l}. \tag{9}$$

By introducing a transfer matrix $\hat{\mathbf{T}}$

$$\hat{\mathbf{T}} = \begin{bmatrix} e^{\beta J} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J} \end{bmatrix}, \tag{10}$$

the expression can be written as

$$Z_N = \sum_{\text{all } \mathbf{s}} \prod_{\langle \mathrm{kl}\rangle}^{N} \hat{\mathbf{T}}_{s_k s_l} = \sum_{\text{all } \lambda^N} \hat{\mathbf{T}}^N, \tag{11}$$

where the sum goes over all eigenvalues λ^N in $\hat{\mathbf{T}}^N$. For the simple 2×2 model, $\hat{\mathbf{T}}$ is diagonalized with

$$\begin{aligned} \lambda_1 &= 2cosh(\beta J) \\ \lambda_2 &= 2sinh(\beta J). \end{aligned} \tag{12}$$

We are left with the analytical partition function

$$Z_N = \lambda_1^N + \lambda_2^N = 2^N \left[(cosh(\beta J))^N + (sinh(\beta J))^N\right]. \tag{13}$$

For $N = 4$, the partition function is given by

$$Z = 4\left[cosh(8\beta J) + 3\right]. \tag{14}$$

The expectation value for the energy per spin $\langle\epsilon\rangle$, is given by

$$\langle\epsilon\rangle = \frac{1}{Z}\sum_{\text{all } \mathbf{s}} \epsilon(s) p(s,T), \tag{15}$$

where the sum goes over the energy per spin times the probability of the system state (at a given temperature) for all possible states $\mathbf{s}$. $1/Z$ is our chosen normalization, where Z is the partition function. By using the same approach as with the partition function, the expectation value for the energy per spin is given by

$$\langle\epsilon\rangle = \frac{\langle E\rangle}{N} = -\frac{16}{NZ}\left[2sinh(8\beta J)\right] \tag{16}$$

for our 2×2 lattice. The expectation value for the energy per spin squared $\langle\epsilon^2\rangle$ is

$$\langle\epsilon^2\rangle = \frac{\langle E^2\rangle}{N^2} = \frac{128}{N^2 Z}\left[2cosh(8\beta J)\right]. \tag{17}$$

The expectation value for the magnetization per spin is given by

$$\langle|m|\rangle = \frac{1}{Z}\sum_{\text{all } \mathbf{s}} m(s) p(s,T), \tag{18}$$

where the sum goes over the magnetization per spin times the probability of the system state (at a given temperature) for all possible states $\mathbf{s}$ normalized by $1/Z$. For our 2×2 lattice this yields the expectation value

$$\langle|m|\rangle = \frac{\langle|M|\rangle}{N} = \frac{8}{NZ}(e^{8\beta J} + 2), \tag{19}$$

for the magnetization per spin, and

$$\langle m^2\rangle = \frac{\langle M^2\rangle}{N^2} = \frac{32}{N^2 Z}(e^{8\beta J} + 4) \tag{20}$$

for the expectation value for magnetization per spin squared. We can also calculate the heat capacity C_V and susceptibility χ per spin from the equations

$$C_V = \frac{1}{N}\frac{1}{k_B T^2}\mathrm{Var}(E) = \frac{1}{N}\frac{1}{k_B T^2}\left(\langle E^2\rangle - \langle E\rangle^2\right), \tag{21}$$

and

$$\chi = \frac{1}{N}\frac{1}{k_B T}\mathrm{Var}(M) = \frac{1}{N}\frac{1}{k_B T}\left(\langle M^2\rangle - \langle|M|\rangle^2\right). \tag{22}$$

For our numerical approach, the MCMC method will be applied (see subsection II A). This algorithm will need

the Boltzmann factor $e^{-\beta\Delta E}$, where ΔE describes the energy difference in the system due to the flip of a single spin. For any arbitrary two dimensional lattice with $L > 2$, ΔE can only take one of five possible values. Computing an array of all the $e^{-\beta\Delta E}$ values and calling these should make the algorithm much more efficient compared to repeatedly calling the exponential function.

ΔE is given by

$$\Delta E = E_{\text{after}} - E_{\text{before}}. \tag{23}$$

Consider a spin in any $L > 2$ square lattice with periodic boundary conditions. Assuming that our chosen spin and all its immediate neighbours have spins $s = +1$, we get

$$\begin{aligned} E_{\text{before}} &= -4J \\ E_{\text{after}} &= 4J, \end{aligned} \tag{24}$$

where E_{after} is the energy after flipping our chosen spin. By equation 23, this yields $\Delta E_1 = 8J$, which is one of the five possible values. Repeating the same procedure with all possible variations of the neighbouring spins and flipping the middle one we get

$$\begin{aligned} \Delta E_2 &= 4J \qquad \Delta E_3 = 0 \\ \Delta E_4 &= -4J \qquad \Delta E_5 = -8J. \end{aligned} \tag{25}$$

By sampling expectation values for the energy and magnetization per spin, the heat capacity and susceptibility for different temperatures we can look for a phase transition. The phase transition we will look for in the Ising model happens at the critical temperature, and the critical temperature $T_c(L)$ can be found as the peak of the graph from the heat capacity and susceptibility as a function of temperature. Doing this for different size lattices we can approximate the critical temperature T_c for an infinitely large system. The critical temperature can be found from the relation

$$T_c(L) - T_c(L = \infty) = \alpha L^{-1} \tag{26}$$

If we look closely at the expression we can see that it follows a linear function $y = ax + b$, where $y = T_c(L)$ and $x = L^{-1}$. This then means that α is the slope and $T_c(L)$ is the intercept. Thus we can find the critical temperature from the intercept of a linear regression for $T_c(L)$ as a function of L. The critical temperature for an infinite 2D Ising model was found in 1944 by Lars Onsager and is expressed as followed

$$T_c(L = \infty) = \frac{2}{\ln\left(1 + \sqrt{2}\right)} = 2.269 J/k_B \tag{27}$$

A. The algorithm

In our numerical calculations we are in equilibrium the whole time; starting from equilibrium due to utilizing the Boltzmann distribution, we will choose our initial state at a random position in our lattice. Being in equilibrium requires that detailed balance is satisfied. The system must also have the property of ergodicity, that means there must always be a possibility to reach another state within a finite number of steps. The Metropolis-Hastings algorithm[2] is one acceptance rule that satisfies this. The Metropolis-Hastings algorithm is a MCMC method in statistical physics which uses a probability distribution (here: the Boltzmann distribution) to obtain a sequence of random samples. The MCMC method is outlined in algorithm 1.

Algorithm 1 Markov Chain Monte Carlo

One Monte Carlo cycle : ▷ To be repeated N times
- Generate candidate state $\mathbf{s}'$ with energy E_{b}
  - → Pick a random spin s_i in candidate lattice
  - → Flip chosen spin
  - → Compute energy E_a of the new spin state $\mathbf{s}_i$
- Find value of $\Delta E = E_a - E_b$
  Corresponding to finding the ratio of probabilities: $p(\mathbf{s}'; T)/p(\mathbf{s}_i; T)$

if $\Delta E \leq 0$ **then**
  Accept the new state $\mathbf{s}_i$ ▷ Cycle done: store values
else
  Generate a random number r from $U(0, 1)$
  Compute $w = e^{-\beta\Delta E}$
  if $r \leq w$ **then**
    Accept the new state $\mathbf{s}_i$ ▷ Cycle done: store values
  else
    Keep current state $\mathbf{s}'$ ▷ Cycle done: store values

By using this algorithm, we can obtain a Markov chain containing numerical estimates of $\langle\epsilon\rangle$, $\langle|m|\rangle$, C_V and χ. By creating plots of these values as functions of temperature T, we can expect to see indications of a phase transition.

When using the MCMC method, all values of the Markov chain depend on each other, therefore we expect there to be a certain burn-in time before the set of values accumulate around the true expectation values. Using a burn-in to throw away samples that are "too far outside" our desired uniform distribution will ensure computed expectation values closer to the true expectation values[2].

When sampling from the Ising model for different temperatures to find the critical temperature and observe the phase transition, we will need a lot of cycles to to get accurate enough values for larger lattices. To reduce the time it takes to compute all the results we will parallelize a part of our program. This will allow multiple threads in our computer to compute that part at the same time. For that we will use openMP and parallelize part that run the MCMC, by running multiple instances of MCMC cycles at the same time. Thus we can reduce the amount of

[2] Whether throwing away some samples actually will cause the wanted outcome is of course dependant on some probability, but this probability is outside the scope of this report, and thus, we will just choose this to be true.

cycles needed in total by taking the average result from the threads.

III. RESULTS AND DISCUSSION

We solved the 2×2 case analytically to compare it to our numerical results. We did this by using the expression for the partition function (eq. 14) and the expressions for the energy, magnetization, heat capacity, and susceptibility per spin presented in section II. For the 2×2 case with temperature $T = 1.0J/k_B$, we found the following values

$$\begin{aligned} \langle \epsilon \rangle &= -1.996J \\ \langle |m| \rangle &= 0.998 \\ C_V &= 0.032k_B \\ \chi &= 0.004. \end{aligned} \tag{28}$$

The same values found numerically were solved using the MCMC method with one million cycles. This gave us the final expectation values

$$\begin{aligned} \langle \epsilon \rangle &= -1.997J \\ \langle |m| \rangle &= 0.999 \\ C_V &= 0.025k_B \\ \chi &= 0.003. \end{aligned} \tag{29}$$

As seen from the graphs below (figure 1), the values we sample numerically for the Ising model fit quite well for the expected values for the energy and magnetization. From the graph we can see that closer to one million cycles the curves flatten out and the expected values stays more or less constant, with only a few small changes. This was done with the smallest possible lattice size and with larger lattices there would be more attempted spin flips per cycle. Which would cause less deviation between each MCMC cycle. That means we would need fewer cycles to achieve the correct results.

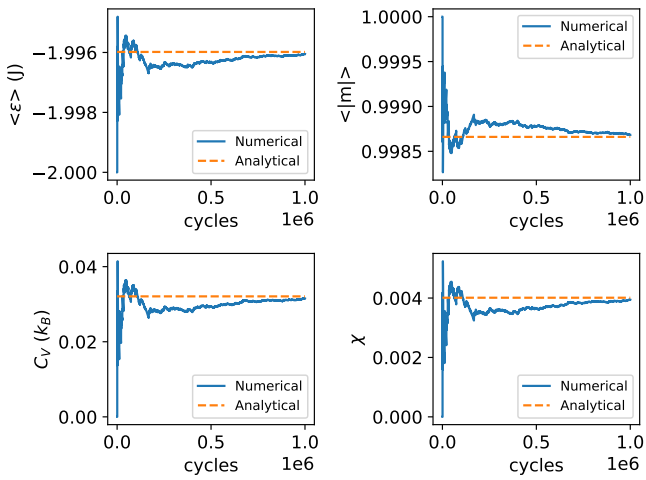

FIG. 1. Figure shows the expected values for the energy per spin $\langle \epsilon \rangle$ (top left graph), magnetization per spin $\langle |m| \rangle$ (top right), the heat capacity C_V (bottom left) and the susceptibility χ (bottom right). The samples where collected from 200000 MCMC cycles for a 2×2 lattice of spins. All the spins where set to $+1$ for the starting lattice.

Next we moved on to the 20×20 case, where we sample the expected values for the energy and magnetization per spin for the temperatures $T = 1.0J/k_B$ and $T = 2.4J/k_B$. We make 30000 MCMC cycles per result. From the graph of the expected values as a function of MCMC cycles (figure 2), we can notice a few things. Increasing the temperature makes it take more cycles for the system to reach a balance, as seen in the graph where it takes longer time to achieve balance for higher temperature. This also makes sense as for lower temperature our system would be more stable. Especially for when the temperature equals $1J/k_B$, where we can see from the graph that the energy and magnetization per spin have its expectation value almost at the highest possible value for the energy and magnetization of our system. We also notice that the starting spin configuration for the system matters, though only mostly before the system have reached a balance. It is important to note that the ordered system for $T = 1.0J/k_B$ start in a balance, since a lattice with all equal spin will have the highest possible energy for that system, and for the temperature equal to $1J/k_B$, that state is the most likely and we can therefore not notice any change for that configuration. The time it takes for the system to reach a balance is what we call burn-in. That is when we have too few samples which moves the expectation value away from the balanced point. One possibility is to remove the first few points from the accumulation and then, most likely get a better approximation for the expectation value with less samples. We can also notice the difference between the 2×2 case and the 20×20 case that for the larger lattice we use, which also means more attempted spin swaps in the system, we need less cycles to find a good approximation for the expectation value.

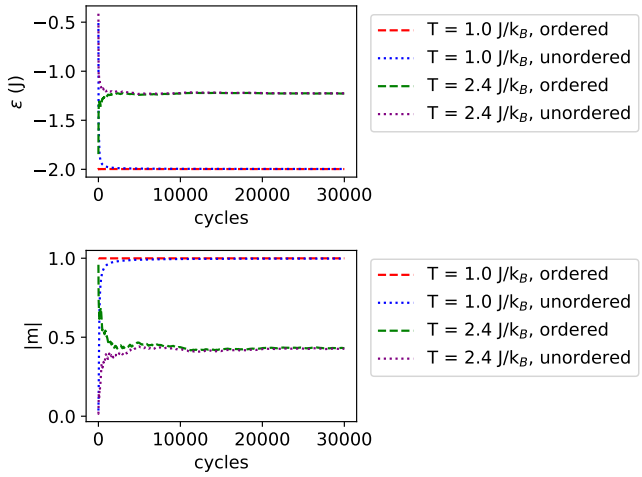

FIG. 2. Figure shows the expected values for the energy $\langle\epsilon\rangle$ and magnetization $\langle|m|\rangle$ per spin for the ordered case (start with all spins equal $+1$) and the unordered case (start with all random spin ± 1, for temperatures $T = 1.0J/k_B$ and $T = 2.4J/k_B$. The burn-in time can be seen for when the expected values approach the more correct value.

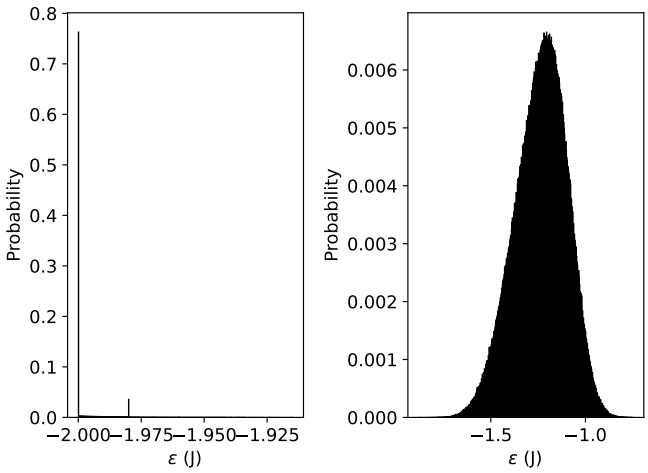

FIG. 3. Histogram for the energy per spin ϵ, with a 20×20 lattice of spins with all the spins being ordered (start with all the spins equal to $+1$). The plot to the left is for $T = 1.0J/k_B$ and the plot to the right is for $T = 2.4J/k_B$.

The histogram (figure 3), shows all the energy samples we collected over one million MCMC cycles for a 20×20 lattice all with ordered starting spin configurations. The samples where collected with temperatures $T = 1.0J/k_B$ (left graph) and $T = 2.4J/k_B$ (right graph). As for $T = 1.0J/k_B$, the probability for the spin configuration to change from the state with largest energy is close to zero, and after one million cycles we can see from the histogram that the probability of the system having maximum energy is close to 75%. This compared to the system with $T = 2.4J/k_B$ where there is almost zero probability of the system being in the state at maximum energy. With the most probable state having close to $-1.2J$ energy per spin, and the shape of the histogram shows that the energy have a Gaussian probability function when the temperature of the system is higher than $1.0J$ per spin. We would then expect that the width of the Gaussian curve will increase as the temperature of the system increases, while also moving the center of the curve as the expectation value. The width of a Gaussian function is equal to the square root of the variance, and as the variance increases then the heat capacity will also increase (eq. 21).

The figure below (figure 4) shows the expectation values for the energy and magnetization per spin, the heat capacity and susceptibility as a function of temperature for different lattice sizes. Where we made 10000 MCMC cycles per thread and we used 2 threads. We could have used more threads for better approximations, but using more threads increased the computation time and it was more important to have enough cycles to get over the burn-in, which would have created weird results. The burn-in varied from 2000 cycles for the smaller lattice sizes and 5000 for the larger lattice sizes. We can then from the peaks of the graphs find the critical temperature $T_c(L)$ for that size lattice. Those peaks indicate a phase transition. We can then read of the graphs what the critical temperatures are

$$\begin{aligned} T_c(40) &= 2.303J/k_B \\ T_c(60) &= 2.304J/k_B \\ T_c(80) &= 2.293J/k_B \\ T_c(100) &= 2.295J/k_B \end{aligned} \tag{30}$$

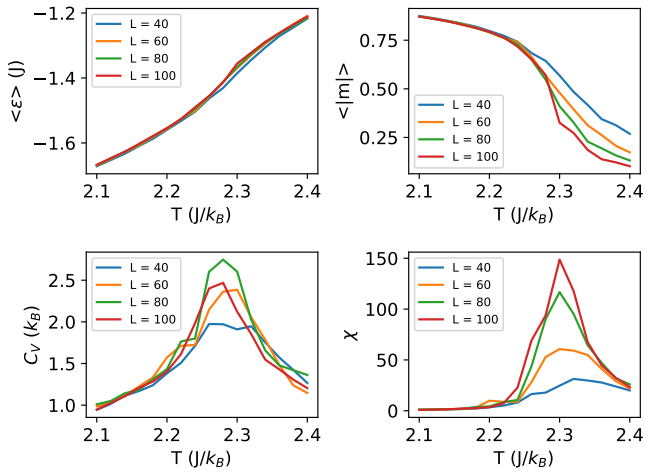

FIG. 4. Figure shows the expectation values for the energy $\langle\epsilon\rangle$ and magnetization $\langle|m|\rangle$ per spin, the heat capacity C_V and susceptibility χ as a function of temperature T for different values of lattice size L. The critical temperature can be found at the peaks of the heat capacity and susceptibility graphs.

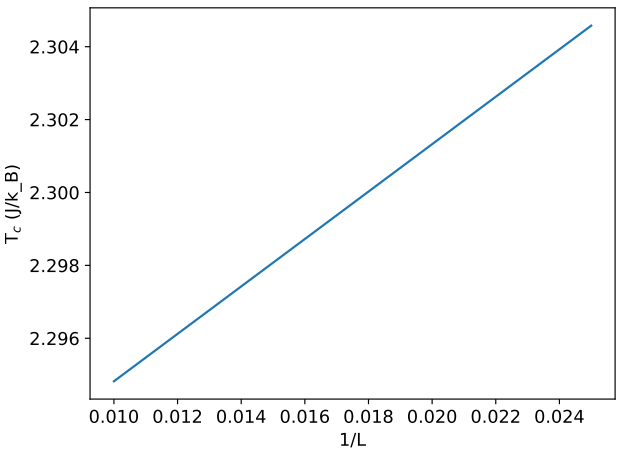

FIG. 5. Figure shows the linear regression for where $y = T_c(L)$, $x = L^{-1}$, the slope equals α and the intercept equals $T_c(L = \infty)$. The linear regression is computed from the critical temperatures found from the phase transition for different lattice sizes (figure 4), given the critical temperatures (eq. 30).

Using the critical temperatures we found we can create a linear regression using the expression (eq. 26) for the critical temperature of an infinite size 2D Ising model $T_c(L = \infty)$. The graph in figure 5 shows the linear regression we computed with the critical temperatures and lattice sizes. We then find the critical temperature for the infinitely large Ising model from the intercept as $T_c(L = \infty) = 2.288$. Compared to the analytical solution found by Lars Onsager $T_c(L = \infty) = 2.269 J/k_B$, which gives a relative error of 0.8%.

IV. CONCLUSION

In this report we have used the Markov Chain Monte Carlo method to compute the energy, magnetization, heat capacity and susceptibility for an $L \times L$ Ising model. We compared the numerical results (eq. 28) with the analytical solutions (eq. 29) for the 2×2 case. Where we found that for that case, the numerical approximation for the expectation values fit well with the analytical results, with relative errors below 1%. We then looked at the burn-in for a 20×20 size lattice for different temperatures and for ordered or unordered starting spin configurations, where there were very little difference whether the starting spins where ordered or unordered. While increasing the temperature would also increase the time it takes for good approximations of the expectation values. We would also compare the density of the energy samples collected after one million MCMC cycles to find the probability distribution for the energy of the states. With the results, we were able to find the phase transition for the Ising model by finding the critical temperature for a given size lattice (eq. 30). Which we could then compute the approximate of the critical temperature for an infinite 2D Ising model $T_c(L = \infty) = 2.288$ and compare it to the analytical result derived by Lars Onsager $T_c(L = \infty) = 2.269$, with relative error of 0.8%.

[1] Montroll, Elliott W. / Potts, Renfrey B. / Ward, John C.(1963): *Correlations and Spontaneous Magnetization of the Two-Dimensional Ising Model.*

[2] Hastings, W. K.(1970): *Monte Carlo sampling methods using Markov chains and their applications*, 1: 97-109.

[3] Utermohlen, Franz(2018): *Mean Field Theory Solution of the Ising Model.*

[4] Hjorth Jensen, Morten (2015): *Computational Physics [Lecture Notes Fall 2015].* , Department of Physics, University of Oslo.