ISING MODEL

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Abstract. In this article we are going to study a widely popular model to simulate phase transitions, namely, the *Ising model* in two dimensions. The aim was to solve this problem numerically in a two dimensional lattice with periodic boundary conditions. Which we did, by using the Metropolis algorithm and Monte Carlo methods.We found that for large number of Monte Carlo cycles the numerical values for mean quantities is almost the same as analytical values. We also found that higher temperature means higher energies. At a given critical temperature $T_C = 2.2692J/k_B$, this model undergoes a phase transition from a magnetic phase to a phase with zero magnetization. Numerically we found that the critical temperature is $T_C = 2.25J/k_B$.

Contents

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1. Introduction

The *Ising model*, named after the physicist, Ernst Ising, is a mathematical model of ferromagnetism in statistical physics. It is the most studied model for interacting spins with respect to simulations of phase transitions. It is meant to simulate a two dimensional model of a magnet composed of many small atomic magnets. However, this model can also be used in analyzing other complex systems, such as gases sticking to solid surfaces or hemoglobin molecules that absorb oxygen. The Ising model was invented by the physicist, Wilhelm Lenz, who gave it as a problem to his student Ernst Ising. The one dimensional Ising model was solved by Ising himself in his 1924 thesis, it has no phase transitions. The two dimensional square lattice Ising model is much harder, and was solved analytically by the Norwegian born chemist, Lars Onsager in 1944.

To simulate this model we will use the Monte Carlo based Metropolis algorithm. Monte Carlo(MC) methods are suitable in situations where alternative methods may be computationally heavy. MC methods rely on repeated random sampling to obtain numerical results. The metropolis algorithm gives us a sampling rule, and allows us to sample the probability distribution function of complicated systems. In this article, we start by presenting the theoretical background of the Ising model, then we explain the algorithms used and some implementation details. Finally we present our results and discuss our findings before giving a conclusion.

2. Theory

Metals like iron, nickel, cobalt and some of the rare earths like gadolinium, exhibit a unique magnetic behavior which is called ferromagnetism. Such materials show a long range ordering phenomenon at the atomic level, which causes the unpaired electron spins to line up parallel with each other in a region called a *domain*. The long range order which creates magnetic domains in ferromagnetic materials arises from a quantum mechanical interaction at the atomic level. Therefore we could think of a metal as composed of, for example, a cubic lattice with atoms at each corner, with a resulting magnetic moment pointing in a particular direction. In many ways, these atomic magnets are like ordinary magnets, and can be thought of little magnet vectors pointing from south to north poles.

2.1. **The Ising Model.**

The Ising model provides a simple way of describing how a magnetic material responds to thermal energy and an external magnetic field. In this model, each domain has a corresponding spin of north or south. The spins can be thought of as the poles of a bar magnet. The model assigns a value of $(+1)$ to the spins pointing up $\uparrow$, that is, to the north, and a value of (-1) to the spins pointing down $\downarrow$, that is, to the south. The position of each spin is given in a lattice, which allows each spin to only interact with its nearest neighbours. We can model the system as,

$$E = -J \sum_{<kl>}^{N} s_k s_l - \mathcal{B} \sum_{k}^{N} s_k \tag{1}$$

Here $s_k = \pm 1$, N is the total number of spins, J is a coupling constant, expressing the strength of the interaction between neighboring spins, and $\mathcal{B}$ is an external magnetic field interacting with the magnetic moment set up by the spins. The symbol $< kl >$ means that we sum over the nearest neighbors only. However in this article, we will study the system with $\mathcal{B} = 0$. The system is then expressed as,

$$E = -J \sum_{<kl>}^{N} s_k s_l \tag{2}$$

where $s_k = \pm 1$, s_k and s_l is the spin of lattice point $k$and l, N is the total number of spins, J is a coupling constant, and we still sum over the nearest neighbors only. In this model all the atoms interact with each other through the spins. If two neighboring spins are aligned in the same direction, they will give a negative contribution to the energy. If two neighboring spins are disaligned, they will give a positive contribution.

The probability of a certain configuration, i is given by the Boltzmann distribution,

$$P_i(\beta) = \frac{e^{-\beta E_i}}{Z} \tag{3}$$

where $\beta = 1/k_B T$, k_B is the Boltzmann constant and T is the temperature. E_i is the energy of state i, and Z is the *partition function* for the canonical ensemble defined as,

$$Z = \sum_{i}^{W} e^{-\beta E_i} \tag{4}$$

here, W is the number of microstates. The number of microstates is give as $W = 2^N$, where N is the number of spins. The partition function acts as a normalization constant. The energy for a given microstate i, is given by

$$E_i = -J \sum_{<kl>}^{N} s_k s_l \tag{5}$$

where we sum over the nearest neighbor only, and N is the total number of spins. We are also interested in the magnetization, M for a given microstate i, this is given by,

$$M_i = \sum_{j=1}^{N} s_j \tag{6}$$

where N is the total number of spins.

2.2. **Statistical quantities.** We are interested in calculating the expectation values of different physical properties of the Isling model. Some of the quantities that characterize the magnetic system can be calculated as shown below.

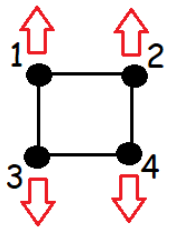


FIGURE 1. An example of a spin configuration in a 2×2 lattice

The *expectation value, the mean energy* can be calculated as

$$\langle E \rangle = \sum_{i=1}^{W} E_i P_i(\beta) = \frac{1}{Z} \sum_{i=1}^{W} E_i e^{-\beta E_i} \tag{7}$$

The *mean magnetization* can be calculated as

$$\langle M \rangle = \sum_{i=1}^{W} M_i P_i(\beta) = \frac{1}{Z} \sum_{i=1}^{W} M_i e^{-\beta E_i} \tag{8}$$

The *absolute value of the mean magnetization* can be also be found,

$$\langle |M| \rangle = \sum_{i=1}^{W} |M_i P_i(\beta)| = \sum_{i=1}^{W} |\frac{M_i e^{-\beta E_i}}{Z}| \tag{9}$$

The *magnetic susceptibility*, χ, tells us if the material is attracted into, or repelled out of a magnetic field. It can be calculated as,

$$\chi = \frac{1}{k_B T} (\langle M^2 \rangle - \langle M \rangle^2) \tag{10}$$

The variance of the magnetization is the quantity $\sigma_M^2 = \langle M^2 \rangle - \langle M \rangle^2$.

The *heat capacity* at constant volume, C_V, tells us how much energy is needed to change the temperature, it can be calculated as,

$$C_V = \frac{1}{k_B T^2} (\langle E^2 \rangle - \langle E \rangle^2) \tag{11}$$

The variance of the energy is the quantity $\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2$.

Here W is the total number of microstates, as before, k_B is the Boltzmann constant, T is the temperature, and Z is the partition function.

2.3. **The 2×2 Ising Model.** In one and two dimensions, the Ising model has analytical solutions to several expectation values, as long as the external magnetic field is zero. In a two dimensional model, with lattice size $L = 2$ and periodic boundary conditions, this model would have $W = 2^{2\times 2} = 2^4 = 16$, different configurations.

Figure 1 shows an example of a spin configuration in a 2×2 lattice. The energy and magnetization with periodic boundary conditions(PBC) can be

TABLE 1. All possible configurations for 2×2 lattice with PBC, here N↑ gives the number of spins pointing up.

N↑	Degeneracy	E_i	M_i
4	1	$-8J$	4
3	4	0	2
2	4	0	0
2	2	$8J$	0
1	4	0	-2
0	1	$-8J$	-4

calculated for the example in figure 1 as,

$$\begin{aligned} E_1 &= -J(s_1s_2 + s_2s_1 + s_1s_3 + s_3s_1 + s_2s_4 + s_4s_2 + s_3s_4 + s_4s_3) \\ &= -J(1 + 1 - 1 - 1 - 1 - 1 + 1 + 1) = 0 \\ M_1 &= \sum_{j=1}^{4} = s_1 + s_2 + s_3 + s_4 = 1 + 1 - 1 - 1 = 0 \end{aligned}$$

We can summarize all possible configurations in table 1 for the 2×2 lattice with periodic boundary conditions. The degeneracy tells us the number of configurations with the same energy.

We can compute the expectation values mentioned above, because for a 2×2 lattice, these quantities have analytical expressions. We have twelve micro states with $E = 0$, two micro states with $E = -8J$, and two micro states with $E = 8J$. The partition function can then be found by,

$$Z = 2e^{8J\beta} + 2e^{-8J\beta} + 12e^{0} = 2e^{8J\beta} + 2e^{-8J\beta} + 12 = 4cosh(8J\beta) + 12$$

where $\beta = 1/k_BT$

$$\begin{aligned} \langle E \rangle = \frac{1}{Z}\sum_i E_i e^{-(\beta E_i)} &= \frac{1}{Z}\Big(- 8J(2)e^{8J\beta} + 8J(2)e^{-8J\beta}\Big) \\ &= \frac{1}{Z}\Big(- 16Je^{8J\beta} + 16Je^{-8J\beta}\Big) \\ &= \frac{-16J}{Z}\Big(e^{8J\beta} - e^{-8J\beta}\Big) = \frac{-16(2)J}{Z}sinh(8J\beta) \\ &= \frac{-32J}{Z}sinh(8J\beta) \end{aligned}$$

Simlarly we can calculate the other quantities,

$$\begin{aligned} \langle E^2 \rangle = \frac{1}{Z}\sum_i E_i^2 e^{-(\beta E_i)} &= \frac{1}{Z}\Big(64J^2(2)e^{8J\beta} + 64J^2(2)e^{-8J\beta}\Big) \\ &= \frac{(2)128J^2}{Z}\Big(e^{8J\beta} + e^{-8J\beta}\Big) = \frac{256J^2}{Z}cosh(8J\beta) \end{aligned}$$

$$\langle M \rangle = \frac{1}{Z}\sum_i M_i e^{-(\beta E_i)} = \frac{1}{Z}\Big(- 4e^{8J\beta} + 4e^{8J\beta} + 8 - 8\Big) = 0$$

$$\langle |M| \rangle = \frac{1}{Z} \sum_i |M_i| e^{-(\beta E_i)} = \frac{1}{Z}\Big(4e^{8J\beta} + 4e^{8J\beta} + 8 + 8\Big) = \frac{1}{Z}\Big(8e^{8J\beta} + 16\Big)$$

$$\begin{aligned}\langle M^2 \rangle = \frac{1}{Z} \sum_i M_i^2 e^{-(\beta E_i)} &= \frac{1}{Z}\Big(16e^{8J\beta} + 16e^{8J\beta} + 4(4) + 4(4)\Big) \\ &= \frac{1}{Z}\Big(32e^{8J\beta} + 32\Big) = \frac{32}{Z}\Big(e^{8J\beta} + 1\Big)\end{aligned}$$

The heat capacity can be found by equation (11),

$$\begin{aligned}C_V &= \frac{1}{k_B T^2}\Big(\frac{256J^2}{Z} cosh(8J\beta) - \Big(\frac{-32J}{Z} sinh(8J\beta)\Big)^2\Big) \\ &= \frac{1}{k_B T^2}\Big(\frac{256J^2}{Z}\Big(cosh(8J\beta) - \frac{4}{Z} sinh^2(8J\beta)\Big)\Big)\end{aligned}$$

The magnetic susceptibility can be found from equation (10),

$$\chi = \frac{32}{Z}\Big(e^{8J\beta} + 1\Big) - 0 = \frac{32}{Z}\Big(e^{8J\beta} + 1\Big)\frac{1}{k_B T}$$

For a given value of J, β, where $\beta = 1/k_B T$, and T, we have analytical solutions for these expectation values. These quantities are functions of T, temperature provided one uses PBC.

2.4. **Phase transitions.** A phase transition is marked by abrupt macroscopic changes as external parameters are changed, such as an increase of temperature. The point where a phase transition takes place is called a critical point. The Ising model in two dimensions undergoes a phase transition of second order. This mean that below the critical temperature T_C, the Ising model exhibits a spontaneous magnetization with $\langle M \rangle \neq 0$. Above T_C the average magnetization is zero. Near T_C, we can characterize the behaviour of many physical quantities by a power law behavior. The mean magnetization is given by,

$$\langle M(T) \rangle \sim (T - T_c)^\beta \tag{12}$$

where $\beta = 1/8$, is the critical exponent. A similar relation applies to heat capacity and susceptibility,

$$C_V(T) \sim |T_C - T|^\alpha \tag{13}$$

$$\chi(T) \sim |T_C - T|^\gamma \tag{14}$$

where $\alpha = 0$ and $\gamma = 7/4$.

3. Algorithms

The algorithm of choice for simulating the Isling model is the approach proposed by Metropolis in 1953. The pathway to finding the steady state can be seen as a Markov chain.

3.1. **Markov chains.** All Monte Carlo schemes are based on Markov processes in order to generate new random states. A Markov chain is a random walk with a selected probability for making a move. The new move is independent of the previous history of the system. The reason for choosing a Markov process is that when it is run for a long enough time starting with a random state, we will eventually reach *the most likely state* of the system. This means that after a certain number of Markov processes we reach an equilibrium distribution. To reach this distribution, the Markov process needs to fulfill the condition of *ergodicity*, and *detailed balance*. Ergodicity means that the Markov process should be able to reach any state of the system from any other state if we run it long enough. At equilibrium, the condition of detailed balance gives us,

$$\frac{P(j \to i)}{P(i \to j)} = \frac{P_i}{P_j} = e^{-\beta(E_i - E_j)} \tag{15}$$

This simplifies our calculations as we never have to evaluate the partition function Z explicitly.

3.2. **The Metropolis algorithm.** The metropolis algorithm full fills the conditions of ergodicity and detailed balance, therefore we can use it to simulate the Ising model. New configurations are generated from a previous one using a transition probability which depends on the energy difference between the initial and final states. The metropolis algorithm considered only the ratios between probabilities, so we do not need to compute the partition function as all.

The algorithm can be described as,

(1) Initialize the system with an initial state with energy E_b. This can be generated randomly. Calculate the energy E_b of this configuration.
(2) Change the in ital configuration by flipping one spin only at a random position in the lattice. Calculate the energy of this new trial state E_t.
(3) Calculate $\Delta E = E_t - E_b$. For the two dimensional case, there are only five values for ΔE. This is explained below.
(4) If $\Delta E \leq 0$, accept the new configuration. This means that the energy is lowered and we are moving towards an energy minimum.
(5) If $\Delta E > 0$, calculate $w = e^{-\beta \Delta E}$. Draw a random number r. If $r < w$, accept the new configuration, else keep the old configuration.
(6) Calculate the new expectation values and update them. Continue the process until you have reached a sufficiently good representation of the states.
(7) Each time we sweep through the lattice, that is, summed over all spins, it is called a *Monte Carlo cycle*. At the end, divide the various expectations by the total number of cycles.

3.3. **Energies in two dimensions.** A crucial step in the algorithm described above is the calculation of the energy difference and the change in magnetization. For the Ising model in two dimensions there are only five values of ΔE. Each time, we flip one spin only. First select a random spin position x, y and assume this spin and its nearest neighbours are all pointing

TABLE 2. All possible configurations for the energy in two dimensions with PBC. Here state i is the initial state, state j is the final state. Similarly E_i is the energy of the inital state, E_j is the energy of the final state, and ΔE is the energy change that we wish to compute.

State i	State j	E_i	E_j	ΔE
$\begin{matrix} & \uparrow & \\ \uparrow & \uparrow & \uparrow \\ & \uparrow & \end{matrix}$	$\begin{matrix} & \uparrow & \\ \uparrow & \downarrow & \uparrow \\ & \uparrow & \end{matrix}$	$-4J$	$4J$	$8J$
$\begin{matrix} & \downarrow & \\ \uparrow & \uparrow & \uparrow \\ & \uparrow & \end{matrix}$	$\begin{matrix} & \downarrow & \\ \uparrow & \downarrow & \uparrow \\ & \uparrow & \end{matrix}$	$-2J$	$2J$	$4J$
$\begin{matrix} & \downarrow & \\ \downarrow & \uparrow & \uparrow \\ & \uparrow & \end{matrix}$	$\begin{matrix} & \downarrow & \\ \downarrow & \downarrow & \uparrow \\ & \uparrow & \end{matrix}$	0	0	0
$\begin{matrix} & \downarrow & \\ \downarrow & \uparrow & \downarrow \\ & \uparrow & \end{matrix}$	$\begin{matrix} & \downarrow & \\ \downarrow & \downarrow & \downarrow \\ & \uparrow & \end{matrix}$	$2J$	$-2J$	$-4J$
$\begin{matrix} & \downarrow & \\ \downarrow & \uparrow & \downarrow \\ & \downarrow & \end{matrix}$	$\begin{matrix} & \downarrow & \\ \downarrow & \downarrow & \downarrow \\ & \downarrow & \end{matrix}$	$4J$	$-4J$	$-8J$

up, then the possible combinations are shown in table 2. The possible energies are $\Delta E \in \{8J, 4J, 0, -4J, -8J\}$, this means we can precalculate these values in the main part, so we dont haveto compute them everytime.

3.4. **Ising class.** The Ising model is implemented in C++ in the class Ising.cpp contains all the methods needed for simulating The metropolis algorithm in order to find all the expected values. The full program can be found by following the link at the front page of this article.

The Ising class consists of many methods but the three most important methods are Initialise , Simulate and Metropolis. Every thing important is i happening there the rest of the methods are there to serve these three methods and because i wanted to object orient my code which makes it easier for both the user and maker the to check for errors and understanding. As the program is built right now, it can be run with command line arguments for spin lattice dimension, temperature domain, the number of Monte Carlo cycles and another argument for temperature for just one value, which called M times by simulate adds up to have a total complexity of $\mathcal{O}(ML^2)$.

TABLE 3. Comparison between Monte Carlo simulations at different length and the analytical solution for a 2×2 system.

M	$\langle E \rangle$	C_V	χ	$\langle \mathcal{M} \rangle$
Analytical	-1.99598	0.03208	0.00401	0
10	-2.2	-1.76	-0.44	-1.1
100	-2.02	-0.1616	-0.0404	-1.01
1000	-2.002	-0.016016	-0.004004	-1.001
10000	-1.996	0.031936	0.00289471	0.03175
100000	-1.99572	0.034486726	0.0044016479	0.214195
1000000	-1.995884	0.032892234	0.0040535744	-0.0076055
10000000	-1.9959950	0.031982240	0.0039823994	-0.014154750

4. RESULTS

In Table 3 one can see how increasing the number of Monte Carlo cycles gives more precise numerical solutions that measure up to the analytic (exact) solution for a 2×2 system. One can see that it is necessary to have towards 10000000 cycles in order to get the best numerical approximations. Having this result in mind, we move forward and make graph of the (mean) Energy and Magnetization as a function of the number of Monte-Carlo cycles. You can see the result in figure 2.

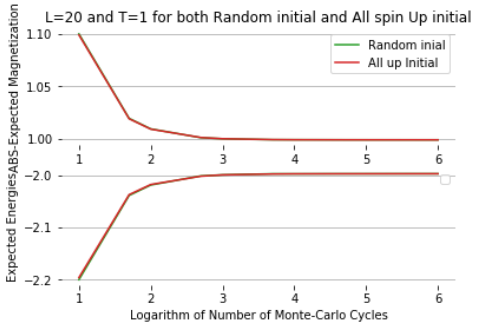
This result shows tells us three things. First, the amount of Monte Carlo cycles necessary in order to establish a steady state, for both Random initial values and all spin in the same direction initial values. This must be known in order to know where it is alright to start calculating the expected values. Second, the different temperatures are a big deciding factor, as the temperature gets bigger the expected values comes out to be more and more inaccurate and skewed. And Third, from figure 2a we can see that the difference between All up initial values and Random initial values is almost zero. We will discuss this deeper in the discussion section.

In figure 3 one can see how the expected values for Energy, absolute value of (mean) Magnetization, Specific heat and Susceptibility changes as a function of Temperature, in domain [2,2.3] with dT(temp steps) =0.05. For different spin lattice dimensions. One can easily spot the rise and fall of all quantities and they approach the critical temperature is $kT_C/J = 2/\ln\left(1+\sqrt{2}\right) \approx 2.269$ with $\nu = 1$, which i will discuss more in the discussion section.

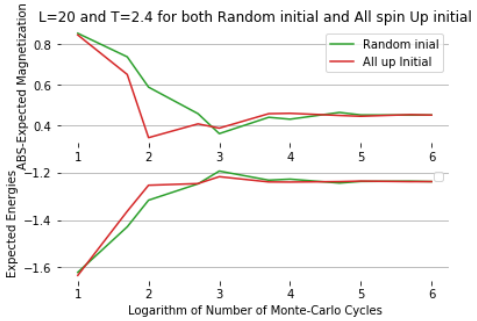
In figure 4, one can see how the number of the Accepted States reacts to different Temperatures(1 and 2.4) for the equilibrium number of Monte Carlo cycles. Which seems to be ¿10000.

5. EVALUATION

I was unable to find the probabilities for the systems Mean Energy, due to insufficient time on this project. But my guess is that the probability for finding the system at a higher energy is most probable at a higher temperature. We were also unable to parallelize our code since the openMPI wouldn't work on our QT creator IDE on windows.



(A) Energy and absolute Magnetization for L=20 and T=1



(B) Energy and absolute Magnetization for L=20 and T=2.4

FIGURE 2. Energy and absolute Magnetization for T=1 A) and T=2.4 B) as a function of Monte-Carlo cycles

6. Discussion

The Monte Carlo Cycles necessary for equilibrium state seems to be $>$ 10000 for all lattice dimensions, and both Random and All up initial conditions, while the increase temperature doesn't seem to have much effect on the equilibrium state it does effect the expected values. In figure 5, one can see how the expected energy rises(increases) with increasing temperatures. Which is what one would expect, since high temperature usually mean high energies.

In figure 3 one can see how the Mean Energies are increasing with temperature for different Lattice dimensions. They are increasing almost in the same way til they the approach the critical temperature and we can start to see different colours and a rapid increase. This means that for big lattice dimensions one finds the Curie T_c temperature $2.2692J/k_B$, according to the following equation.

$$T_c(L \to \infty) = T_c(L) - aL^{-\frac{1}{\nu}} \tag{16}$$

where the exact result gives $\nu = 1$ and a is a constant. We can see that at around $2.25J/k_B$ temperature, the Energies fluctuates the most. The same happens with all the other expected quantities. Specific Heat is a bit inaccurate but still exhibits some of the same described traits.

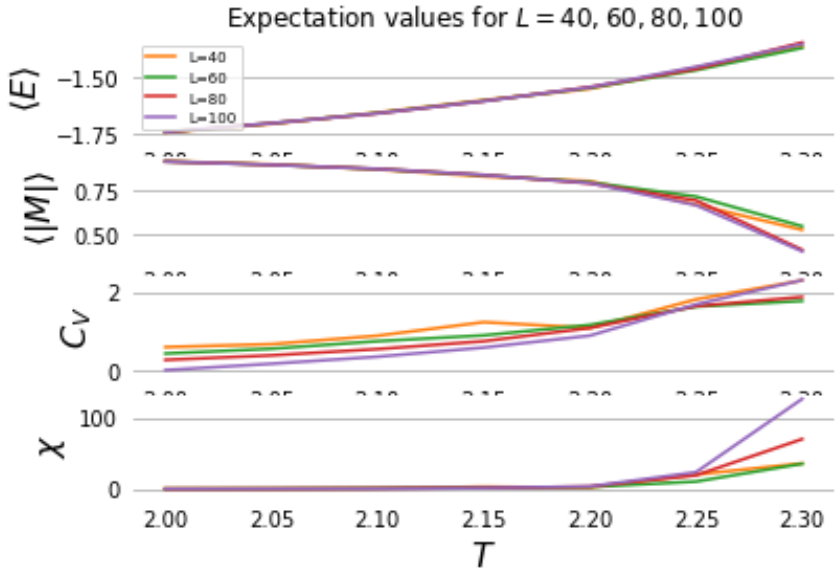


FIGURE 3. Mean Energy, absolute Mean magnetisation, Specific Heat and Susceptibility for L=40,60,80,100 as a function of temperatures $T = [2, 2.3]$.

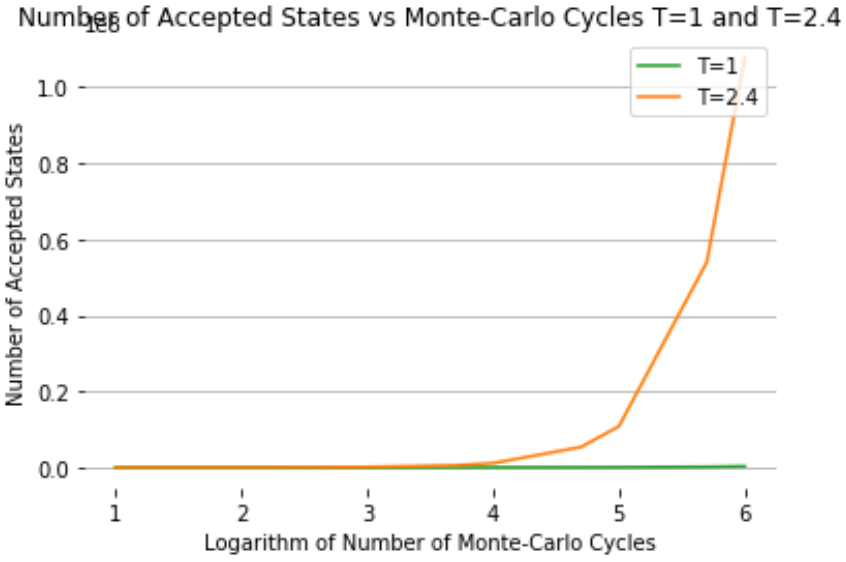


FIGURE 4. Figure showing that the number of accepted states for a higher-temperature system ($T = 2.4$) rises at equilibrium point, while the accepted states for for a lower-temperature system ($T = 1$) stays the constant at equilibrium, MC-cycles = 10^4.

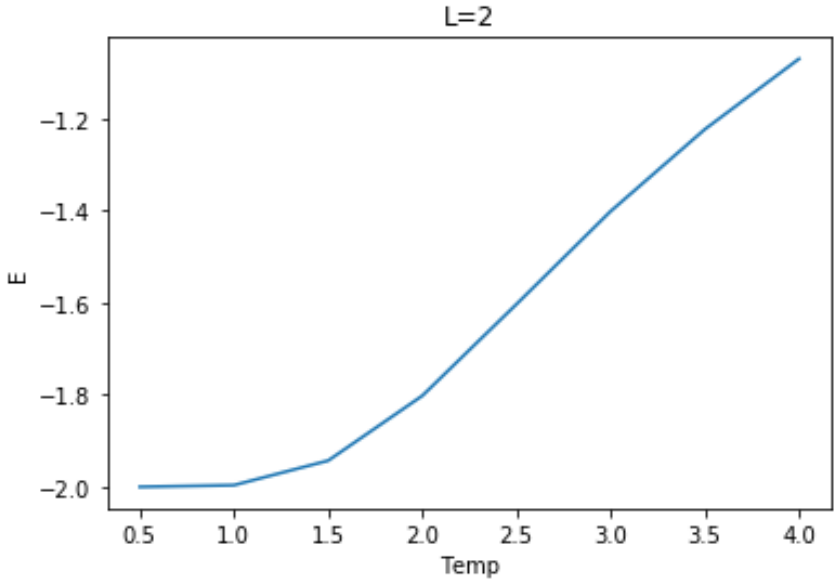


FIGURE 5. Energy as a function of different temperatures $T = [0.5to4]$ for dt=0.5, for 2×2 Lattice.

7. Conclusion

We studied the 2D Lattice Ising model using the Monte Carlo based Metropolis algorithm numerically with periodic boundary conditions. We start with simulating the 2×2 lattice and comparing our results with the analytical ones. We find that our numerical results fit quite well with the analytical result for large number of Monte Carlo Cycles. For the results to match theory we see that we need almost more then 10^4 MC cycles.

Then we studied the Monte Carlo cycles path to equilibrium for different temperatures and different initial conditions and different spin Lattice dimensions. We saw that it is generally needed more than 10^4 MC cycles before reaching equilibrium. For both low and high temperatures, systems equilibrium is reached almost at the same amount of Monte Carlo cycles with both Random and All up(same direction) initial values. From the results we see that the values are fluctuating around equilibrium with high temperatures, which makes sense since the temperatures are high, the entropy state is higher. For the low temperature, low entropy state, we see very small fluctuations. We were unable to find the probabilities and were unable to Parallelizing the code because of time and technical issues, respectively. By studying macroscopic properties around the phase transition we are able to find the critical temperature of the Ising model, to be around $2.25J/k_B$ numerically while the analytical value is $2.2692J/k_B$.

8. References

- All codes can be found in the github repository `https://github.com/moonnesa/FYS3150-2020`

- Morten Hjorth-Jensen. Computational Physics, Lecture notes, Fall 2015, chapter 13. 2015
- En.wikipedia.org. 2020. Ising Model. [online] Available at: `https://en.wikipedia.org/wiki/Ising_model` [Accessed 15 November 2020].