Fys3150 Project 4

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Abstract

The Ising model is investigated through analytical and numerical methods. The behaviour of larger scale systems are analyzed and used to determine the Curie temperature T_C numerically. In order to solve the Ising system Monte Carlo simulations using the Metropolis algorithm were ran. For a 2×2-lattice we found that the numerical result were sufficiently close to the analytic value when $N = 10^6$.

Onsager found the analytical value for the Curie temperature for a 2×2-lattice to be $T_C \approx 2.269$. This is the temperature for which the two dimensional Ising model contains a magnetic phase transition.

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1 Introduction

The goal of this numerical project is to study magnetic phase transitions in a ferromagnetic material. To do this we will be using the Ising model, named after Ernst Ising. The one-dimensional Ising model contains no phase transition, and was the topic of Ising's 1924 thesis. The two-dimensional lattice version of the Ising model and was only first analytically solved by Norwegian chemist Lars Onsager in 1944. His analytical values will be used as a benchmark for the numerical accuracy of the implementation.

In order to study the Ising model for larger two-dimensional systems a numerical solver is implemented which Monte-Carlo cycles a Metropolis algorithm scheme. For each differently sized lattice system the heat capacity C_V and the magnetic susceptibility χ_M are calculated for multiple temperatures. From the pair of these thermodynamic quantities the critical temperature for the phase transition can be approximated. Throughout this paper we present energies and temperatures scaled with J and kT/J respectively. Thus, the spin and the magnetization are dimensionless quantities.

2 Theory

2.1 The Ising Model

The Ising model is popularly used to study binary systems, such as a collection of spinning particles. At a given critical temperature T_C the Ising model models a phase transition from a magnetic phase to a non-magnetic phase. In one and two dimensions the Ising model has exact solutions for several expectation values. The simplest form for the energy of the Ising model is

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

with $s_k = \pm 1$, N representing the total number of spins and J is a coupling constant expressing the strength of the interaction between neighboring spins. The symbol $\langle kl \rangle$ indicates that the sum is only carried out over the nearest neighboring spins only. In addition, we assume ferromagnetic ordering $J > 0$. This form of the energy for the Ising model will be used as a numerical benchmark throughout this project. In addition, we will need to calculate the mean energy

$$\langle E \rangle = \sum_{i=1}^{C} E_i P_i(\beta) = \frac{1}{Z} \sum_{i=1}^{C} E_i e^{-\beta E_i} \tag{2}$$

where $P_i(\beta)$ is the Boltzmann distribution. Further the mean magnetization is

$$\langle M \rangle = \sum_{i=1}^{C} M_i P_i(\beta) = \frac{1}{Z} \sum_{i=1}^{C} M_i e^{\beta E_i} \tag{3}$$

where C represents the total number of possible configurations. The thermodynamic quantities which will be studied in this project can be constructed from the above expressions in the following way. First the heat capacity at constant volume C_V

$$C_V = \frac{1}{kT^2} \big(\langle E^2 \rangle - \langle E \rangle^2 \big) \tag{4}$$

similarly the magnetic susceptibility is given by

$$\chi = \frac{1}{kT}\big(\langle M^2\rangle - \langle M\rangle^2\big) \tag{5}$$

2.2 Ising Model in Two Dimensions

For our first consideration we will be studying a simple 2×2 lattice model in order to obtain an analytical solution to verify subsequent models. This model has 2^4 possible configurations, with energy of a given configuration given by equation (1) and a magnetization given by

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

Below is a compilation of the energies, magnetization and degeneracy of the possible configurations of this 2×2 lattice model. Using table 1 we can now calculate the expectation values $\langle E\rangle$, $\langle M\rangle$,

s_+	$\Omega(E_i)$	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

Table 1: The various possible configurations for the 2×2 Ising model

$\langle C_V\rangle$, as well as the magnetic susceptibility χ. We start by finding an expression for the partition function of our system

$$Z = \sum_{i=1}^{N} e^{\beta E_i} = 4\cosh\big(8J\beta\big) + 12 \tag{7}$$

Using this expression for the partition function the expectation values for the energy and magnetization are

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

$$\langle M\rangle = 0 \tag{9}$$

Further the means of the square energy and magnetization are

$$\langle E^2\rangle = \frac{256J^2\cosh\big(8J\beta\big)}{4\cosh\big(8J\beta\big) + 12} \tag{10}$$

$$\langle M^2\rangle = \frac{8\big(e^{8J\beta} + 1\big)}{\cosh\big(8J\beta\big) + 3} \tag{11}$$

Now for the expressions for the heat capacity at constant volume and the magnetic susceptibility

$$C_V = \frac{1}{kT^2}\frac{64J^2(3\cosh\big(8J\beta\big) + 1)}{(\cosh\big(8J\beta\big) + 3)^2} \tag{12}$$

$$\chi = \frac{1}{kT} \frac{8\left(e^{8J\beta} + 1\right)}{\cosh\left(8J\beta\right) + 3} \tag{13}$$

These values were then compared to the numerical ones obtained from our Monte Carlo simulation.

2.3 Phase Transition

As mentioned above it was first showed by Lars Onsager that there existed phase transitions in the two-dimensional Ising model. This stands in contrast to the one-dimensional case, for which there exists no phase transition. This phase transition in the two-dimensional model occurs at the critical temperature. At this temperature, the spins rapidly change direction causing the thermodynamic quantities to exhibit discontinuities. The quantities can be modeled as

$$\begin{aligned} \langle M(T) \rangle &\sim (T_C - T)^{\beta} \\ C_V(T) &\sim |T_C - T|^{\gamma} \\ \chi(T) &\sim |T_C - T|^{-\alpha} \end{aligned} \tag{14}$$

where $\beta = 1/8$, $\gamma = 7/4$ and $\alpha = 0$ are critical exponents. Through so-called finite size scaling relations it is possible to relate the behaviour of finite lattices with the results for an infinitely large lattice. Scaling the critical temperature as

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu} \tag{15}$$

where a is a constant and ν defined by

$$\xi(T) \sim |T_C - T|^{-\nu} \tag{16}$$

we now set $T = T_C$ and obtain a mean magnetization

$$\langle M(T) \rangle \sim L^{-\beta/\nu} \tag{17}$$

a heat capacity

$$C_V(T) \sim L^{\alpha/\nu} \tag{18}$$

and susceptibility

$$\chi(T) \sim L^{\gamma/\nu} \tag{19}$$

These equations can then be used to approximate the critical temperature in the thermodynamic limit.

2.4 Metropolis Algorithm

Monte-Carlo simulations are used to model the time evolution of a system. In our particular case the algorithm of choice is the Metropolis algorithm. Following is a brief description of the implementation of the Metropolis algorithm for the two-dimensional Ising model.

1. Establish an initial state. This can be either ordered in some way, or generated drawing from a uniform distribution.

2. Next we flip one of the spins, and compute the energy of this new state. Using this energy we find the change in the energy of the system. For the two-dimensional Ising model it turns out there are only five ΔE's, which can be pre-computed.

3. If $\Delta E \leq 0$ we accept this new state to model the natural tendency for systems to fall to lower energies. Else we calculate $w = e^{-\beta \Delta E}$ and compare this with a random number r. If $w \geq r$ then we accept the new configuration, otherwise we keep the old one.

4. If $\Delta E \leq 0$ or $w \geq r$ then we update variables for the mean energy, mean energy squared, mean magnetization, mean magnetization squared and the absolute value for the magnetization, making sure to normalize them properly. In addition there is a counter for the number of accepted spin flips.

5. When the various values from above have settled, we use them to calculate the heat capacity and the magnetic susceptibility.

To study larger lattices, with larger numbers of Monte Carlo cycles, over greater temperature ranges. Python's multiprocessing for parallel computing, as well as cluster computing was utilized. This allowed for results which otherwise would have been unreachable.

2.5 Parallelizing the Ising Model

Some of the calculations in this article required parallelization in order to get results in any meaningful amount of time. Using Python does sacrifice some run time, however due to its rapid prototyping capability we decided on using Python for our simulations. Parallelization is fairly straightforward, as most things are in Python. Below is a pseudo-code explanation of the process

1. Setup a Python multiprocessing Pool

2. Use multiprocessing map method

That's it. Map is passed the metropolis function and a range of either cycles or temperatures and runs each calculation on an available cpu-core. [1]

3 Results

3.1 2×2 Ising model

Below are the results from the 2×2-lattice model. We see after 10^6 Monte Carlo cycles that the calculated thermodynamic values agree well with the exact values.

[1] As explained later we ran parallel calculations where we weren't supposed to. This is discussed more in the results section.

MC-cycles	E	$\|M\|$	C_V	χ
10^1	-7.2000	3.8000	5.759999	0.360000
10^2	-7.9200	3.9800	0.633600	0.039600
10^3	-7.9600	3.9860	0.318399	0.043804
10^4	-7.9856	3.9952	0.114996	0.014377
10^5	-7.9835	3.9943	0.131568	0.017448
10^6	-7.9834	3.9945	0.132333	0.016370
10^7	-7.9836	3.9945	0.131052	0.016425

Table 2: Convergence of the various thermodynamic properties as a function of Monte Carlo cycles. To obtain these values np.seed(0) was used.

3.2 20×20 Ising model

Next we ran the simulation for a lattice with $L = 20$, and recorded how the mean energy and absolute magnetization converged during the Monte Carlo sweeps for the temperatures 1 and 2.4. We remind that the temperatures are scaled with kT/J. Below are graphs of the results when the lattice is both initialized disorderly and with all spin up.
[2]

3.3 Larger Lattices

Next we wished to look at the behaviour of the Ising model as the lattice dimension increases. As mentioned in the footnote above, this type of simulation lends itself well to parallelization. This is because it is possible to run the simulation for each temperature on a separate cpu-core, allowing for a potential six times increase in computational speeds.

[2]When first solving task C, I felt that the text was a bit vague. Therefore, I first simulated in the same fashion as we are supposed to for the various temperatures in task E. Where I ran multiple simulations of the 20×20 Ising system with $N \in [1, 10000]$ cycles. Running this on a normal computer takes a very long time, but I was able to parallelize the code using Python's multiprocessing as well as running the code on UiO's beehive computing platform. Because all this time otherwise would be wasted I have decided to attach the plots generated in an appendix, because I believe they do show, in a sense, the same behaviour as we were asked to analyze.

Figure 1: For $T = 1$ both the energy and the magnetization converge rather quickly. After approximately 10000 cycles we see that there is relatively little change in the values. I.E the system has reached equilibrium.

Figure 2: For $T = 2.4$ the energy becomes relatively stable after 50000 cycles, while the magnetization is still settling.

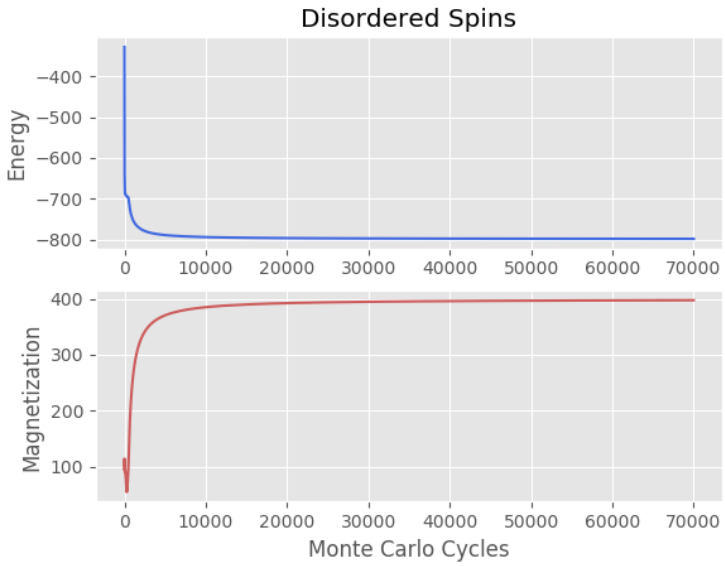

Figure 3: Again, for $T = 1$, only this time the spins are disordered. We see that both the energy and magnetization are fairly close to equilibrium around $N = 15000$

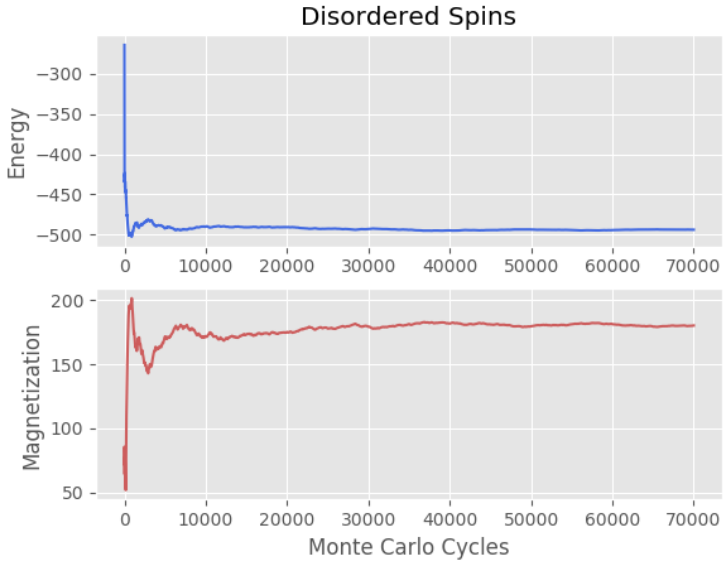

Figure 4: For $T = 2.4$ we again see fluctuations in the magnetization due to the temperature.

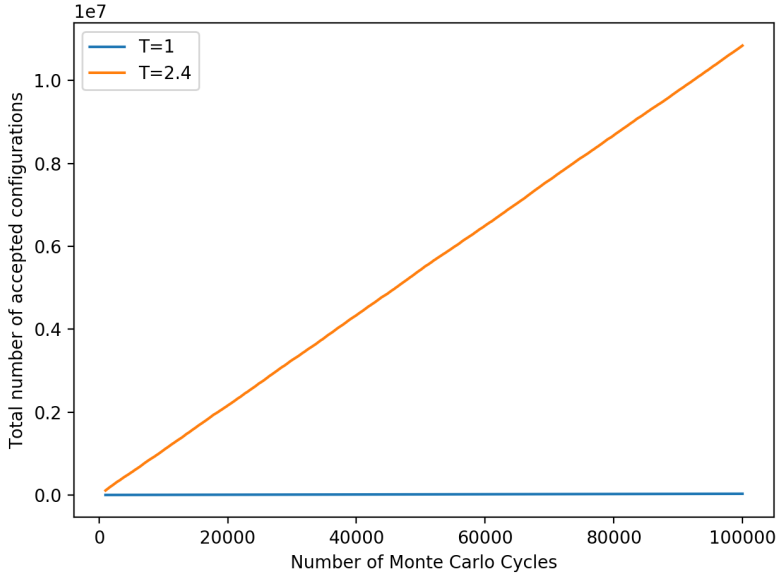

Figure 5: Number of accepted configurations as a function of Monte Carlo cycles for lattice size $L = 20$

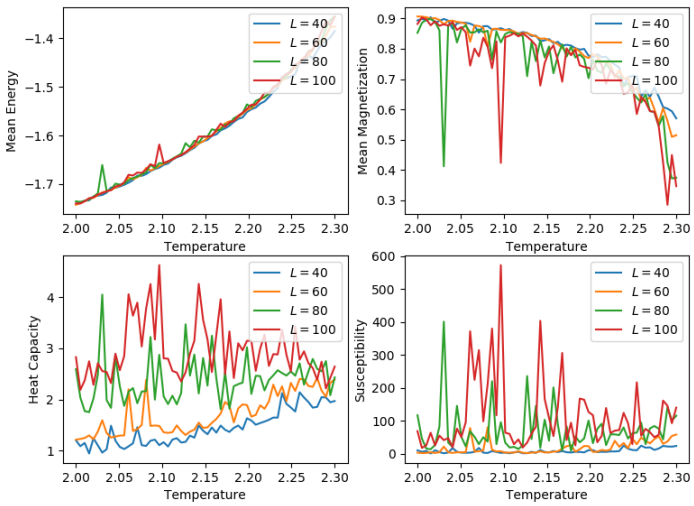

Figure 6: Mean energy, mean magnetization, heat capacity and susceptibility for lattice sizes $L \in [40, 60, 80, 100]$. Simulation ran for 60 temperatures with $\Delta T = 0.005$. There is obviously something wrong with the simulation at this point. Throughout this project my code has gone through so much troubleshooting that it's all messy making it very hard to actually determine what is going wrong. It does seem that the mean energy and magnetization start rising more around the critical temperature but the heat capacity and susceptibility are clearly wrong.

3.4 Discussion and Conclusion

Even though the Ising model is fairly simple in its formulation it manages to capture the complexity of real world lattice systems. Analytical solutions exist for the 2×2 Ising lattice, but are hard to come by for larger systems. Therefore, Monte Carlo methods are used to study these systems. IN this article we decided on using the Metropolis algorithm, although plenty others exist. For the 2×2-lattice we achieved great numerical precision when performing a large number of Monte Carlo sweeps.

In order to run simulations for larger lattices parallelization of Python code was used, along with cluster computing. From here on out the findings are not very solid. While the code is supposed to return the correct values, as was verified with the $L = 2$ case. We had some problems when calculating the various thermodynamic properties. We were not able to extract the critical temperature from the thermodynamic properties. We suspect this is caused by the tolerance for the number of Monte Carlo cycles. Running very long simulations for a lot of temperatures with large lattices proved to be a challenge.

I think the biggest take-back from this assignment is to improve when initially starting such a comprehensive project. When solving the first tasks we opted to use prototype driven development using Python, because this is familiar to us and a great way to get familiar with the problem at hand. However, this approach quickly became messy in the later stages of the assignment where large chunks of code needed to be altered to obtain the results asked for. Making more modular code would also be a great help here.

Further work on this topic would probably fairly rapidly produce much better results than the ones presented here, as I really do fell I am on the cusp of locating this error. However, due to time constraints there is not really much more to be done.

A : 'Wrong' Calculation

Below are the figures generated from running 10000 metropolis runs. Here we also see that for $T = 1$ the energy and magnetization get stable a lot faster than for $T = 2.4$.

B

Github link: `https://github.com/Linueks/fys3150/tree/master/project_4`

C

Collaborated with Joakim Flatby a bit on the code, our codes are not exactly identical but we both have had several bugs making the work difficult throughout this project. Our reports are completely independent.

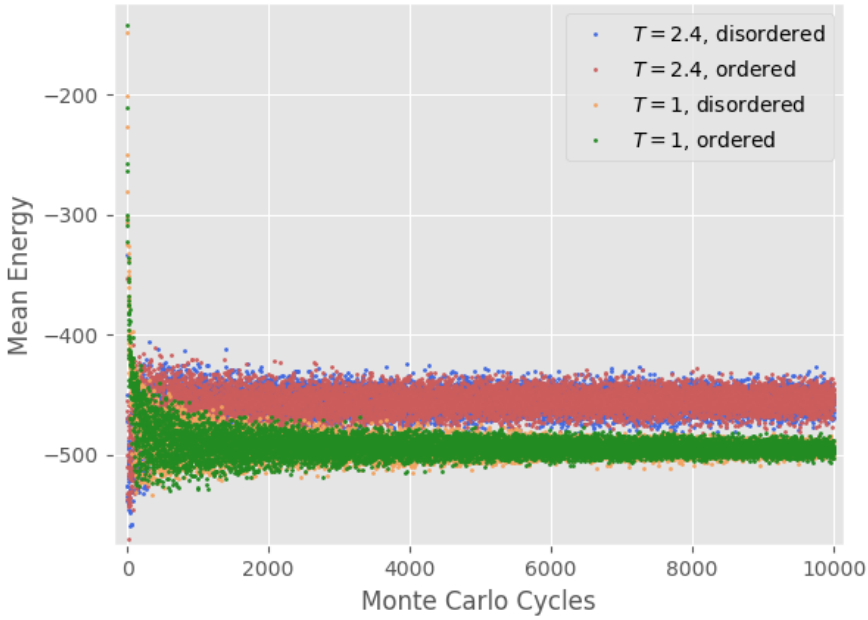

Figure 7: The energies converge fairly rapidly for $T = 1$, and slower for $T = 2.4$

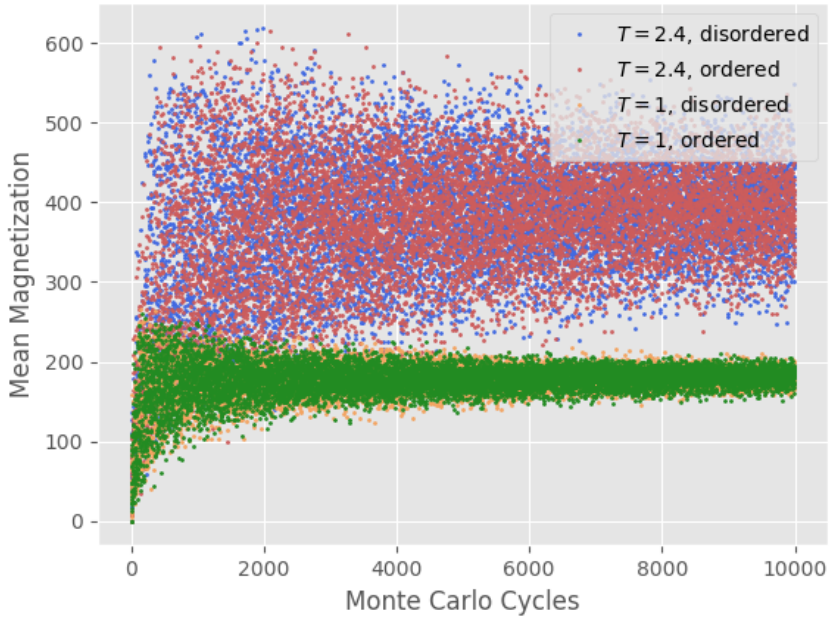

Figure 8: For $T = 1$, the mean magnetization converges within a reasonable amount of time. However, for