Project 4

Marit Kollstuen

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Abstract

Ferromagnetic phase transitions have been studied using the Ising model in two dimensions with Monte Carlo (MC) simulation applied. The model was found to replicate the analytic values of a 2×2 lattice after around 1e7 MC-cycles. The simulation reached an equilibrium solution after around 10~000 MC-cycles for T=1.0 and after around 50~000 cycles for T=2.4 when applied to a 20×20 lattice. The energy distribution for T=2.4 yielded a slightly higher variance than the calculated variance. When running the model for lattice sizes of 40×40 , 60×60 , 80×80 and 100×100 , the result suggested a critical temperature around T=2.275, which is fairly close to the result of Onsager [4], which is $T_C=2.269$

1 Introduction

The aim of this project is to study phase transitions in magnetic systems by applying the Ising model in two dimensions. The Ising model is a mathematical model of ferromagnetism, which is a highly complex physical phenomenon, by the use of statistical physics. The model was first solved in one dimension by Ernst Ising [5], and later in two dimensions by Lars Onsager [4]. The Ising model is widely popular due to its simplicity and efficiency, in addition to it having an analytic solution for the square-lattice case[2]. This makes it possible to perform benchmark calculations that serves as a validation of the model.

The report is an attempt to simulate and describe the phase transitions of a ferromagnetic system. This also gives us an opportunity to study other matters such as for which configuration it is most likely for a system in equilibrium to be in at a given temperature, and how long it takes for a system in a specific initial state to reach equilibrium.

The motivation of this project is to get an insight in statistical physics in terms of Monte Carlo simulations and random walks. This can be applied to a variety of sciences. Personally, I am studying geophysics, and see this as an opportunity to learn more about statistical physics that may be applied to highly non-linear systems. Typically, these systems are simplified using parameterizations, but may benefit from being looked upon as a problem within statistical physics. This was, for instance explored in 2013 by Christopher K. Wikle et.al. [7] .

The report is structured such that in the first section (Section 2), the reader is provided with the theoretical insight of the Ising model and the theory behind the calculations performed in the results' section (Section 3). Further, the results are discussed in Section 4, and I have reached my conclusions in Section 5.

2 Theory

2.1 The Ising model in two dimensions

The Ising model provides a way of describing how a magnetic material correspond to thermal energy and an external magnetic field. In our domain, we have a system that can take two values for the spins, which are ± 1 . The model studies phase transitions at finite temperature for magnetic system [1]. The energy of the Ising model is given by:

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

In which J is a coupling constant of interaction strength between neighbouring spins. The summation over $\langle kl \rangle$ denotes the summation over nearest neighbour only over all spins N. s_l and s_k denotes the spins, and can take values of ± 1 . B denotes the external magnetic field of the system, which will be omitted in this analysis.

In order to estimate expectation values such as the mean energy $\langle E \rangle$ and magnetization $\langle M \rangle$ at a given temperature, we need a probability distribution function (PDF). This is given by the Boltzmann distribution:

$$P_i(\beta) = \frac{e^{-\beta E_i}}{Z} \tag{2}$$

where $\beta = 1/k_BT$, k_B is the Boltzmann constant, E_i is the energy of a microstate i. Z is the partition function (or normalization constant) defined as:

$$Z = \sum_{i=1}^{M} e^{-\beta E_i} \tag{3}$$

Which sums over all M microstates. For the remainder of the calculations, the temperature is scaled and has units Tk_B/J , but will be referred to as T. From this, we can deduce that transitions to a state with lower energy is more likely than transitioning to a state with higher energy.

The expectation values for the energy (the mean energy) can be calculated as a function of the partition function by:

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

$$\tag{4}$$

With variance:

$$\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2 = \frac{1}{Z} \sum_{i=1}^M E_i^2 e^{-\beta E_i} - \left(\frac{1}{Z} \sum_{i=1}^M E_i e^{-\beta E_i}\right)^2 \tag{5}$$

Which, when divided by k_BT^2 , becomes the specific heat at constant volume:

$$C_v = \frac{1}{k_B T^2} (\langle E^2 \rangle - \langle E \rangle^2) \tag{6}$$

Similarly, the mean magnetization is given by:

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

$$\tag{7}$$

With the susceptibility of the system given by the variance of Equation 7 divided by $1/k_BT$:

$$\chi = \frac{1}{k_B T} (\langle M^2 \rangle - \langle M \rangle^2) \tag{8}$$

2.2 Analytical solution for a 2×2 lattice

It is possible to find analytical solutions to Equation 3 when considering a 2×2 lattice, as there are but 16 microstates. These microstates are listed in Table 2.2 for temperature T=1.0. The microstates are calculated using periodic boundary conditions, which means that each spin sees four neighbouring spins [1]. Thus, at the endpoints, the spins takes the value of the spin at the opposite endpoint. (For a larger lattice, however, this becomes close to impossible, as an $n \times n$ lattice has $2^{n \times n}$ microstates.)

No. spins up	$\mathbf{\Omega}(\mathbf{E})$	${f E}$	\mathbf{M}
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: Total energy, E, (with periodic boundary conditions) and magnetization, M, of the different configurations, Ω at T=1.0

For a 2×2 lattice, we have lattice dimension L=2 and $s=2^4=16$ configurations. Thus the partition function becomes:

$$Z = \sum_{i=1}^{16} e^{-\beta E_i}$$

$$= 12e^{0.\beta J} + 2e^{-8\beta J} + 2e^{8\beta J}$$
(9)

By using the hyperbolic cosine identity $\frac{e^z+e^{-z}}{2}=\cosh z$, Equation 9 becomes:

$$Z = 12 + 4\cosh(8\beta J) \tag{10}$$

The expectation value for the energy is then given by [1]:

$$\langle E \rangle = -\frac{\partial \ln(Z)}{\partial \beta}$$

$$= -\frac{8J \sinh(8\beta J)}{\cosh(8\beta J) + 3}$$
(11)

The analytical solution of the heat capacity C_v is then:

$$C_{v} = \frac{1}{kT^{2}} \frac{\partial^{2} \ln(Z)}{\partial \beta^{2}}$$

$$= \frac{1}{kT^{2}} \frac{\partial}{\partial \beta} \left(-\frac{8J \sinh(8\beta J)}{\cosh(8\beta J) + 3} \right)$$

$$= \frac{1}{kT^{2}} \frac{64J^{2}(-\sinh^{2}(8\beta J) + \cosh^{2}(8\beta J) + 3\cosh(8\beta J)}{(\cosh(8\beta J) + 3)^{2}}$$
(13)

The analytical expectation value for the magnetization is simply:

$$\langle M \rangle = \frac{1}{Z} \sum_{i=1}^{M} M_i e^{-\beta E_i}$$

$$= \frac{1}{Z} (4e^{8\beta J} + 8e^0 + (-8e^0) + (-4e^{8\beta J}))$$

$$= 0$$

The mean absolute value of the magnetic moment is given by:

$$\langle |M| \rangle = \frac{1}{Z} \sum_{i=1}^{M} |M_i| e^{-\beta E_i}$$

$$= \frac{1}{Z} (4e^{8\beta J} + 8e^0 + 8e^0 + 4e^{8\beta J})$$

$$= \frac{4 + 2e^{8\beta J}}{\cosh(8\beta J) + 3}$$
(14)

And, finally, the susceptibility is given by:

$$\chi = \frac{1}{kT} \sigma_M^2
= \frac{1}{kT} [\langle M^2 \rangle - \langle M \rangle^2]
= \frac{1}{kTZ} \sum_{i=1}^M M_i^2 e^{-\beta E_i} - 0
= \frac{32}{kTZ} (e^{8\beta J} + 1)
= \frac{8(e^{8\beta J} + 1)}{kT(\cosh(8\beta J) + 3)}$$
(15)

2.3 Phase transitions

The Ising model in two dimensions is expected to exhibit some second order phase transitions [1]. An important quantity in the study of phase transitions is the correlation length ξ , which can be related to the size of the lattice (in the case of a finite lattice). In the case of a second-order transition, the correlation length diverges at the critical point. The two phases on either side of the critical point is expected to become identical [1]. The Ising model exhibits a second-order phase transition since the heat capacity and susceptibility diverges for an infinite lattice. Since this report explores results from finite lattices, however, the C_v and χ will not diverge, but instead it is expected to show a broad maximum around T_C with a sharpening peak as L becomes larger. Near (but below) T_C , the mean magnetization of the Ising model is given by:

$$\langle M(T) \rangle \sim (T - T_C)^{\beta}$$
 (16)

where $\beta = 1/8$ is a critical exponent. A similar relation can be seen for the heat capacity:

$$C_V(T) \sim |T - T_C|^{\alpha} \tag{17}$$

and the susceptibility:

$$\chi(T) \sim |T - T_C|^{\gamma} \tag{18}$$

In which $\alpha = 0$ and $\gamma = 7/4$. The correlation length defines the correlation of the spins as T approaches T_C , and increases as we get closer to the critical temperature. The divergent behaviour of ξ near T_C is given as:

$$\xi(T) \sim |T_C - T|^{-\nu} \tag{19}$$

The relation between the critical temperature for a finite lattice of size $L \times L$, $T_C(L)$, and the critical temperature for an infinitely large lattice, $T_C(L = \infty)$ is given by:

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu}$$
 (20)

In which a is a constant and ν is defined by Equation 19. In this report, I will use the exact result $\nu=1$ and apply this to Equation 20 in order to estimate T_C in the thermodynamic limit $L\to\infty$, which has the analytic result after Onsager: $kT_C/J=2/\ln(1+\sqrt{2})\approx 2.269$ [4].

When inserting $T = T_C$ in Equations 16 to 18, we get the following expressions:

$$\langle M(T) \rangle \sim (T - T_C)^{\beta} \to L^{-\beta/\nu}$$
 (21)

$$C_V(T) \sim |T - T_C|^{\alpha} \to L^{\alpha/\nu}$$
 (22)

$$\chi(T) \sim |T - T_C|^{\gamma} \to L^{\gamma/\nu}$$
 (23)

2.4 Monte Carlo methods

The Monte Carlo (MC) simulation can aid us in simulating the physical process we are dealing with in the Ising model. The simulation only requires that the process can be described by a PDF. Many simulations (trials) are performed and the results are sampled according to a sampling rule, which in this case is the Metropolis algorithm, which is presented in the section below The results are then taken as an average over the number of observations. One can predict the statistical error (variance) in the average result, and thus an estimate of the number of Monte Carlo trials needed to achieve a given error.

2.4.1 Markov chains

A Markov process is a process in which a conditional probability is independent of all states but the immediate predecessor. The corresponding sequence of states is called a Markov chain [3]. In the case of this report, our Markov chain determined whether a move is to be made or not based on the change from the old state of the system to the new one, ΔE .

The derivation of the transition probabilities for our system is a lengthy one, but the essence is that it allows us to perform the simulation without involving the partition function (Equation 3) [2]. We are simply left with:

$$e^{-\beta(E_i - E_j)} = e^{-\beta\Delta E} \tag{24}$$

In which i, j are different energy states and i < j[2].

In our 2D model, $e^{-\beta\Delta E}$ can take five values, that are: -8J, -4J, 0, 4J, 8J.

2.4.2 Metropolis algorithm

The Metropolis algorithm determines the sampling rule for the simulation. The essence of the test is simply whether the new state after flipping one spin is higher or lower than the previous state. If the new energy is lower, we accept the move and if it is higher, it is a bit more difficult for the move to be accepted. The way the test is implemented in the algorithm is:

In which Equation 24 is implemented. For a transition to a lower state, Equation 24 becomes positive and large, and the move will be accepted anyway. Other transitions Equation 24 might still be larger than the random number, and might be accepted, but most likely not. Thus, the system will equilibriate after some cycles.

MC-cycles	$\langle {f E} angle$	$\langle {f M} angle$	$\mathbf{C_v}$	χ
1e2	-2.0	1	0	3.9600
1e3	-1.9996	1	0.0032	3.9960
1e4	-1.9980	0.9973	0.0637	3.9969
1e5	-1.9953	0.9987	0.0298	3.9927
1e6	-1.9958	0.9986	0.0339	3.9928
1e7	-1.9960	0.9987	0.0317	3.9929
Analytical:	-1.9960	0.9987	0.0321	3.9933

Table 2: Results for $\langle E \rangle$, $\langle |M| \rangle$, C_v and χ as a function of MC-cycles compared to analytical results

2.5 Parallelization and CPU time

Since we are dealing with a vast number of MC-cycles, which is computationally heavy, a part of the report is emphasized on lowering the CPU time. The algorithm outlined above was implemented using Python 3.6 with numba-decorated functions to lower the CPU time [6]. The decorators utilized are prange, which specifies that a loop can be parallelized, and njit, which is a compilation mode that generates code that does not access the Python C API [6]. These two decorators lower the CPU time. The CPU time for some configurations can be seen in Table 4 in Appendix A.

3 Results

3.1 The Ising model for a 2×2 lattice

In table 2, the analytic results of the partition function (from the configurations listed in 2.2) and the results from the simulation of the Ising model for a 2×2 lattice is listed. It is clear from the table that a certain number of MC-cycles are needed in order to achieve satisfactory results. For 10 million MC-cycles, the results are almost identical to the analytical values to the fourth decimal (third for C_v).

3.2 The ising model for a 20×20 lattice

Figures 1 to 4 are providing an overview of how many MC-cycles are needed in order to acheve a steady-state (equilibrated) solution to the Ising model. When the temperature is 1.0 (Figure 1 and 2), an ordered (i.e. all spins up) configuration equilibrates quite quickly at the analytic expectation value in Table 2. With a random configuration (i.e. spins can be up or down), however, it takes a few more trials in order to achieve a steady-state solution. The expectation values for the energy with a random initial configuration in Figure 1 starts of at approximately -0.7 and converges quickly to between -1.99 and -2.0. After about 10 000 cycles, both random and ordered configuration converges towards the analytic solution in Table 2.

The expectation values for magnetization in Figure 2 yields pretty much the same picture, but the random initial state converges from below rather than from above and both random and initial state stabilizes around the analytic solution in Table 2.

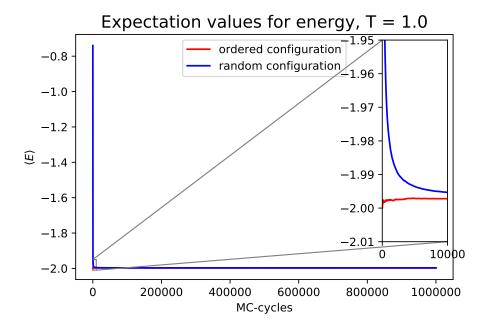


Figure 1: Expectation values of energy at T = 1.0 as a function of MC-cycles (1e6 cycles). Enhanced part is the part before the Ising model equilibrates

When the temperature is 2.4, as in Figures 3 and 4, the picture is somewhat different. For the energy (Figure 3), both ordered and random initial configuration oscillates for a while before stabilizing around approximately -1.24. Both the initial random and ordered configurations starts off way off the equilibration point, and converges from opposite directions. It takes more cycles for the system to equilibrate. This happens after around 50 000 cycles.

The expectation values for magnetization in Figure 4 are oscillating quite a bit more than for the energy, before they both stabilize at around 0.45. Other than that, this figure resembles the behaviour of Figure 3 a lot. The system stabilizes after about 100 000 cycles.

Figure 5 displays the number of accepted states during a simulation over 1e4 MC-cycles when the temperature is 1.0. With an ordered spin configuration, there is not much that is happening, and the number of accepted states rises linearly with a slope of around 0.3 accepted states per MC-cycle. With a random initial spin configuration, however, the system initially accepts more state, until equilibrium is reached, and the slope resembles that of the ordered spin configuration.

Again, when the temperature is 2.4 (Figure 6), the system becomes more exciting. Both the initial random and ordered configuration experiences more accepted states per MC-cycle, and the slope of the graph is steadily steep with about 100 accepted states per MC-cycle. The initial ordered spin configuration has a slightly steeper slope than that of the initial random spin configuration.

The probability that the simulation will yield a given energy is drawn in Figure 7 as a count of the number of times that energy appeared (note that the histogram is normalized). The simulation is ran over 1e6 MC-cycles and the sampling is initiated after the first 10 000 cycles has been ran. The

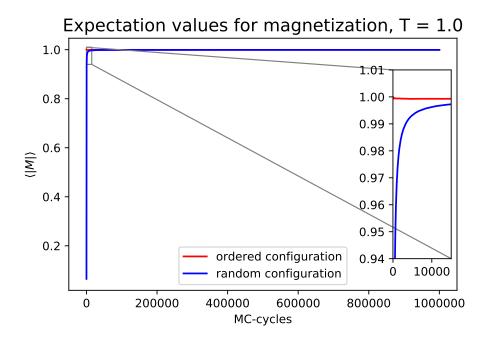


Figure 2: Expectation values of magnetization at T = 1.0 as a function of MC-cycles (1e6 cycles). Enhanced part is the part before the Ising model equilibrates

energy distribution is centered around -2 and -1.98 with a few outliers. The variance calculated from the Ising model (blue) differs a lot from the variance calculated from the linear fit by Python.

The same probability distribution is provided in Figure 8, with temperature, T=2.4 and sampling started after 100 000 cycles. The distribution almost resembles the standard normal distribution fitted to the data. The variance calculated in the Ising model is quite similar to the estimated variance.

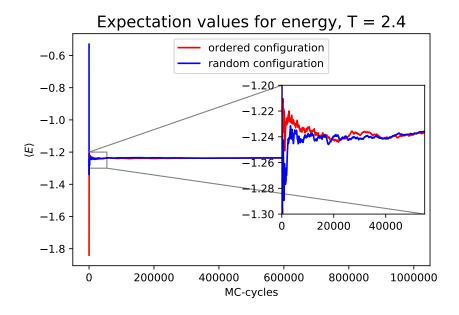


Figure 3: Expectation values of energy at T=2.4 as a function of MC-cycles (1e6 cycles). Enhanced part is the part before the Ising model equilibrates

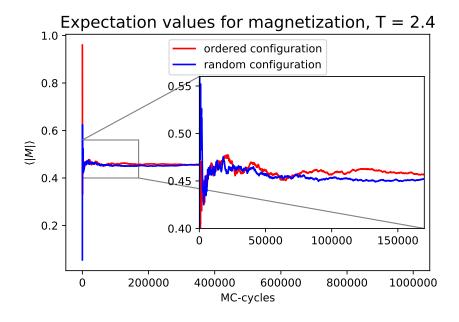


Figure 4: Expectation values of magnetization at T=2.4 as a function of MC-cycles (1e6 cycles). Enhanced part is the part before the Ising model equilibrates

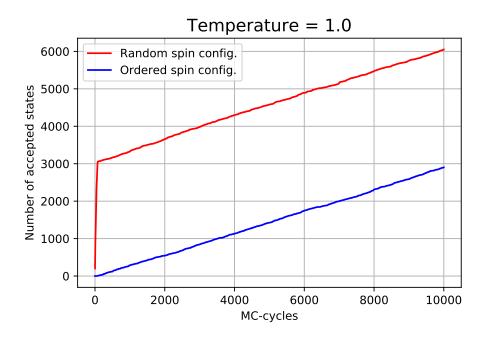


Figure 5: Number of accepted states in the Metropolis algorithm for temperature T=1.0 for 1e4 MC-cycles

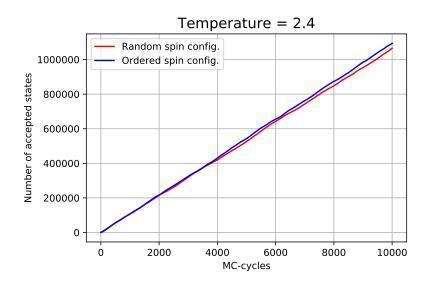


Figure 6: Number of accepted states in the Metropolis algorithm for temperature T=2.4 for 1e4 MC-cycles

Energy distribution with T = 1.0MC-cutoff: 1.0% $\sigma^2 = 7.63e - 03$ 250 Normalized number of occurences $\sigma^2 = 3.95e - 02$ 200 150 100 50 0 -1.96 -1.92 -2.00-1.98-1.94-1.90Energy per spin

Figure 7: Energy distribution after equilibration for temperature T=1.0

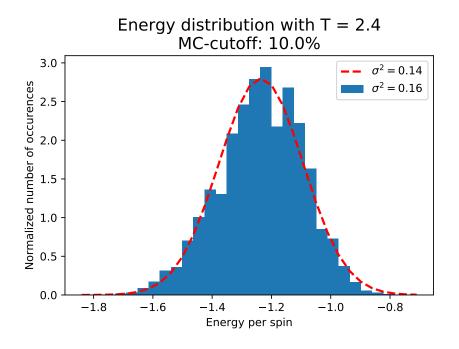


Figure 8: Energy distribution after equilibration for temperature T=2.4

3.3 Phase transitions

Figures 9 to 12 are depicting the phase transitions of the Ising model as the lattice, L, becomes larger and the temperature span includes the critical temperature, T_C . The temperature span was set to be from 2.1 to 2.5 with $\Delta T = 0.05$, and the simulation was ran for 1e6 MC-cycles.

From Figure 9 it is clear that as the temperature increases, the energy of the system does so as well. The results is more or less the same for the various lattice sizes, except for a small diverging behaviour around T_C . At that point, the largest lattic maintains the highest energy.

The heat capacity in Figure 11, as a function of energy can be seen in accordance with Figure 9. At the diverging point in energy in Figure 9, there is a peak in the heat capacity, with L = 100 yielding the highest peak.

In Table 3, the analytic values of the mean magnetization and susceptibility at $T = T_C$ are listed. Seen in context with the magnetization in Figure 10 and the susceptibility in Figure 12, it shows some accordance in terms of magnetization, but the susceptibility seems to have approximately half of the analytic value.

The magnetization in Figure 10, shows that for low temperatures, the system is yielding the same magnetization for all lattice sizes, but for higher temperatures, the magnetization is diverging, and especially after T_C . L=100 yields the lowest magnetization for the highest temperature in the simulation. The susceptibility in Figure 12 yields a peak for $T < T_C$ for small lattices and a critical temperature of approximately T=2.275 for L=100.

Lattice size	$\langle {f M}({f T}) angle$	$\chi(\mathbf{T})$
40	0.631	636.217
60	0.599	1293.495
80	0.578	2139.969
100	0.562	3162.278

Table 3: Analytic values of Equations 21 and 23 at $T=T_c$ with $\beta=1/8,\ \alpha=7/4$ and $\nu=1$

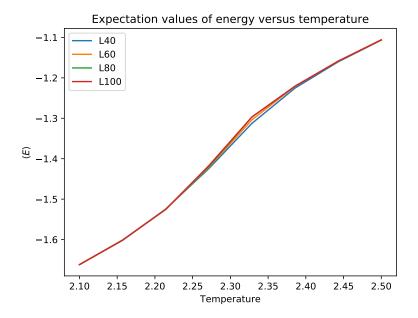


Figure 9: $\langle E(T) \rangle$ for various lattice sizes

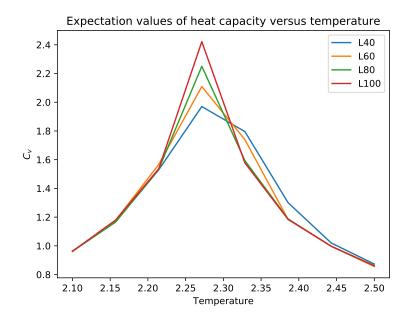


Figure 10: $C_v(T)$ for various lattice sizes

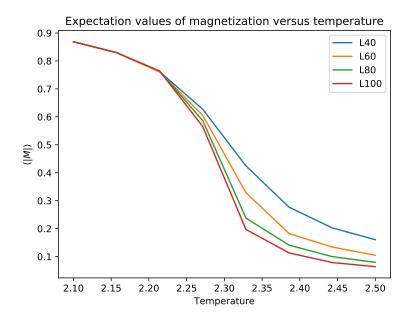


Figure 11: $\langle M(T) \rangle$ for various lattice sizes

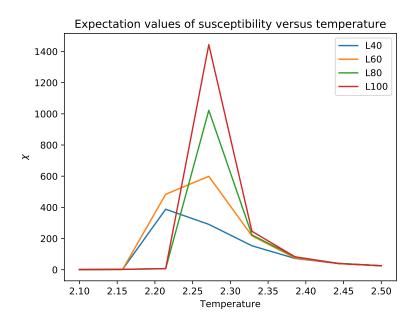


Figure 12: $\chi(T)$ for various lattice sizes

4 Discussion

The initial test of whether the Ising model manages to reproduce the analytic results for a 2×2 lattice (Table 2) shows that it actually reproduces them correctly after 1e7 cycles. Therefore, the same algorithm is applied to a larger lattice, and the results are trusted to be plausible.

The expectation values of energy and magnetization are calculated in Figure 1 to 4. These show that in the case of T=1.0, the Ising model quickly reaches an equilibrated state. Therefore, only the first 1% of the 1e6 MC-cycles are omitted in the sampling of the energies in Figure 7. The low number of accepted states (Figure 5) are due to the fact that for low temperatures, the most likely configuration is such that all spins are aligned in one specific direction [1]. We can also see from the same figure that it does not make a big difference whether the initial configuration is random or ordered as the slope of the graph is the same in the end.

In the case of temperature T=2.4, the number of accepted states is far higher (Figure 6). It is also clear from Figure 3 and 4 that the equilibration time increases as the temperature gets higher. Therefore, 10% of the 1e6 MC-cycles has been ommitted in the sampling of the energies in Figure 8.

The energy distribution for T=1.0 depicted in Figure 7 shows that the distribution of the temperature corresponds quite well with the expectation values calculated in Table 2. The variance is, however very different from the variance yielded by the linear fit, which makes some sense, since the distribution is not normal.

When the temperature is 2.4, however, the distribution in Figure 8 resembles a normal distribution to a much larger degree, and the variance from the data and the linear fit is much more similar. Most likely, the uniform distribution arises from the fact that for higher temperatures than T_C , the system is close to disorder [1], and the resulting energies are then spred around the equilibration point, even after cutting off the first 10% of the MC-cycles.

Lastly, I have looked at how the model behaves when several temperatures (including T_C) are spanned, and for several lattices (Figures 9 to 12). The mean energy (Figure 9) is steadily rising as a function of temperature, with a small divergence concerning the lattice sizes at the area around T_C , which is expected.

The heat capacity (Figure 11), being related to the mean energy by being the first derivative (Equation 12), has a peak for all lattice sizes at this point, with the highest peak for L = 100.

When it comes to the mean magnetization (Figure 12), the values at $T \approx T_C$ corresponds quite well with the analytic values in Table 3. It can also be seen that the values of mean magnetization is diverging for high temperatures, which implies that for higher temperatures, the system becomes more chaotic, which makes sense.

The susceptibility (Figure 12) is not corresponding that well to the values in Table 3, but are systematically yielding about half the analytic value for all lattice sizes, which could imply that there is a systematic mistake in my calculations. Nevertheless, the peak of the susceptibility is located at around T = 2.275, which is fairly close to Onsager's result of $T_C = 2.269$.

5 Conclusion

My implementation of the Ising model yields values close to the analytic values of expectation values of energy, $\langle E \rangle$, mean absolute magnetization, $\langle |M| \rangle$, specific heat, C_V , and susceptibility, χ for a 2 × 2 lattice when ran through the MC-algorithm 1e6 – 1e7 times.

When applied to a larger lattice of 20×20 , the model uses about 10 000 cycles at T=1.0 to equilibrate, and about 50 000 cycles at T=2.4. The spread in the energy distribution for T=1.0 is lower than what the calculated variance would suggest which is probably due to the stability of the system at low temperatures. When the temperature is 2.4, the energy distribution is shaped like a normal distribution, and the variance is close to what's calculated.

The estimation of T_C is done by calculating the $\langle E \rangle$, $\langle |M| \rangle$, C_V and χ for different lattice sizes and a range of temperatures. The general shape of the results seems reasonable, but the results for the susceptibility seems to be systematically half of what is should be according to Table 3. I could have attempted to run the model with smaller ΔT and more MC-cycles to see if this would have yielded different results.

The critical temperature read off the Figures 9 to 12, is $T_C \approx 2.275$, which is quite close to the result of Onsager [4].

6 Documentation

The material used in this project can be found in the group member's repository in GitHub: https://github.com/marikoll/FYS4150_projects/tree/master/project_4

The Python 3.6 scripts and figures can be found at:

https://github.com/marikoll/FYS4150_projects/tree/master/project_4/python_code Note: The codes have been developed in cooperation with Johanne Mehren and Stine Sagen

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A Appendix:

Lattice size	MC-cycles	Temperature(s)	CPU-time [sec]
2×2	1e2 1e3 1e4 1e5 1e6 1e7	1.0	6.29
20 × 20	1e7	1.0 2.4	1056.34
$ \begin{array}{c} 40 \times 40 \\ 60 \times 60 \\ 80 \times 80 \\ 100 \times 100 \end{array} $	1e6	2.1 - 2.5	8090.35

Table 4: CPU times for various lattice sizes, input MC-cycles and temperatures