Statistical physics and the Ising model

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Abstract

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1 Introduction

The aim of this project is to simulate a 2-dimensional binary system consisting of spins pointing either up or down in a square lattice. As the lattice size increases, such a system can rapidly become difficult, if not impossible to solve analytically due to the increasingly complex correlations between all the spins. Therefore, being able to model this problem numerically can prove to be of great interest for predicting the behaviour of real binary systems at different temperatures. We will make use of the Ising model for estimating the values of several properties of the system, such as the energy and magnetization, as well as simulating the phase transition from a magnetic phase to a phase with no magnetization. Join us, as we dive into the wonders of the Ising model, Monte Carlo simulations and 10 hour run times.

2 Theory

2.1 The Ising Model

The Ising model is built upon the idea that magnetic dipole moments of atomic spins can be represented by discrete variables, which can be in one of two states, $+1$ or -1. Furthermore, the discrete variables are arranged in a lattice where each of the variables or spins, as we will denote them from now on, is allowed to interact with its nearest neighbours only. The energy of the Ising model (without an externally applied magnetic field) is given by

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

where $s_k = \pm 1$ is the direction of the spin, $J > 0$ is the coupling constant (with a ferromagnetic ordering), expressing the strength of the interaction between neighboring spins, N is the total number of spins, and $< kl >$ indicates that we sum over nearest neighbors only.

Moreover, in this project we will use periodic boundary conditions.

The magnetic moment, or mean magnetization is defined as

$$M = \sum_{i=1}^{N} s_i \tag{2}$$

which we get by summing over all spins.

2.2 System Properties

In statistical physics, one is dependent on a probability distribution to calculate anything at all. Therefore, in this project we will use the Boltzmann distribution as the probability distribution function (PDF) to calculate all our findings throughout this project.

The Boltzmann distribution is given by

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

where P_i is the probability of the system being in state i, E_i is the energy of that state, $\beta = \frac{1}{k_B T}$, where k_B is the Boltzmann constant and T is the temperature of the whole system.

While Z is the partition function for the canonical ensemble, also called the normalization constant and is defined as

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

where N now represents the number of states.
In general, most systems have an infinity of microstates making thereby the computation of Z practically impossible.

2.3 2×2 Lattice

One of the simplest 2-dimensional cases, we have a 2×2 lattice, with only a possibility for values $+1$ or -1, also denoted as spin up and spin down, there exists 2^4 microstates. This can be visualised by figure 1.

By using equation (1) & (2) to the different microstates in figure 1, we obtain the results shown in table 1.

Number of spins up	Degeneracy	Energy	Magnetization
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: Energy and Magnetization for the microstates in Fig 1

In this project we are only focusing on the energy E, magnetization M, specific heat C_V and the magnetic susceptibility χ. Luckily, for this system, there exists analytical solutions, for these quantities.

Firstly, we get that the partition function

$$Z = \sum_{i}^{N} e^{-\beta E_i} = 2\big(6 + e^{8J\beta} + e^{-8J\beta}\big)$$

For a canonical ensemble, the expectation value for the energy is defined as

$$\langle E \rangle = -\frac{\partial \ln Z}{\partial \beta} \tag{5}$$

and the specific heat expressed from the energy

$$\langle C_V \rangle = \Big(\frac{\partial \langle E(T) \rangle}{\partial T} \Big)_V \tag{6}$$

However, we will use another approach to calculate the expectation values, and use Monte Carlo sampling to estimate the expectation values, as demonstrated below.

$$\langle E \rangle = \frac{1}{Z} \sum_i^M E_i e^{-\beta E_i} \tag{7}$$

$$\langle E^2 \rangle = \frac{1}{Z} \sum_i^M E_i^2 e^{-\beta E_i} \tag{8}$$

$$\langle M \rangle = \frac{1}{Z} \sum_i^M M_i e^{-\beta E_i} \tag{9}$$

$$\langle |M| \rangle = \frac{1}{Z} \sum_i^M |M_i| e^{-\beta E_i} \tag{10}$$

$$\langle M^2 \rangle = \frac{1}{Z} \sum_i^M M_i^2 e^{-\beta E_i} \tag{11}$$

To find the specific heat and the magnetic susceptibility, it can be shown that they are related to the variance of the energy and magnetization in the following way

$$\langle C_V \rangle = \frac{\sigma_E^2}{k_B T^2} = \frac{1}{k_B T^2} \Big(\langle E^2 \rangle - \langle E \rangle^2 \Big) \tag{12}$$

$$\langle \chi \rangle = \frac{\sigma_M^2}{k_B T} = \frac{1}{k_B T} \Big(\langle M^2 \rangle - \langle M \rangle^2 \Big) \tag{13}$$

but, in this project we will use the absolute mean magnetization $|M|$, instead of the mean magnetization M in all of the calculations, including the magnetic susceptibility.

The final expressions for all the expectation values are

$$\langle E \rangle = \frac{16J\left(e^{-\beta 8J} - e^{\beta 8J}\right)}{Z} \tag{14}$$

$$\langle C_V \rangle = \frac{512J^2\left(3e^{\frac{8J}{k_B T}} + 3e^{-\frac{8J}{k_B T}} + 2\right)}{Z^2 k_B T^2} \tag{15}$$

$$\langle M \rangle = 0 \tag{16}$$

$$\langle |M| \rangle = \frac{8\left(e^{8J\beta} + 2\right)}{Z} \tag{17}$$

$$\langle \chi \rangle = \frac{32}{Z k_B T}\left(1 + e^{8J\beta} - \frac{2}{Z}\left(e^{8J\beta+2}\right)^2\right) \tag{18}$$

The exciting and long algebraic derivation of these quantities can be found in Appendix A.

2.4 Phase Transitions & Critical Temperature

Near the critical temperature T_C, often named the Curie temperature, one can characterize the behavior of the thermodynamic quantities by a power law behavior. For the Ising model, the mean magnetization is given by

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

where $\beta = 1/8$. Similar relations exist for the heat capacity and susceptibility

$$C_V(T) \sim |T_C - T|^{\alpha}, \tag{19}$$

$$\chi(T) \sim |T_C - T|^{\gamma}, \tag{20}$$

with $\alpha = 0$ and $\gamma = 7/4$. Another important quantity is the correlation length, which is expected to be of the order of the lattice spacing for $T >> T_C$. Because the spins become more and more correlated as T approaches T_C, the correlation length increases as we get closer to the critical temperature. The divergent behavior of ξ near T_C is

$$\xi(T) \sim |T_C - T|^{-\nu}. \tag{21}$$

A second-order phase transition is characterized by a correlation length which spans the whole system. Since we are always limited to a finite lattice, ξ will be proportional with the size of the lattice. Through so-called finite size scaling relations it is possible to relate the behavior at finite lattices with the results for an infinitely large lattice. The critical temperature scales then as

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu}, \tag{22}$$

with a a constant and we will set $\nu = 1$. By rearranging the terms

$$T_C(L) = \frac{1}{L}a + T_C(L = \infty), \tag{23}$$

we can see that the critical temperature evolves linearly, being inversely proportional to the number of spins L in each dimension, and with a constant coefficient $T_C(L = \infty)$. This is the temperature we are looking to estimate, and this can be done by finding $T_C(L)$ for a set of L's and plotting the temperatures against $\frac{1}{L}$. $T_C(L)$ can be found as the corresponding temperatures

of the peak values of C_V or χ. When we have calculated multiple $T_C(L)$, we can then perform a linear regression to the data points and read off the constant term of the equation, being the intercept with the temperature-axis.

2.5 Markov Chains

When studying a physical system which evolves towards equilibrium, and want to understand how the system evolves with time, then Markov chains is the preferred way of accomplishing this.

Markov processes 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 Markov process is used repeatedly in Monte Carlo simulations in order to generate new random states. 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. In thermodynamics, this means that after a certain number of Markov processes we reach an equilibrium distribution. This mimicks the way a real system reaches its most likely state at a given temperature of the surroundings.

For the Markov processes, the time development of a systems PDF, is defined as

$$w_i(t+1) = \sum_j W_{ij} w_j(t)$$

or in matrix form

$$\hat{w}(t+1) = \hat{W}\hat{w}(t)$$

where $w_i(t)$ is the time dependent PDF of the state i, W_{ij} is the transition probability of going from state j to i and both quantities are normalized. If we have that $\hat{w}(t=\infty) = \hat{W}\hat{w}(t=\infty)$, we say that we have reached the most likely state of the system, the so-called steady state also referred to the equilibrium state.

By rewriting the transition probability W_{ij} into a product of two probabilities

$$W_{ij} = T_{ij} A_{ij}$$

where T_{ij} is the probability for making the transition from state j to state i (suggesting moves), and A_{ij} is the probability for accepting the proposed move from state j to the state i (accepting or rejecting moves).

We can then express the time development w_i as

$$w_i(t+1) = \sum_j \Big[w_j(t) T_{ij} A_{ij} + w_i(t) T_{ji} \big(1 - A_{ji}\big) \Big]$$

assuming that T and A are time-independent.

By utilizing that all the probabilities are normalised (as mentioned above), one can rewrite the equation above as

$$w_i(t+1) = w_i(t) + \sum_j \Big[w_j(t) T_{ij} A_{ij} - w_i(t) T_{ji} A_{ji} \Big]$$
$$w_i(t+1) - w_i(t) = \Big[w_j(t) T_{ij} A_{ij} - w_i(t) T_{ji} A_{ji} \Big]$$

In the limit $t \to \infty$, it can be shown that

$$w_i(t+1) = w_i \quad \text{and} \quad w_i(t) = w_i$$

which leads to

$$\sum_j w_j(t) T_{ij} A_{ij} = \sum_j w_i(t) T_{ji} A_{ji}$$

However, the condition that the rates should equal each other is in general not sufficient to guarantee that we, after many simulations, generate the correct distribution. We may risk to end up with so-called cyclic solutions. To avoid this issue, one introduces an additional condition, namely that of detailed balance [1].

$$W_{ij} w_j = W_{ji} w_i$$
$$w_j(t) T_{ij} A_{ij} = w_i(t) T_{ji} A_{ji}$$
$$\frac{T_{ij} A_{ij}}{T_{ji} A_{ji}} = \frac{w_i}{w_j}$$

3 Method

3.1 The Metropolis Algorithm

The Metropolis algorithm takes advantage of the Markov processes.

If we apply the detailed balance principle on our system with the Boltzmann distribution as the PDF, we end up with

$$w_i = \frac{e^{-\beta E_i}}{Z}, \quad \& \quad w_j = \frac{e^{-\beta E_j}}{Z}$$
$$\frac{T_{ij} A_{ij}}{T_{ji} A_{ji}} = \frac{w_i}{w_j} = e^{-\beta \left(E_i - E_j \right)} = e^{-\beta \Delta E}$$

We observe that the partition function is cancelled, which means we never need to evaluate Z, which leads to saving a ton of difficult calculations.

The simplest form of the Metropolis algorithm (sometimes called for brute force Metropolis) assumes that the transition probability T is symmetric, that means $T_{ij} = T_{ji}$, we then get

$$\frac{A_{ij}}{A_{ji}} = e^{-\beta \Delta E}$$

From the expression above we observe that the lower energies are the most probable. However, we cannot only accept moves to the lower energy states only. That would lead to biased statistical averages, since it would violate the condition ergodicity, which says that it should be possible for any Markov process to reach every possible state of the system from any given initial point, if the simulations is carried out for a long enough time.

A solution to this problem, is to define the acceptance probability A as

$$A_{ij} = \begin{cases} e^{-\beta \Delta E}, & \Delta E > 0 \\ 1, & \text{else} \end{cases}$$

implying that if we move to a state with a lower energy, we always accept this move with acceptance probability $A_{ij} = 1$. If the energy is higher, we need to check this acceptance probability with the ratio between the probabilities from our PDF.

3.2 Monte Carlo & Metropolis

In a calculation of the Ising model in two dimensions, the number of configurations is given by $2N$ with $N = L \times L$ the number of spins for a lattice of length L. Fortunately, the Metropolis algorithm considers only ratios between probabilities and we do not need to compute the partition function at all. The algorithm goes as follows

Metropolis Algorithm

1. Initialise the lattice in a configuration with energy E_{start}, by either starting in a fixed configuration or at a random configuration.
2. Choose a random position in the lattice, and change the configuration by flipping e.g., one spin only. Compute the energy of this configuration, E_{new}.
3. Calculate $\Delta E = E_{\text{new}} - E_{\text{start}}$.
4. If $\Delta E \leq 0$ we accept the new configuration.
5. If $\Delta E > 0$, calculate $w = e^{-(\beta \Delta E)}$.
6. Compare w with a random number $r \in [0, 1]$. If $r \leq w$, accept the new configuration, else we keep the previous configuration.
7. Next, update the various expectations values.
8. Repeat steps (2)-(7) for a given number of Monte Carlo cycles, which is constituted by each sweep through the lattice.
9. Divide the expectation values by the number of Monte Carlo cycles.

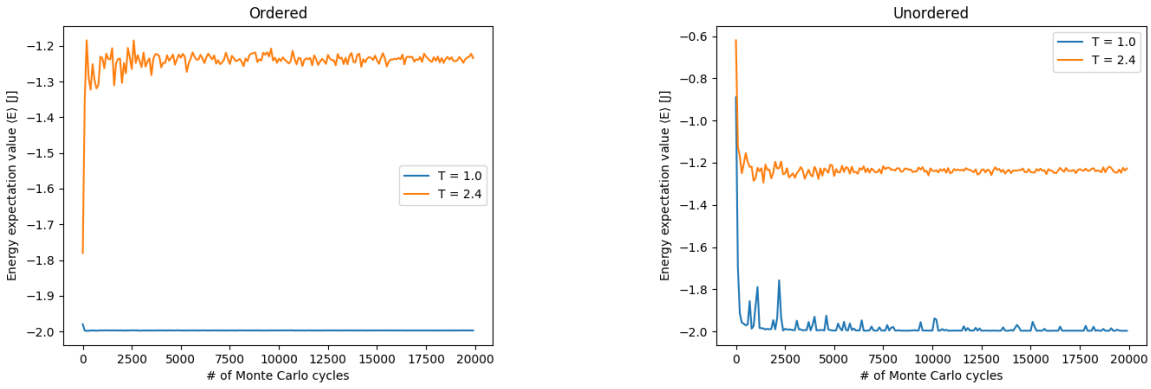
4 Implementation

Programs used in this project can be found on https://github.com/jensbd/FYS4150/tree/master/Project4 and the readme.txt on the github repository explains how to run the scripts. All calculations are done in C++, while the plotting is done in Python.
The C++ programs are mainly based on the program "IsingModel.cpp" and other codes found in the course's github repository https://github.com/CompPhysics/ComputationalPhysics [1]. We have also utilized the C++ library Armadillo [3] [4]. In addition, we have also used the numpy functions polyfit and polyval to perform linear fittings.

5 Results

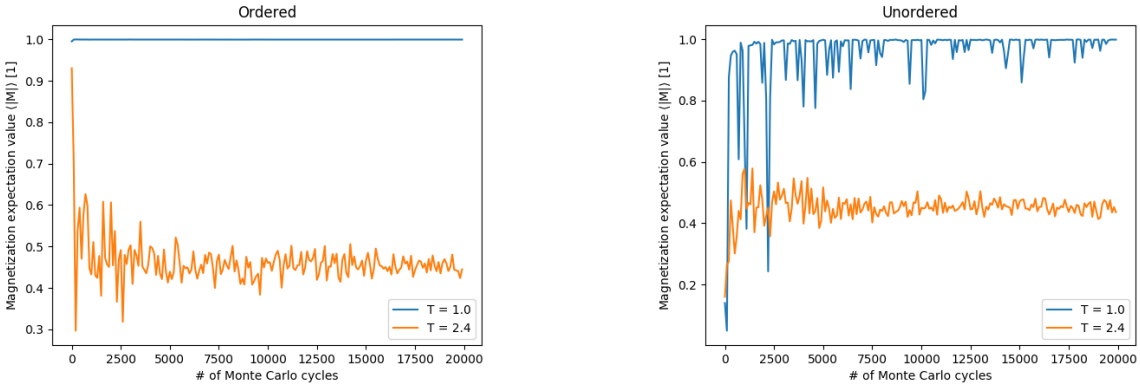
Table 2: Expectation values per spin for $L = 2$ and $T = 1.0\, kT/J$

	MC cycles (N)	$\langle E \rangle$	$\frac{\sigma_E}{\sqrt{N}}$	$\langle \lvert M \rvert \rangle$	$\frac{\sigma_{\lvert M \rvert}}{\sqrt{N}}$	$\langle C_V \rangle$	$\langle \chi \rangle$
	10^4	-1.9934	0.0046	0.99770	0.00169	0.0526	0.00717
	10^5	-1.9964	0.0011	0.99882	0.00037	0.0284	0.00351
	10^6	-1.9961	0.0004	0.99871	0.00012	0.0313	0.00383
	10^7	-1.9960	0.0001	0.99865	0.00004	0.0322	0.00404
	10^8	-1.9960	0.00004	0.99865	0.00001	0.0321	0.00403
Analytical		-1.9960		0.99866		0.0321	0.00401



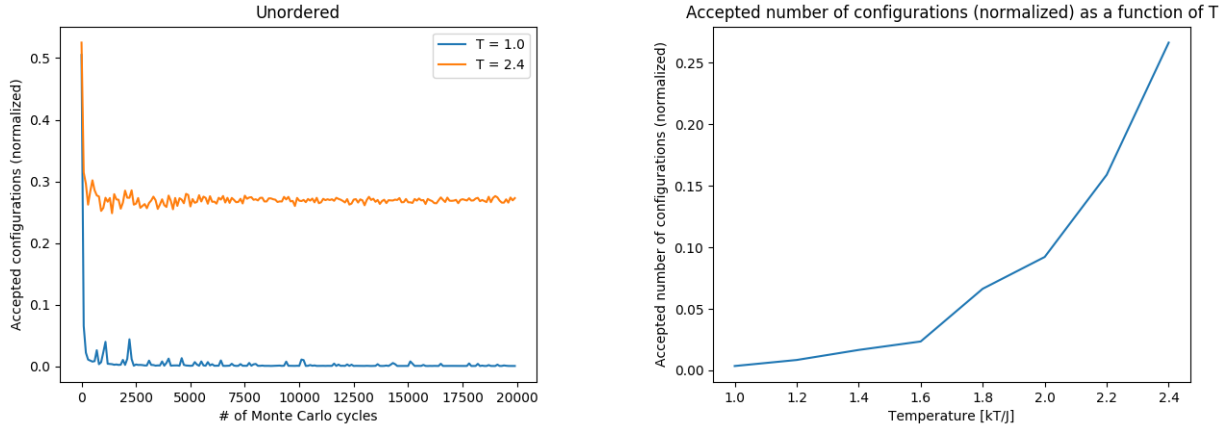
(a) (b)

Figure 1: Expectation values of the energy for two temperatues, as well as ordered (a) and unordered (b) initial states of the spin lattice. At 10 000 Monte Carlo cycles, a very stable behaviour is shown for both temperatures and initial states, with small variations in energy.



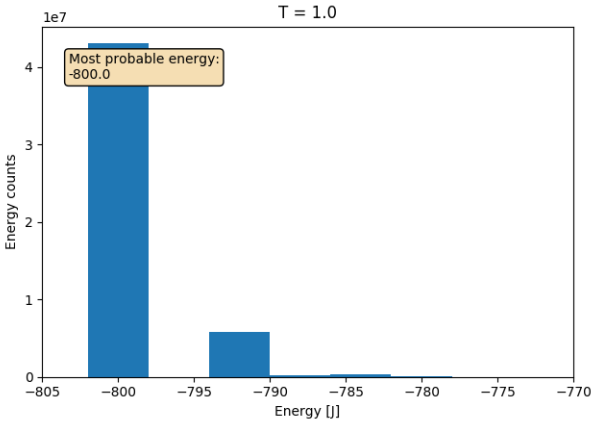
(a) (b)

Figure 2: Expectation values of the magnetization for the same temperatues and initial lattice states as above. There are more significant variations here, but stabilisiation is also achieved at 10 000 Monte Carlo cycles.

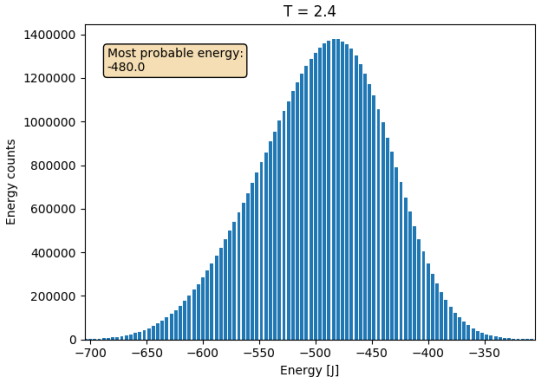


(a) (b)

Figure 3: Number of accepted spin configurations (normalized) as function of Monte Carlo cycles (a) and temperature (b). The same stabilisation at 10 000 Monte Carlo cycles as for the energy and magnetization is observed. In addition, the number of accepted configurations are shown to increase with increasing temperature.

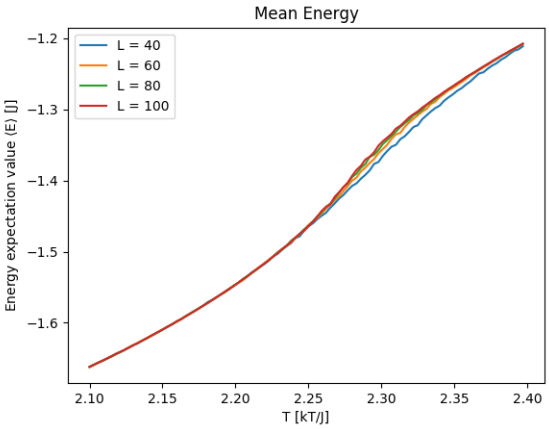


(a) $\sigma = 3.05$

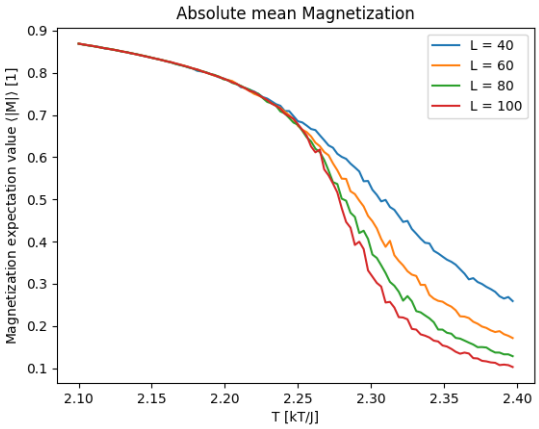


(b) $\sigma = 57.20$

Figure 4: Histograms showing probability distributions of the energy for temperatures 1.0 and 2.4. For $T = 1.0$ a significant majority of configurations are in the lowest energy state, but for $T = 2.4$, a much wider spread is observed, closely resembling the normal distribution.

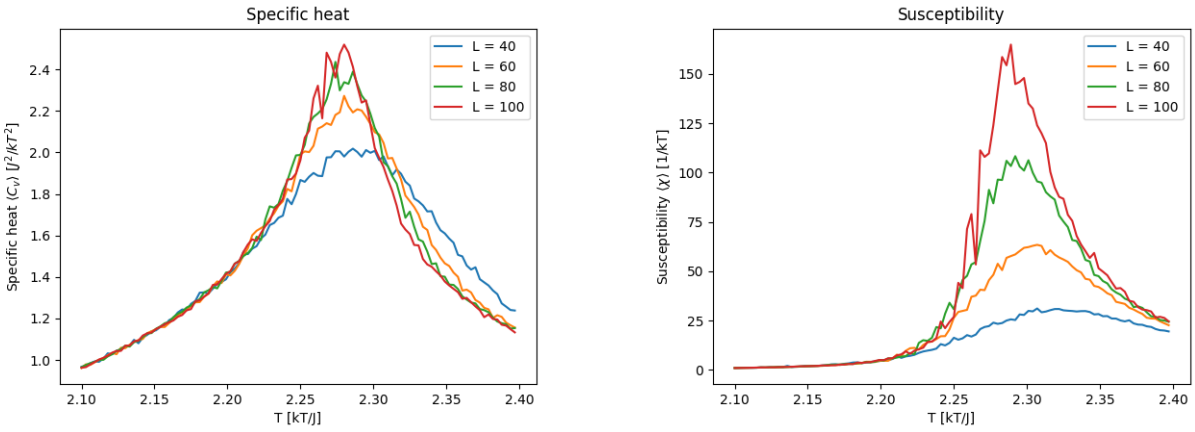


(a)



(b)

Figure 5: Expectation values for energy and magnetization as function of temperature for Lattice sizes $L = [40, 60, 80, 100]$. When T passes $2.25\,kT/J$, the plots begin to diverge from each other, although only slightly for the energy.

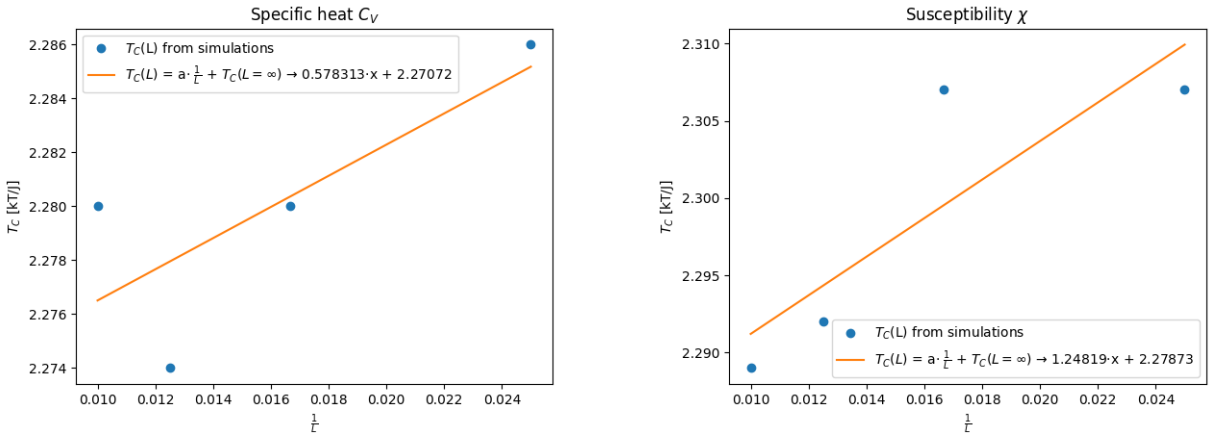


(a) (b)

Figure 6: Expectation values for specific heat and susceptibility as function of temperature for Lattice sizes $L = [40, 60, 80, 100]$. Both plots show clear peaks, corresponding to the critical temperature $T_C(L)$.

Table 3: The calculated temperatures from the maximum values of the specific heat and susceptibility from figure 6a and 6b.

Critical temperatures T_C [kT/J]		
L	C_V	χ
40	2.286	2.307
60	2.28	2.307
80	2.274	2.292
100	2.28	2.289



(a) (b)

Figure 7: Linear regression of the points from table 4. The estimated critical temperature from taking the averages of the intercepts of the plots above is $T_C = 2.27472$

Table 4: Estimation of the critical temperature T_C in the thermodynamic limit $L \to \infty$, with respect to the specific heat and susceptibility.

$L \approx \infty$	
Estimated	T_C
C_V	2.271
χ	2.279
Lars Onsager	$\frac{2}{\ln(1+\sqrt{2})} \approx 2.269$

Table 5: Timing selected runs for both a parallelised and unparallelised program

CPU-time [s]		
Monte Carlo Cycles	**Parallelised**	**Not parallelised**
10^1	0.05	0.13
10^2	0.34	1.16
10^3	3.03	11.38
10^4	42.96	120.99
10^5	494.48	1230.96

6 Discussion

Table 2 shows that after 10^5 Monte Carlo cycles, the numerical results for the energy and magnetization are within three leading digits after the decimal point compared with the analytical ones. On the other hand, the specific heat and susceptibility requires 10^7 Monte Carlo cycles to achieve the same accuracy.
These results could perhaps be explained by the fact that C_V and χ are dependent of fluctuations of the energy and magnetization, but since we are simulating such a small lattice at low temperatures, which will not fluctuate away from the equilibrium state, therefore we need a higher number of Monte Carlo cycles to simulate this, so that we can end achieve satisfactory results. Using more than 10^8 cycles will give even smaller errors, but it requires a substantial increase in computation time. Thus, $10^3 - 10^6$ Monte Carlo cycles were used throughout this project.

The analysis methods in this project is only valid for systems at equilibrium, therefore we need to investigate how our systems converges to the most likely state. Figures (1) and (2) illustrates how a lattice with both a random and ordered initial spin configuration reaches equilibrium, with respect to the mean energy and absolute mean magnitization.

We observe from figure (1) & (2) that the mean energy and absolute mean magnetization for a ordered initial spin configuration, stabilises differently depending on the temperature. For $T = 1.0$ we clearly see that the energy and magnetization has stabilised around 10^3 cycles, while $T = 2.4$ requires a higher number of cycles and stabilises around 10^4 cycles. In the case of the random initial spin configuration, it stabilises around 10^4 cycles for both $T = 1.0 \& T = 2.4$.

In figure (5a), we can see that the acceptance ratio has a clear dependence on the temperature. At $T = 1.0$ the acceptance ratio goes to zero, while for $T = 2.4$ it stabilises around 0.3. This behaviour can be explained by the thermal energy which is too low to cause a change in state, however at $T = 2.4$ the thermal energy is high enough to make more states available which means the acceptance ratio is higher than 0.

Figure (4) illustrates the probability distribution of the system at different temperatures, $T = 1.0$ and $T = 2.4$. At $T = 1.0$, the lowest energy state, $E_0 = -800J$, clearly is the most favoured one. However, when the temperature is increased to $T = 2.4$, a different energy state seems to be the most favoured one. Actually, the probability distribution takes the form of a gaussian/normal distribution around the most likely state at $T = 2.4$. We also observe at the lower temperature, the spread in energy is quite small, with a standard deviation of $\sigma_E = 3.05$, compared to the system at a higher temperature with a standard deviation of $\sigma_E = 57.20$.

By examining the results presented in figure (5) and (6) we can observe our system near the critical temperature, with respect to all quantities. From the power law discussed earlier, we know that the specific heat and the magnetic susceptibility should have a peak near the critical temperature indicating a magnetic phase transition. Our results seems to fit well with this theory.

Furthermore, the tabulated values in table (3) has been plotted as $T_C(L) = a \times \frac{1}{L} + T_C(L = \infty)$ to make a linear fit, to estimate the critical temperature for $L \to \infty$, which can be seen in figure (7). Our estimate is then the intercept of the linear model. The results from the linear fit in figure (7) has been summarized in table 4, and compared with the exact result for the critical

temperature discovered by Lars Onsager. We see that the results from the specific heat is the closest to the exact answer.

In table (5), we have presented the CPU-time for some selected runs of our program for both an unparallelised and parallelised version. We notice a considerably speed up concerning the CPU-time, when the number of Monte Carlo cycles increases. As one would expect, running the calculations on multiple CPU's gives considerably faster calculations compared to one CPU.

7 Conclusion

In this project we have implemented the infamous Ising model for a magnetic system in two dimensions, that consists of particles with either spin up or spin down. We have compared the analytical values for a 2×2 lattice with numerical values generated from the model, where it requires at least 10^7 Monte Carlo cycles to achieve a close agreement. More cycles could have been used to increase the accuracy of the results further, but this would demand a higher capacity for computational resources, which we are lacking.
Next, the size of the system was increased to a 20×20 lattice, where it was discovered that 10^4 Monte Carlo cycles were needed for the system to reach the equilibrium state, for both an ordered and unordered initial spin configuration. In addition, it was found out that the number of accepted spin configurations was directly proportional to the temperature.
It was also found that the expectation value of the mean energy and the spread of it increased when the temperature increased, indicating that when the temperature rises so does the number of available states.
Finally, the phase transitions of the system at sizes $L = 40, 60, 80$ and $L = 100$ was examined. The critical temperature was estimated to be $T_C = 2.271$, which is close to the exact solution $T_C \approx 2.269$, discovered by Lars Onsager.

For an evaluation of our work, we have seen how simple it is to implement the Ising model to simulate a real solid. Further improvements on this project, would be to utilize the parallelization of the code on a higher scale, and run it on more CPU's to simulate larger lattice sizes to get better estimates to the real world where lattice sizes is infinitely large. One could then, also attempt to take even smaller temperature step sizes, ΔT, to find better approximations to the critical temperature, T_C. All these improvements would create more data, which will lead to better statistical approximations and accurate results. This unique experience will be of great value when we further dive into new and undiscovered materials.

Appendices

A Analytic Derivation

This is the derivation for all the expectation values for a 2×2 lattice.

Partition Function Z

$$\begin{aligned} Z &= \sum_{i}^{N} e^{-\beta E_i} \\ &= \sum_{i=1}^{N=16} e^{-\beta E_i} = 12 + e^{-\beta 8J} + e^{-\beta 8J} + e^{\beta 8J} + e^{\beta 8J} \\ &= 2(6 + e^{\beta 8J} + e^{-\beta 8J}) \end{aligned}$$

where $\beta = \frac{1}{k_B T}$, k_B is Boltzmann's constant and T is the temperature of the system.

Expectation value for the energy $\langle E(T) \rangle$

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

$$\frac{\partial \ln Z}{\partial \beta} = \frac{\partial(\ln 2(6 + e^{\beta 8J} + e^{-\beta 8J}))}{\partial \beta} = \frac{\partial(\ln 2 + \ln(6 + e^{\beta 8J} + e^{-\beta 8J}))}{\partial \beta} = \frac{\partial(\ln(6 + e^{\beta 8J} + e^{-\beta 8J}))}{\partial \beta}$$

$$u = 6 + e^{\beta 8J} + e^{-\beta 8J}, \qquad \partial u = 8J\big(e^{\beta 8J} - e^{-\beta 8J}\big)\partial\beta \quad \rightarrow \quad \partial\beta = \frac{\partial u}{8J\big(e^{\beta 8J} - e^{-\beta 8J}\big)}$$

$$\begin{aligned} \frac{\partial \ln Z}{\partial \beta} &= \frac{\partial \ln u}{\partial u} \times 8J\big(e^{\beta 8J} - e^{-\beta 8J}\big) \\ &= \frac{1}{u} \times 8J\big(e^{\beta 8J} - e^{-\beta 8J}\big) = \frac{8J\big(e^{\beta 8J} - e^{-\beta 8J}\big)}{6 + e^{\beta 8J} + e^{-\beta 8J}} \end{aligned}$$

$$\langle E(T) \rangle = -\frac{\partial \ln Z}{\partial \beta} = -\frac{8J\big(e^{\beta 8J} - e^{-\beta 8J}\big)}{6 + e^{\beta 8J} + e^{-\beta 8J}} = \frac{8J\big(e^{-\beta 8J} - e^{\beta 8J}\big)}{6 + e^{\beta 8J} + e^{-\beta 8J}} = \frac{8J\big(e^{-\beta 8J} - e^{\beta 8J}\big)}{\frac{1}{2}Z}$$

$$\langle E(T) \rangle = \frac{16J\big(e^{-\beta 8J} - e^{\beta 8J}\big)}{Z}$$

Expectation value for the specific heat $\langle C_V \rangle$

$$\langle C_V \rangle = \Big(\frac{\partial \langle E(T) \rangle}{\partial T}\Big)_V = \frac{\partial}{\partial T}\Big(\frac{8J\big(e^{-\frac{8J}{k_B T}} - e^{\frac{8J}{k_B T}}\big)}{6 + e^{\frac{8J}{k_B T}} + e^{-\frac{8J}{k_B T}}}\Big)$$

$$u = 8J\big(e^{-\frac{8J}{k_B T}} - e^{\frac{8J}{k_B T}}\big), \qquad \frac{\partial u}{\partial T} = u' = \frac{64J^2}{k_B T^2}\Big(e^{-\frac{8J}{k_B T}} - e^{\frac{8J}{k_B T}}\Big)$$

$$v = 6 + e^{\frac{8J}{k_B T}} + e^{-\frac{8J}{k_B T}}, \qquad \frac{\partial v}{\partial T} = v' = \frac{8J}{k_B T^2}\Big(e^{-\frac{8J}{k_B T}} - e^{\frac{8J}{k_B T}}\Big)$$

$$\langle C_V \rangle = \Big(\frac{\partial \langle E(T) \rangle}{\partial T}\Big)_V = \frac{u' \times v - u \times v'}{v^2}$$

$$= \frac{\frac{64J^2}{k_B T^2}\Big(e^{-\frac{8J}{k_B T}} - e^{\frac{8J}{k_B T}}\Big)\Big(6 + e^{\frac{8J}{k_B T}} + e^{-\frac{8J}{k_B T}}\Big) - 8J\big(e^{-\frac{8J}{k_B T}} - e^{\frac{8J}{k_B T}}\big)\frac{8J}{k_B T^2}\Big(e^{-\frac{8J}{k_B T}} - e^{\frac{8J}{k_B T}}\Big)}{\Big(6 + e^{\frac{8J}{k_B T}} + e^{-\frac{8J}{k_B T}}\Big)^2}$$

$$= \frac{\frac{64J^2}{k_B T^2}\Big(6e^{\frac{8J}{k_B T}} + 6e^{-\frac{8J}{k_B T}} + 4\Big)}{\Big(6 + e^{\frac{8J}{k_B T}} + e^{-\frac{8J}{k_B T}}\Big)^2} = \frac{\frac{64J^2}{k_B T^2}\Big(6e^{\frac{8J}{k_B T}} + 6e^{-\frac{8J}{k_B T}} + 4\Big)}{(\frac{1}{2}Z)^2}$$

$$\langle C_V \rangle = \frac{512J^2\Big(3e^{\frac{8J}{k_B T}} + 3e^{-\frac{8J}{k_B T}} + 2\Big)}{Z^2 k_B T^2}$$

The heat capacity is also related to the variance of the energy

$$\langle C_V \rangle = \frac{\sigma_E^2}{k_B T^2}$$

where σ_E^2 is the variance of the energy and is defined as

$$\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2$$

Expectation value for the mean magnetization $\langle M \rangle$ is defined as

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

$$= \frac{1}{Z}\big(4e^{8J\beta} + 4 \times 2 \times e^0 + 4 \times 0 \times e^0 + 2 \times 0 \times e^{8J\beta} - 4 \times 2 \times e^0 - 4e^{8J\beta}\big)$$

$$\langle M \rangle = 0$$

where M_i is the magnetization of state i and E_i is the energy of the equivalent state.

The absolute mean magnetization $\langle |M| \rangle$ is defined as

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

$$= \frac{1}{Z}\big(|4|e^{8J\beta} + 4 \times |2| \times e^0 + 4 \times |0| \times e^0 + 2 \times |0| \times e^{8J\beta} + 4 \times |-2| \times e^0 + |-4| \times e^{8J\beta}\big)$$

$$\langle |M| \rangle = \frac{8\big(e^{8J\beta} + 2\big)}{Z}$$

and the expectation value of $\langle M^2 \rangle$ is

$$\begin{aligned}
\langle M^2 \rangle &= \frac{1}{Z} \sum_{i}^{M} M_i^2 e^{-\beta E_i} \\
&= \frac{1}{Z} \Big((4^2) e^{8J\beta} + 4 \times (2^2) \times e^0 + 4 \times (0^2) \times e^0 + 2 \times (0^2) \times e^{8J\beta} - 4 \times (2^2) \times e^0 + (-4^2) e^{8J\beta} \Big) \\
\langle M^2 \rangle &= \frac{32}{Z} \big(1 + e^{8J\beta} \big)
\end{aligned}$$

The corresponding variance σ_M^2 is

$$\sigma_M^2 = \langle M^2 \rangle - \langle M \rangle^2$$

The variance defines the susceptibility χ

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

but in this project we will work with the susceptibility χ defined as

$$\begin{aligned}
\langle \chi \rangle &= \frac{1}{k_B T} \Big(\langle M^2 \rangle - \langle |M| \rangle^2 \Big) \\
&= \frac{1}{k_B T} \left(\frac{32}{Z} \big(1 + e^{8J\beta} \big) - \Big(\frac{8(e^{8J\beta} + 2)}{Z} \Big)^2 \right) \\
\langle \chi \rangle &= \frac{32}{Z k_B T} \left(1 + e^{8J\beta} - \frac{2}{Z} \big(e^{8J\beta + 2} \big)^2 \right)
\end{aligned}$$

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