

Ising Model

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Abstract

The Ising Model, developed by Dr. Ernst Ising, is a mathematical model of ferromagnetism in statistical physics. It allows the identification of phase transitions as a simplified model of reality as well as investigating other observables. The Ising model can often be difficult to evaluate numerically if there are many states in the system, which gives motivation to use Monte Carlo methods such as the Metropolis algorithm. The aim of this discussion is to investigate observables and evaluate the behavior of the system when using the Metropolis algorithm. It turns out that the Ising Model is a good model for investigating expectation values such as energy and magnetization, and the single flip Metropolis algorithm is good for lower temperatures, but need some time to reach a steady state on big lattices around the critical temperatures.

Introduction

In statistical mechanics an ideal system is one in which the particles do not exert significant forces on each other. Then it is often possible to break the system down into subsystems and treat these systems one at a time and then sum over the subsystems in the end. In the real world, many systems are not ideal and we call them nonideal systems. In fact, spontaneous magnetization is a nonideal system and you have to treat the whole system at once. Predicting the behavior of such nonideal systems, consisting of many mutual interacting particles is often difficult. Often it is not possible to calculate thermodynamic quantities exactly, and you have to resort to approximations.

In classical electromagnetism, magnetization is the vector field that expresses the density of permanent or induced magnetic dipole moments in a magnetic material. The origin of the magnetic moments responsible for magnetization can be either microscopic electric currents resulting from the motion of electrons in atoms, or the spin of the electrons or the nuclei. Ferromagnetism[3] is the basic mechanism by which certain materials form permanent magnets, or are attracted to magnets. They carry out spontaneous magnetization which is the appearance of an ordered spin state (magnetization) at zero applied magnetic field in ferromagnetic and ferrimagnetic materials below a critical point called the Curie temperature or T_C . In other words ferromagnetic material is a

material that can be magnetized by an external field and remain magnetized after the external field is removed. In physics one distinguishes between several types of magnetism. Ferromagnetism is the strongest type which is the only one that typically creates forces strong enough to be felt. There are also other types of substances that respond weakly to magnetic fields, such as paramagnetism, diamagnetism and antiferromagnetism. This discussion will focus on ferromagnetic material on look at the behavior around the critical point where a phase transition is expected.

Ising Model

The Ising Model is used for modelling ferromagnetic and anti-ferromagnetic materials. The model represents a lattice occupied by atoms where each atom can have dipole moments or spin, as seen in the figures below. The quantum mechanical nature of spin causes the electron to only be able to be in two states where the magnetic field is pointing up or down. This is called a binary system. When these microscopic dipoles are aligned in the same direction, their individual magnetic fields add together causing a measurable macroscopic field. One should notice that materials can divide themselves into smaller chunks or domains which are magnetized differently from the net magnetization. Ferromagnetic materials 1a are strongly ordered and have a net magnetization $\langle M \rangle \neq 0$ for $T < T_C$. They are able to maintain spontaneous magnetization even under the absence of external fields. When the temperature is above T_C , the tendency to stay ordered is disrupted due to competing effects from thermal motion and behaves like a paramagnetic substance 1d where $\langle M \rangle = 0$. For a ferromagnetic substance the coupling parameter $J > 0$. For an antiferromagnetic substance 1b where the exchange interactions between the electrons tend to favour the alignment of neighbouring atoms with opposite spin $J < 0$.

↑	↑	↑	↑
↑	↑	↑	↑
↑	↑	↑	↑
↑	↑	↑	↑

(a) Ferromagnet ordering: Below T_C , spins are aligned parallel in magnetic domains.

↑	↓	↑	↓
↓	↑	↓	↑
↑	↓	↑	↓
↓	↑	↓	↑

(b) Antiferromagnetic ordering: Below T_N , spins are aligned anti-parallel in magnetic domains.

↑	↓	↑	↓
↓	↑	↓	↑
↑	↓	↑	↓
↓	↑	↓	↑

(c) Ferrimagnetic ordering: Below T_C , spins are aligned anti-parallel, but do not cancel.

↑	↑	↑	↓
↓	↓	↓	↑
↓	↓	↑	↑
↓	↑	↓	↓

(d) Paramagnetic ordering: Above T_C , spins are randomly oriented. (Any of the other configurations.)

Each atom can adopt two states, as explained above, corresponding to $s = \{-1, 1\}$ where s represents the spin. In this discussion $s_\uparrow = 1$ and $s_\downarrow = -1$. The spin interaction is dependent of the coupling parameter J_{ij} between the adjacent atoms. We use periodic boundary conditions which are a set of boundary conditions which are often chosen for approximating large (infinite) system. It will be explained in the next chapter. The model is defined in the Canonical Ensemble (N, V, T) and the energy of a configuration is given in terms of the Hamiltonian:

$$E(s) = -J_{ij} \sum_{\langle ij \rangle} s_i s_j - h \sum_i s_i$$

where $\langle ij \rangle$ indicates that s_{ij} is the spin of particle and h is the external field strength. In this discussion we are looking at a situation with no external magnetic field, so $h = 0$ and then the last term vanishes. In the canonical ensemble the partition function[2] is given by:

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

where M is the number of all microstates, $\beta = 1/k_B T$, k_B is the Boltzmann constant and E_i is the energy of the system in configuration i . In order to calculate expectation values such as the mean energy $\langle E \rangle$ as a function of T , it

is necessary to introduce the probability distribution (Boltzmann distribution):

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

The energy in the sense of a canonical ensemble is expressed as an expectation value since energy can be exchanged with the surroundings. The mean energy $\langle E \rangle$ and the corresponding variance σ_E^2 can be calculated with the probability distribution:

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

Using the same approach as for energy, the mean value of the absolute value of the magnetization $\langle M \rangle$ and the corresponding variance σ_M^2 is found to be:

$$\begin{aligned}\langle |M| \rangle &= \frac{1}{Z} \sum_i^M |M_i| e^{-\beta E_i} \\ \sigma_M^2 &= \langle M^2 \rangle - \langle M \rangle^2 \\ &= \frac{1}{Z} \sum_{i=1}^{M'} M_i^2 e^{-\beta M_i} - \left(\frac{1}{Z} \sum_{i=1}^{M'} M_i e^{-\beta M_i} \right)^2\end{aligned}$$

From the variances of the energy, we can obtain the specific heat capacity C_V and the susceptibility χ , by dividing our expressions for the variance with $k_B T^2$ and $k_B T$ respectively:

$$\begin{aligned}\chi &= \frac{1}{k_B T} \sigma_M^2 \\ &= \frac{1}{k_B T} (\langle M^2 \rangle - \langle M \rangle^2) \\ C_V &= \frac{1}{k_B T^2} \sigma_E^2 \\ &= \frac{1}{k_B T^2} (\langle E^2 \rangle - \langle E \rangle^2)\end{aligned}$$

Example of Configuration	Spin Up	Degeneracy	Energy	Magnetization
$\begin{array}{cc} \uparrow & \uparrow \\ \uparrow & \uparrow \end{array}$	4	1	$-8J$	4
$\begin{array}{cc} \downarrow & \uparrow \\ \uparrow & \uparrow \end{array}$	3	4	$0J$	2
$\begin{array}{cc} \uparrow & \uparrow \\ \downarrow & \downarrow \end{array}$	2	4	$0J$	0
$\begin{array}{cc} \uparrow & \downarrow \\ \downarrow & \uparrow \end{array}$	2	2	$8J$	0
$\begin{array}{cc} \uparrow & \downarrow \\ \downarrow & \downarrow \end{array}$	1	4	$0J$	-2
$\begin{array}{cc} \downarrow & \downarrow \\ \downarrow & \downarrow \end{array}$	0	1	$-8J$	-4

Figure 2: Energy states for a 2×2 Lattice

A simple 2×2 Lattice with Periodic Boundary Conditions

Periodic Boundary Conditions for a one-dimensional case means that the right neighbour of the last spin s_N is assumed to take the value of s_1 and that the left neighbour of the first spin s_1 takes the value of s_N . In a two-dimensional case with two spins in each dimension we consider a matrix like:

$$\begin{array}{cccc} & (s_3) & (s_4) & \\ (s_2) & s_1 & s_2 & (s_1) \\ (s_4) & s_3 & s_4 & (s_3) \\ & (s_1) & (s_2) & \end{array}$$

where the PBC neighbours are given in parenteces, such that the right neighbour of the last spin on each row takes the value of the first spin on the corresponding row and the left neighbour of the first spin on each row takes the value of the last spin on the corresponding row. We'll have to adopt the same strategy for the columns such that the top neighbour of the first spin in each column takes the value of the last spin in the same column and the bottom neighbour of the last spin in each column takes the value of the first spin in the same column. We don't consider the diagonal neighbours. Figure 2 shows a diagram of the different energy states in the particular case when $L = 2$ with periodic boundary conditions. Note that the left most column shows an example of a configuration for that specific energy, such that there will be other configurations that gives the same energy when the degeneracy > 1 .

Analytic calculations

We'll use that $T = \beta = J = 1$ in the following calculations. The partition function becomes:

$$\begin{aligned} Z &= \sum_{i=1}^M e^{-\beta E_i} \\ &= 2e^{8\beta J} + 12e^0 + 2e^{-8\beta J} \\ &= 2(6 + 2 \cosh(8\beta J)) \\ &= 4(3 + \cosh(8)) \end{aligned}$$

The expectation value of the energy $\langle E \rangle$ becomes:

$$\begin{aligned} \langle E \rangle &= \frac{1}{Z} \sum_{i=1}^M E_i e^{-\beta E_i} \\ &= \frac{1}{Z} (2(-8J e^{8\beta J}) + 2(8J e^{-8\beta J})) \\ &= \frac{1}{Z} (-16J (e^{8\beta J} - e^{-8\beta J})) \\ &= \frac{-32(\sinh(8))}{4(3 + \cosh(8))} \\ &= \frac{-8(\sinh(8))}{3 + \cosh(8)} \\ &\approx -7.98 \\ \langle E \rangle / \text{spins} &\approx 1.99 \end{aligned}$$

where we have divided by the spins to obtain the mean energy per spins. The expectation value of the absolute value of the magnetization $\langle |M| \rangle$ becomes:

$$\begin{aligned}
\langle |M| \rangle &= \frac{1}{Z} \sum_i^M |M_i| e^{-\beta E_i} \\
&= \frac{1}{Z} \left(1 \cdot 4e^{-\beta(-8J)} + 4 \cdot 2e^{-\beta(0J)} + 4 \cdot 0e^{-\beta(0J)} + 2 \cdot 0e^{-\beta(8J)} + 4 \cdot 2e^{-\beta(0J)} + 1 \cdot 4e^{-\beta(-8J)} \right) \\
&= \frac{1}{Z} (4e^{8J\beta} + 8e^0 + 8e^0 + 4e^{8J\beta}) \\
&= \frac{1}{Z} (8e^{8J\beta} + 16e^0) \\
&= \frac{8(2 + e^8)}{4(3 + \cosh(8))} \\
&= \frac{2(2 + e^8)}{3 + \cosh(8)} \\
&\approx 3.99
\end{aligned}$$

$$\langle |M| \rangle / \text{spins} \approx 0.99$$

To find the susceptibility we need to calculate:

$$\begin{aligned}
\langle M^2 \rangle &= \frac{1}{Z} \sum_i^M M_i^2 e^{-\beta E_i} \\
&= \frac{1}{Z} \left(1 \cdot 16e^{-\beta(-8J)} + 4 \cdot 4e^{-\beta(0J)} + 4 \cdot 0e^{-\beta(0J)} + 2 \cdot 0e^{-\beta(8J)} + 4 \cdot 4e^{-\beta(0J)} + 1 \cdot 16e^{-\beta(-8J)} \right) \\
&= \frac{1}{Z} (16e^{8J\beta} + 16e^0 + 16e^0 + 16e^{8J\beta}) \\
&= \frac{1}{Z} (16e^{8J\beta} + 32 + 16e^{8J\beta}) \\
&= \frac{1}{Z} (32(1 + e^{8J\beta})) \\
&= \frac{32(1 + e^{8J\beta})}{Z} \\
&= \frac{32(1 + e^{8\beta})}{4(3 + \cosh(8))} \\
&= \frac{8(1 + e^{8\beta})}{3 + \cosh(8)} \\
&= \frac{8(1 + e^8)}{3 + \cosh(8)} \\
&\approx 15.97
\end{aligned}$$

The susceptibility is given by:

$$\begin{aligned}\chi &= \frac{1}{k_B T} (\sigma_M^2) \\ &= \langle M^2 \rangle - \langle |M| \rangle^2 \\ &\approx 0.004\end{aligned}$$

after we have divided by the spins. To calculate the variance we need:

$$\begin{aligned}\langle E^2 \rangle &= \frac{1}{Z} \sum_{i=1}^M E_i^2 e^{-\beta E_i} \\ &= \frac{1}{Z} (2(64J e^{8\beta J}) + 2(64J e^{-8\beta J})) \\ &= \frac{1}{Z} (128J (e^{8\beta J} + e^{-8\beta J})) \\ &= \frac{128(\cosh(8))}{4(3 + \cosh(8))} \\ &= \frac{32(\cosh(8))}{3 + \cosh(8)} \\ &\approx 31.94\end{aligned}$$

The heat capacity is given by:

$$\begin{aligned}C_V &= \frac{1}{k_B T^2} \sigma_E^2 \\ C_V &= \frac{1}{k_B T^2} (\langle E^2 \rangle - \langle E \rangle^2) \\ &= 0.032\end{aligned}$$

after we have divided by spins.

A short description of the Algorithm/Code

The code can be found at: <https://github.com/andehus/isingmodel.git>

A short description of the main steps in the metropolis algorithm[1] and how to code works follows below.

Algorithm

1. Create an initial energy state by positioning yourself at a random configuration in the lattice.

2. Flip one spin so that the initial configuration is changed and define a trial state.
3. Calculate the difference in energy between the initial state and the trial state.
4. We want to move towards the energy minimum, so if the difference in energy $\Delta E \leq 0$ we accept the configuration. Go to step 7.
5. If the difference in energy is positive we calculate $w = e^{-(\beta \Delta E)}$
6. Compare w with random number. If r is less or equal to w, then accept. If not, keep the old config.
7. Update variables
8. Go to step 2 and repeat
9. Divide by cycles, spin and write to file

Code

main() Starts the timing of the algorithm, reads the command line parameters and set up file handling.

We loop over the temperature call for **metropolissampling()**, **writeto-file()**

metropolis() We set up a random generator, define a spinmatrix and variables E and M. Call for **initLattice()** which sets the spin config. We create an array for ΔE and calculate $e^{-(\beta \Delta E)}$ before looping over Monte Carlo cycles since they are known. Then we loop over cycles and for each cycle we loop over the lattice to calculate dE. We draw a random number and if that number is less than the energy difference, we accept the configuration and flips one spin. This process happens for all cycles at a given temperature. In the end we update our expectation values and proceeds to the next temperature step and repeat the process.

initLattice() Sets the init spin configuration, magnetic moment and energy.

Comparing analytic and experimental values

Figure 3 shows a diagram of calculated values when running our simulation for the 2×2 Lattice for $T = 1.0$.

MC cycles	$\langle E \rangle / n_{spins}$	$\langle M \rangle / n_{spins}$	C_V / n_{spins}	χ / n_{spins}	Time(sek)
10^1	-2.0	1.0	0.0	0.0	0.000131
10^2	-2.0	1.0	0.0	0.0	0.000141
10^3	-1.998	0.9995	0.015984	0.000999	0.000348
10^4	-1.9968	0.9989	0.02555904	0.00339516	0.002775
10^5	-1.99536	0.9984	0.037033882	0.00494976	0.027949
10^6	-1.996054	0.998664	0.031505716	0.0040628604	0.26822
10^7	-1.9959822	0.99865925	0.032090629	0.0040203096	2.61538
Analytic	-1.9959821	0.9986607327	0.032082331	0.00401073951	

Figur 3: Comparison between numerical and analytic calculations for different number of Monte Carlo cycles

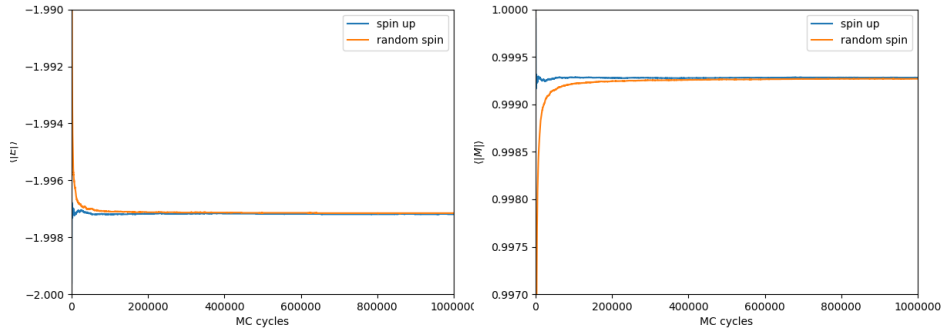
All values are divided by spins ($n_{spins} = 4$). According to the table above, we should have at least 10^6 Monte Carlo cycles to get a reasonable result. This is after three runs, so the statistics could of course be improved by running many times. It also depend on the variable and the error gets bigger when calculating the specific heat and susceptibility which depend on the squared values. So already after 10^3 Monte Carlo cycles is the simulation giving acceptable results for the energy and magnetic moment at $T = 1.0$. One can also observer from the timing in the right column that adding and order of Monte Carlo cycles will increase time with approximaty one order, except in the beginning where a significant part of the time is used to filehandling, writing to file, etc... I could have placed the timing function just around the metropolis algorithm, but usually the program is runned by a number of cycles such that this time is vanishing compared to the algorithm.

A 20×20 Lattice

Monte Carlo Cycles

It would be interesting to investigate how the algorithm behave with the number of Monte Carlo cycles and how much the starting spin configuration would impact the result.

Low temperature $T = 1.0$



Figur 4: Mean energy (Left) and mean magnetization (Right) as a function of Monte Carlo cycles at $T = 1.0$.

Figure 4 shows the mean energy and the mean magnetization as a function of Monte Carlo cycles for low temperature $T = 1.0$. We would expect that the final set of configurations that define the established equilibrium at $T = 1.0$, will be dominated by those configurations where most spins are aligned in one specific direction. It is preferable to use a starting configuration with ordered spin (all pointing upwards) at $T = 1.0$. As we can see, after a short time, the steady state is reached for an ordered spin configuration. When using random spin configuration, the algorithm perform a guess, which most likely will put us far away from the ground state. The differences between ordered and random starting configuration will be less significant as one increases the number of Monte Carlo cycles.

Higher temperature (around the T_C)

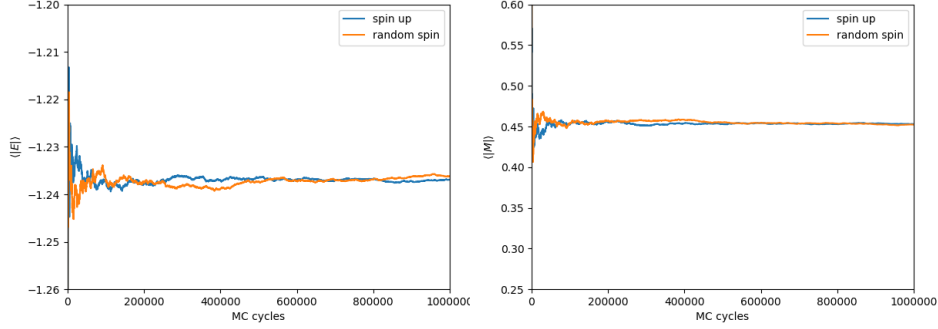


Figure 5: Mean energy (Left) and mean magnetization (Right) as a function of Monte Carlo cycles at $T = 2.4$.

Figure 5 shows the mean energy and the mean magnetization after we have increased the temperature to $T = 2.4$, which is around the critical temperature. One would expect that for higher temperatures it is better to use a random spin configuration as starting point, because a disordered configuration as start configuration brings us closer to the average value at the given temperature. One would expect that it would be better to use an initially random ordered spin configuration since the temperature is further away from the ground state temperature. Since the expectation values oscillates around the equilibrium point when the steady state is reach, is not easy to see exactly when both curves have reached the steady state. On the other hand, we don't know the perfect initial spin configuration for $T = 2.4$, so when the algorithm performs the guess, it might be a bad guess. More cycles are needed to reach the steady state with an ordered configuration. The single spin flip based Metropolis algorithm might not be the best choice when studying properties of the Ising model near T_C .

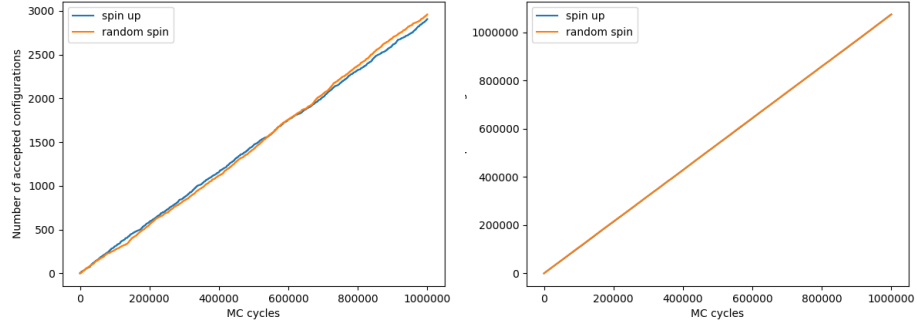


Figure 6: Total number of accepted configurations as a function of Monte Carlo cycles for $T = 1.0$ (Left) and $T = 2.4$ (Right)

Figure 6 shows how the number of accepted configurations behave as a function of Monte Carlo cycles. The configurations are added per 100 cycle. At $T = 1.0$ most of the configurations are rejected and often only accepts 1 – 2 configurations per cycle, which means that the total number of accepted calculations is about 1/3 of the number of Monte Carlo cycles. For $T = 2.4$ a lot more configurations are accepted per cycle (about 100), which also explains why it takes more time to reach the equilibrium state.

Probability distribution

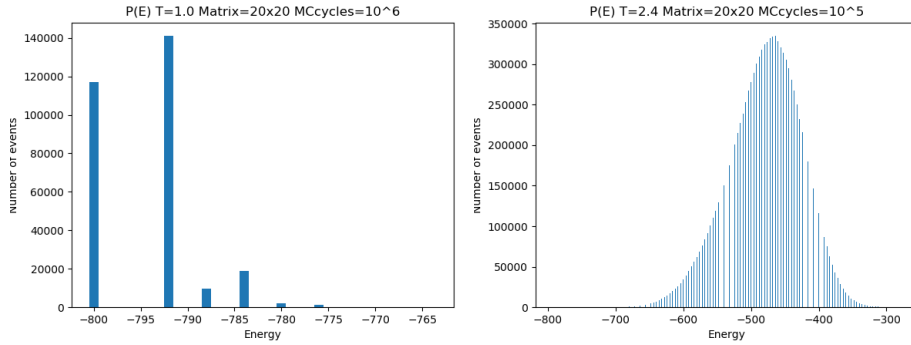


Figure 7: Probability distribution for $T = 1.0$ (Left) and $T = 2.4$ (Right)

From the plots above 7 we see that the system at $t = 1.0$ has a distribution which is more narrow than for $t = 2.4$. This implies that the variance is bigger for $t = 2.4$. This also denotes that the system at $t = 1.0$ stabilizes quicker, while the system at $t = 2.4$ seems to be less stable. From the simulation at $t = 1.0$,

the calculated variance $\sigma_E^2 = 0.023$ and at $t = 2.4$ the variance $\sigma_E^2 = 1.38$. The greater variance at $t = 2.4$ corresponds to what we observed on the histograms with more spreading for this temperature.

Numerical studies of phase transitions

As the temperature increases, the tendency to stay ordered reduces because of thermal fluctuations and the net magnetization, which is a function of net order in the system starts dropping. Beyond temperature T_C , there is no more tendency to stay ordered and due to complete disorderness, the net magnetization per site drops to zero. I first ran the simulation with time steps $\Delta t = 0.05, 0.01, 0.005$, where I decreased the area (with some margin to not miss the maximum) around the critical temperature and increased the resolution to find a more precise maximum value. Calculations with small temperature steps and great lattice size can be time consuming, but one might gain a lot in parallelizing the code. So I tried to split the simulation into different parts and run the code on about 10 different computers (during a couple of nights when nobody else was using the machines) with a time step $\Delta t = 0.001$, where each machine calculated expectation values in a smaller temperature interval depending on the CPU and available computers. This part of the code was parallelized and optimized for four cores. Figure 8 below shows the Energy for different lattices as a function of the Temperature. The results are produced with the metropolis algorithm with 10^6 Monte Carlo cycles with a time step $\Delta t = 0.001$.

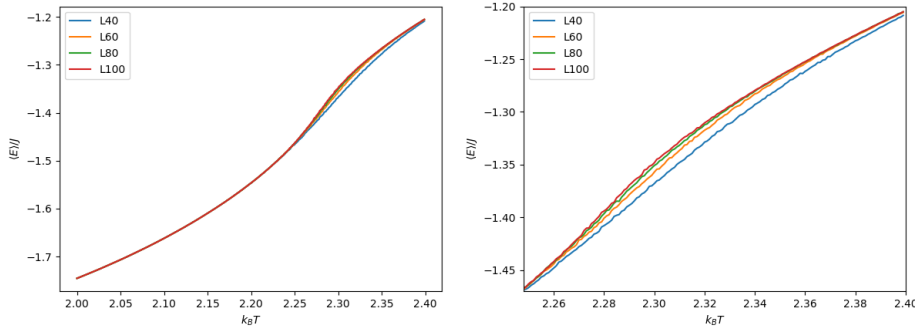


Figure 8: Average energy per spin as a function of the lattice size for the two-dimensional Ising model. The plot on the left shows the same simulation, but on a smaller interval.

In the energy plots above we can see that the energy increases with temperature. The global trend is the same for all lattice sizes, however one can notice that when approaching the critical temperature, it increases a bit faster. This effect is clearer for the greater lattices with our Monte Carlo method. Figure 9

shows the magnetization plot, one notices that the absolute value of the magnetization decreases with higher temperature, and we see a clear drop around the critical temperature. It represents the phase transition moment when the spins are pointing in random directions and cancelling each other in absolute value.

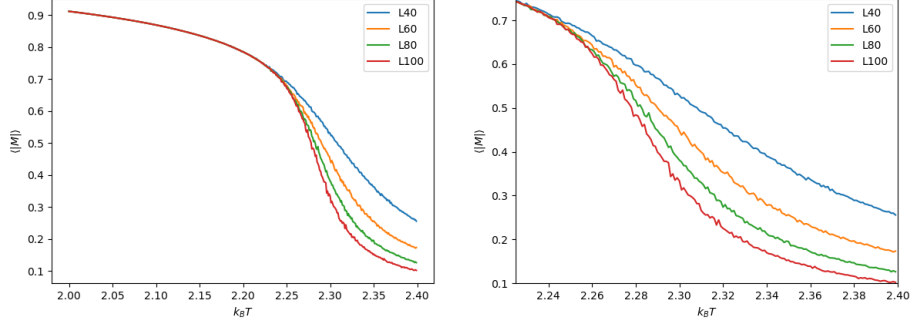


Figure 9: The expectation value of the absolute value of the magnetization as a function of the lattice size for the two-dimensional Ising model.

Figure 10 shows how the specific heat capacity varies with temperature and lattice size. One can observe a peak around the critical temperature. The behavior is clearer for greater lattice size and as we increase the lattice size the peak gets sharper.

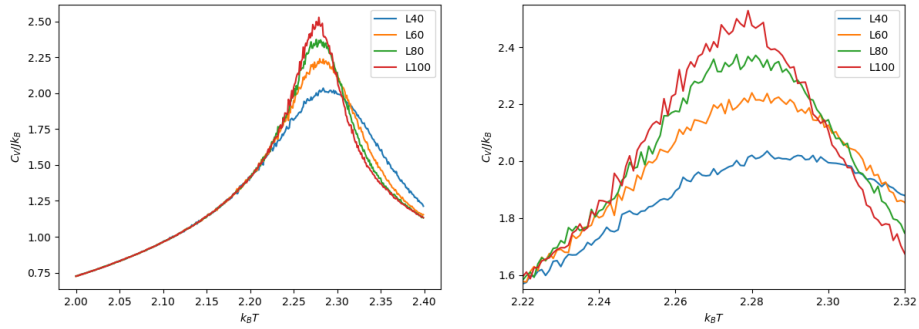
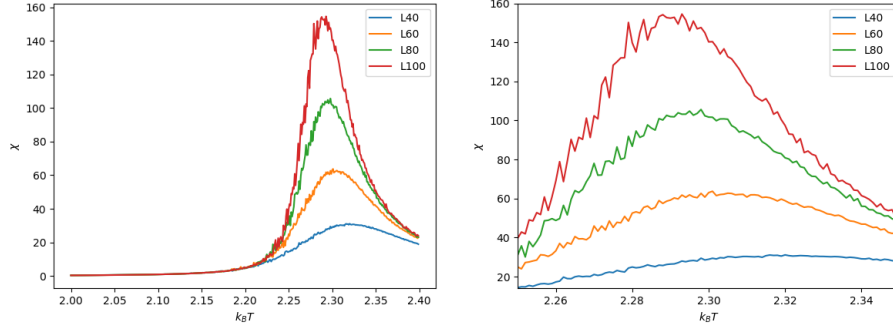


Figure 10: The expectation value of the absolute value of the magnetization as a function of the lattice size for the two-dimensional Ising model.

Figure 11 shows the susceptibility χ as a function of temperature and lattice size. This shows a peak around the critical temperature as we saw in the plot of the specific heat capacity, but the peak is even sharper. Like for specific heat the behavior is more apparent for greater lattice size.



Figur 11: The expectation value of the absolute value of the magnetization as a function of the lattice size for the two-dimensional Ising model.

Extracting the critical temperature

To calculate the critical temperature the following equation[1]:

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

has to be solved for $T_C(L = \infty)$. With $\nu = 1$:

$$T_C(L = \infty) = T_C(L) - a\frac{1}{L}$$

When L tends to infinite, then $a\frac{1}{L}$ tends to 0. Therefore we can estimate $T_C(L = \infty)$ with a linear interpolation of functions of $T_{max}(C_V)$ for a given L to get the value which intercepts with the y-axis. Using $L = 40, 60, 80, 100$ we will get four maximum values for C_V which each correspond to a temperature. With plotting the temperature as a function of $1/L$, finding the slope and extend it to intercept with the y-axis we obtain the value $T_C \approx 2.278$ which is not that far away from Lars Onsagers result $T_C \approx 2.269$.

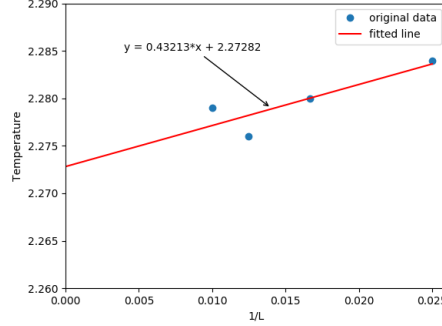


Figure 12: A linear fit of the points corresponding to the temperature of the max value of C_V for $L = 40, 60, 80, 100$ with a resolution $\Delta t = 0.001$.

Conclusion

The Ising Model seems to be a good method for investigating and identifying phase transitions of ferromagnets. The selected expectation values are reasonable and the prediction of the critical temperature is close enough for our purpose. For even greater lattices and more precision one might have to consider other algorithms since the single flip metropolis algorithm shows some weakness around the critical temperature. Reaching the steady state around T_C is time consuming when precision is important. So, then it takes a lot of time to obtain good values for the critical temperature. I have used mpi to parallelize the processing of the simulation. I initially experienced issues with never-ending processes on some computers. After some investigations, I found out that some processes were not respecting the cycles amount, which caused infinite loops. I found out that I did not implement the `MPI_Bcast()` for the cycles variable which secures that information is shared across all processes. Even though debugging and implementation can take a bit more time, the efficiency is much better and decreases the run time on bigger tasks significantly when optimized correctly. When timing the algorithms and comparing the use of mpi/parallelization I notice that there is no time gain in smaller computations. It was actually slower for small L . For small lattices such as $L = 1000$ the time was 3.67s without mpi and 5.3s with mpi. For $L = 10000$ the time was 36.76 without mpi and 42.4s with mpi. That is because the parallelization gains have to be higher than the parallelization overhead and it only happens for demanding enough processing. We do observe that when increasing with a factor of 10, the time is increased by approximately the same factor for a non parallelized run.

Referanser

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