Monte Carlo simulation of Ising model

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The code used in this study is available here:
https://github.com/vebjoro/fys4150_project_4.

Abstract

We study the second order phase transition from a paramagnetic phase to a ferromagnetic phase in a two dimensional material represented by an Ising model. The first and second moments of the energy and magnetization are calculated for various system sizes at various temperatures using a Markov Chain Monte Carlo simulation. We estimate the probability density function of a system of 20×20 spins as well as burn in time for this system. Finally we do simulations of four systems of increasing size from 40×40 spins up to 100×100 spins to estimate the critical temperature of the Ising model in the thermodynamic limit. Our best estimate is, to three significant digits $T_C \approx 2.28 J/k_B$ with an estimated relative error of 0.3% compared to Onsagers analytical result [1].

1 Introduction

The spontaneous magnetization of a paramagnetic material at cold temperatures is an example of a so called critical phenomenon, a phenomenon occurring near the end of the equilibrium curve of a phase transition. Critical phenomena are thoroughly studied, but are still not completely understood[2]. The paramagnetic to ferromagnetic phase transition, which is the focus for this study, is an example of a second order phase transition. It is possible to address these kind of phase transitions analytically, however the techniques involved can get quite advanced [2]. This study will take a numerical approach, which is arguably more straight forward.

The Ising model is a two state model in which the nodes of the system, which can have the states ± 1, or $\uparrow, \downarrow$ depending on preference, displays correlations and importantly a second order phase transition between an ordered state and a disordered state. This makes it a suitable model to study real materials that display this kind of phase transition. The goal of this study is to find the critical temperature of the phase transition in the Ising model numerically in the thermodynamic limit. As an infinite system cannot be represented on a computer we will have to perform multiple simulations of systems of different sizes and try to extrapolate the results to a system of infinite grid size. The simulations are performed using a parallel implementation of the Markov Chain Monte Carlo method sampling states from the Boltzmann distribution for a given temperature. First we have a general discussion about phase transitions and the Ising model. Then we perform some analytical calculations on the Ising model for a system of four spins in a 2×2 lattice to validate our numerical implementation. The Markov Chain Monte Carlo method is presented and some numerical details are discussed. Moving on we present the results for our simulations of a 20×20 lattice

of spins. Finally we discuss our simulations for larger systems up to a size of 100×100 and use our results to estimate the critical temperature of the spontaneous magnetization.

2 Theory

2.1 The Ising model

The Ising Model is a discrete mathematical two-state model in which the states, in our case spin up and down, have some interaction energy associated with them. The model has many applications and displays a phase transition between an ordered and a disordered phase. In this study the order parameter represents the magnetization M of the material, then the ordered phase is interpreted as ferromagnetic, and the disordered phase as paramagnetic.

The model contains a two dimensional (2D) lattice on which we arrange particles of a separate magnetic moment at each lattice site. Each individual spin s_i has only two possible states: $s_i = -1$ and $s_i = +1$. The total interaction energy of the system is described by the equation

$$E(\mathbf{s}) = -J \sum_{\langle kl \rangle}^{N} s_k s_l, \tag{1}$$

where $\langle kl \rangle$ denotes each pair of neighbouring spins, J is a unit energy and N is the total number of spins in the system. Only nearest neighbouring spins make contributions to the energy. Thermal fluctuations effect the degree to which the spins are correlated, with no thermal fluctuations all spins will be pointing in the same direction, minimizing the energy. Since we don't take an external magnetic field into account, all spins up and all spins down are equivalent states. When increasing the temperature, the spins have a higher probability of being in an excited state, that it opposite to some of its neighbours. As the spins interact the excitations can propagate through the system in a wave like manner as a quasiparticle called a magnon. [3] A magnetic analog of phonons. As the temperature increases, fluctuations become more prominent. Close to the critical temperature the spin correlations abruptly diminish and the overall magnetization in the system goes to zero. Finding the critical temperature at which the magnetization vanishes is the main objective of this study.

An analytical estimate of the critical temperature for the phase transition in the Ising model was performed by Onsager in 1944[1]. In the infinite limit the critical temperature is given by

$$T_C = \frac{2}{\ln(1+\sqrt{2})} \approx 2.269 J/k_B. \tag{2}$$

It also turns out there is a scaling relation between the critical temperatures of finite systems and the thermodynamic limit

$$T_C(L) = \frac{a}{L} + T_C(L = \infty). \tag{3}$$

We can use this to estimate $T_C(L = \infty)$. A linear regression of T_C against $1/L$ will produce a line that intercepts the T-axis at $T_C(L = \infty)$.

2.2 Phase transitions

Many materials that are paramagnetic at higher temperature become ferromagnetic as we cool them past a critical temperature, T_C. The system changes from a disordered state, in which it doesn't form large regions of same signed spins, to an ordered state, in which the spins are predominantly like signed. Phase transitions can be categorized as being discontinuous transitions (first order) or continuous transitions (second order, or possibly higher). Spontaneous magnetization falls into the category of second order phase transitions.

This implies that the system will occupy a unique state at the critical point in which all the spins are correlated across the entire system. [2]

When studying a phase transition between an ordered phase and a disordered phase it makes sense to look at the covariance of the spins, that is the degree to which the state of a spin depends on the state of some other spin. Since all the spins are correlated at the critical temperature the covariance will diverge at this point. Identifying the critical temperature is then simply a matter of looking for a spike in the covariance.

The covariance of the spins is called the magnetic susceptibility, and is given by

$$\chi = \frac{1}{N}\frac{1}{k_B T}\left(\langle M^2\rangle - \langle |M|\rangle^2\right), \tag{4}$$

where the factor $\frac{1}{N}$ is to normalize by the number of spins, and k_B is the Boltzmann constant. This will ease the comparison between different system sizes. The magnetic susceptibility has the physical interpretation of the ease with which the system changes its magnetization. With this in mind it seems intuitive that the system undergoes spontaneous magnetization at the point where the susceptibility diverges.

The covariance in the energy is the specific heat capacity of the system, given by

$$C_V = \frac{1}{N}\frac{1}{k_B T^2}\left(\langle E^2\rangle - \langle E\rangle^2\right), \tag{5}$$

also normalized by the number of spins. This can be interpreted as the telling us how much energy must be added to the system for it to increase its temperature per mass.[1] The expectation value for the energy $\langle E\rangle$, the first moment of the energy, can be written as the first derivative of a thermodynamic potential F with respect to the inverse temperature [2]

$$\langle E\rangle = \frac{\partial(\beta F)}{\partial\beta} \tag{6}$$

In a similar manner the specific heat capacity, the second moment about the mean energy, can be written as a second derivative of the thermodynamic potential

$$C_V = -\frac{1}{k_B T^2}\frac{\partial^2(\beta F)}{\partial^2\beta}. \tag{7}$$

We mentioned above that the phase transition we are studying is continuous in $\langle E\rangle$, however it is not continuous in C_V. The heat capacity diverges, just like the susceptibility. The phase transition is categorized as second order because there is a discontinuity in the second derivative of F and the second moment of the order parameter M.

2.3 Analytical solutions for a 2×2-case

In a 2×2-case it is feasable to calculate the expectation values for the mean magnetization per spin and the mean energy per spin analytically.

Since we are ignoring external magnetic fields, the directions of the spins don't matter, only their interactions. There are four significantly different states of the system. All up, three up, and two different combinations of two up-states.

$$\begin{matrix}\uparrow & \uparrow\\ \uparrow & \uparrow\end{matrix}, \quad \begin{matrix}\downarrow & \uparrow\\ \uparrow & \uparrow\end{matrix}, \quad \begin{matrix}\uparrow & \uparrow\\ \downarrow & \uparrow\end{matrix}, \quad \begin{matrix}\uparrow & \downarrow\\ \downarrow & \uparrow\end{matrix} \text{ and } \begin{matrix}\downarrow & \uparrow\\ \uparrow & \downarrow\end{matrix}.$$

The energy, magnetism and degeneracy of these states are listed in 2.3. Here we have included six states, differentiating up from down.

[1] Per spin in our model.

Number of ↑	Energy	Magnetization	Degeneracy
4	-8 J	4	1
3	0	2	4
2	0	0	4
2	8 J	0	2
1	0	-2	4
0	-8 J	-4	1

The expectation value for the energy per spin $\epsilon = \frac{E}{N}$, is given by

$$\langle \epsilon \rangle = \sum_{\text{all } \mathbf{s}} \epsilon(\mathbf{s}) p(\mathbf{s}; T) \tag{8}$$

The probabilities are given by the Boltzmann distribution

$$p(\mathbf{s}; T) = \frac{1}{Z} e^{-\beta E(\mathbf{s})}, \tag{9}$$

where $\beta = \frac{1}{k_B T}$ is the inverse temperature, a measure of the thermal energy fluctuations. The partition function Z is essentially a normalization constant for each specific temperature given by

$$Z = \sum_{\text{all } \mathbf{s}} e^{-\beta E(\mathbf{s})}. \tag{10}$$

In our 2×2-case at the temperature $T = 1$ J$/k_B$ the partition function turns out to be

$$Z = 2\left(e^{-8} + e^{8}\right) + 12. \tag{11}$$

Then we can find the expectation value for $\langle \epsilon \rangle$ as

$$\begin{aligned} \langle \epsilon \rangle &= \sum_{\text{all } \mathbf{s}} \epsilon(\mathbf{s}) p(\mathbf{s}; T) \\ &= \sum_{\text{all } \mathbf{s}} \frac{E(\mathbf{s})}{N} \frac{1}{Z} e^{-\beta E(\mathbf{s})} \\ &= \frac{2}{Z}\left(\frac{8J}{4} e^{-\beta 8J} - \frac{8J}{4} e^{\beta 8J}\right) \\ &= \frac{4\left(J e^{-8\beta J} - J e^{8\beta J}\right)}{Z} \\ &\approx -1.9960 J. \end{aligned} \tag{12}$$

Equivalently we find the expectation value of the absolute value of the mean magnetization to be

$$\langle |m| \rangle = \frac{1}{Z}\left(2e^{8} + 4\right) \approx 0.99866. \tag{13}$$

The second moment about 0 of energy per spin and the magnetization per spin is given by

$$\begin{aligned} \langle \epsilon^2 \rangle &= \sum_{\text{all } \mathbf{s}} \epsilon^2(\mathbf{s}) p(\mathbf{s}; T) \\ &= \frac{8J^2}{Z}\left(e^{-\beta 8J} + e^{\beta 8J}\right), \end{aligned} \tag{14}$$

and

$$\begin{aligned}\langle |m|^2 \rangle &= \sum_{\text{all } \mathbf{s}} |m|^2(\mathbf{s}) p(\mathbf{s}; T) \\ &= \frac{1}{Z}\left(2e^{-\beta 8J} + 2\right),\end{aligned} \tag{15}$$

From this we can find the magnetic susceptibility and the specific heat capacity. To do the calculation we use the total energy and magnetization, this is easily found by multiplying $\langle \epsilon \rangle$ and $\langle |m| \rangle$ by the number of spins N and the second moments, 14 and 15, by N^2.

Using equations 4 and 5 we find that

$$C_V \approx 0.032\, k_B \tag{16}$$

$$\chi \approx 0.0040\, 1/J. \tag{17}$$

$$\tag{18}$$

3 Method

3.1 Markov Chain Monte Carlo algorithm

For a given temperature T, the probability for a given micro state is given by the Boltzmann distribution 9. The interaction energy in 9 makes it quite challenging to deal with analytically, we turn to numerics. To find the probability distribution of macro states of the system at a given temperature, we are applying a Markov Chain Monte Carlo (MCMC) algorithm. A Markov Chain is a random sequence in which the probability of the next state is dependent on the current state, but not on the previous history of states. This makes it suitable to use in modelling systems with thermal fluctuations. The physical processes are simulated in random way, but there is still a degree of correlation forcing the system has to evolve from one state to the next. This ensures that our simulation cannot leap into an improbable state, it has to evolve there just like a physical system. We are not interested in the specific micro state of the system, but of the first and second moments of the energy and magnetization at any given temperature. To find these statistical quantities, we need information about the probability distribution for energy and magnetization. As the system size increases, the accessible energy states become quasi continuous. Then the probability of a given energy tends to zero, and it makes more sense to describe the system by a probability density function rather than a probability distribution. Then we can obtain a finite probability by integrating the probability density over the given domain. We find the moments we need to describe the system by estimating the probability density function (PDF) of the system at a given temperature. Since we cannot represent a continuum of states on a computer we draw a finite number of samples according to the PDF and assume this to be a good approximation of the full PDF.

Algorithm 1 Markov Chain Monte Carlo

randomise initial state **s**
for $j = 0, 1, ..., N$ (number of cycles) **do**
  procedure CYCLE(...)
    for $i = 0, 1, ..., L^2$ (number of spins) **do**
      procedure FLIP(...)
        generate proposed **s'** by flipping a random spin
        A = $\min\left(1, \frac{p(\mathbf{s}')}{p(\mathbf{s_i})}\right)$
        $r \leftarrow U(0, 1)$
        if $r < A$ **then**
          $s_{i+1} \leftarrow s'$
        else
          $s_{i+1} \leftarrow s_i$

The samples are generated by proposing a new state and rejecting or accepting the new state according to the Boltzmann distribution. The process of generating a sample called a Monte Carlo cycle (MC-cycle). This procedure corresponds to the inner loop in 1. By sampling this way our samples should, after a sufficient number of cycles be a good approximation of the true PDF of the system. In each MC-cycle a random spin is chosen and the relative probability of flipping it is calculated according to the Boltzmann distribution. If the relative probability of the state is higher than 1 the acceptance A is set to 1, if not the acceptance is equal to the relative probability. Then a random number r between 0 and 1 is generated and if the acceptance A is larger than r, $A > r$ the spin flip is accepted. Generating one sample takes N such proposed spin flips. The mean energy and magnetization are calculated and stored at the end of each MC-cycle.

3.2 Periodicity

As an infinite lattice would be impossible to simulate, we have to impose boundary conditions. We use periodic boundary conditions, this is equivalent to repeating our finite lattice indefinitely. To implement this on a computer, we extend the lattice on all sides and mirror the opposing edge over to this extended space. To be more precise, our actual grid is represented by a matrix of size L^2. Rows and columns representing our physical system are indexed from 1 to L, while ghost rows and ghost columns have indices $\{0, L + 1\}$. To make the lattice periodic we copy the last row L to the ghost row 0 and the first row 1 to the ghost row $L + 1$. The same is done for columns.

3.3 Burn in time

We are only able to draw a finite number of samples from our system, and it is difficult to know whether our samples are in fact representative for the whole PDF or not without knowing the PDF in advance. Of course, we don't know the PDF in advance. This makes it difficult to start of our simulation in a probable state, there is a good chance that the state we initialize our system in is very improbable. Since our sampling is done by random walkers making finite time steps it can take a long time (many MC-cycles) to reach the highest probability area of our PDF, which is where we should collect most of our samples. To avoid over representation of marginal states we run a number of MC-cycles without sampling. This way there is a higher chance that our limited number of samples are in fact collected according to the true PDF.

3.4 Parallelization

When simulating the model over multiple temperatures, our program comes to be a more computationally expensive program. To be able to run more cycles over more temperature intervals, we parallelize parts of the code. We use OpenMP, which is a C++ API for code parallelization. It allows us to easily distribute processes to multiple cores. In our program we assign each core a lattice of a different temperature configuration respectively. In the next section we're discussing the efficiency increase due to this implementation.

4 Results and Discussion

4.1 Analytical comparison for 2×2 lattice

We simulate a 2×2 lattice with a burn in time of 10 Monte Carlo cycles (MC-cycles). This is sufficient for such a small number of spins, since the state space is in this case quite small. We collect 10^6 samples during our simulations. Our numerical results can be compared to the analytical solutions given in equations 12, 13, 16 and 17. The result is shown in the table 1.

Value	Numerical	Analytical	Relative error
$\langle e \rangle$	-1.995	-1.996	6.2×10^{-5}
$\langle m \rangle$	0.9866	0.99869	3.4×10^{-5}
C_V	0.032	0.031	3.1×10^{-2}
χ	0.0040	0.0039	2.1×10^{-2}

Table 1: Analytical and numerical results for a 2×2 lattice.

We notice that the error in the second moments are roughly three orders of magnitude higher than those of the first moments. This highlights the importance of doing many samples. Since C_V and χ will be the most important quantities to identify the phase transition this many samples will be necessary to be able to estimate T_C with a sufficient accuracy.

4.2 Numerical estimates for 20×20 lattice

To study the effect of the initial state on the final results of the simulation we perform four simulations on a 20×20-lattice using 10000 MC-cycles. The simulations are done at two different temperatures $T = 1\, J/k_B$ and $T = 2.4\, J/k_B$. For each temperature, the system is initialized in two ways. The first one is an ordered state with all spins pointing up. In the other one, the spins are initialized according to a uniform random distribution with a mean of 0.

During the simulation, we update the mean values $\langle \epsilon \rangle$ and $\langle |m| \rangle$ for each cycle. The evolution of the calculated mean values over the number of MC-cycles at temperature $T = 1 J/k_B$ is shown in figures 1 and 2. At low temperatures the system tends to be in an ordered state, thus we can see from the figures that the mean value of the samples don't change as our random walker moves through state space. We started out in a highly probable state and the walker tends not to move far from the starting state in any given direction. The graphs for the disordered states quickly converge towards the same average values as the ordered systems. The walker is far more likely to move towards an ordered system than away from it. During the first couple of thousand samples the estimate for the average values of the estimated PDF uses a disproportionate amount of samples from a low probability area in state space. Our estimated mean values are not representative of the true PDF.

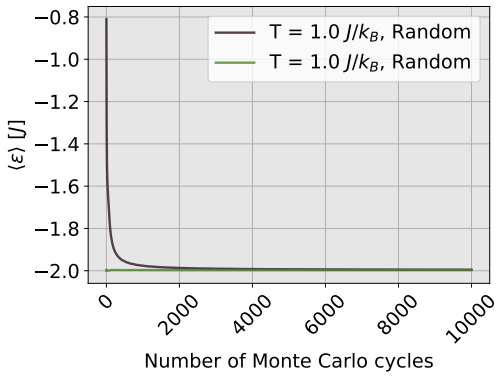

Figure 1: Expected energy over number of Monte Carlo cycles. $T = 1.0 \frac{J}{k_B}$

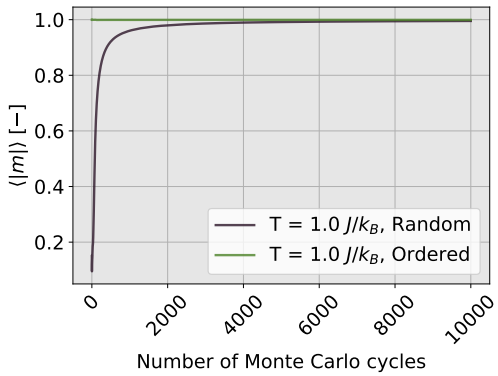

Figure 2: Expected magnetization over number of Monte Carlo cycles. $T = 1.0 \frac{J}{k_B}$

At $T = 2.4\ J/k_B$, as shown in figure 3 and figure 4, there is some wiggling before the mean values settle on a stable value. Both our initial states miss the expectation value of the true PDF by a similar amount. Neither a completely ordered state nor a uniformly disordered state have a particularly high probability in the true PDF. In general we are not able to guess at high probability states according to the unknown distribution, and we need do a burn in to have increase the likelihood of starting the system in a high probability state. In figure 4 we can clearly see the walker starting in the random state overshooting the mean value after a few time steps. This kind of wiggle can indicate that a higher number of different states now have a relatively high probability. The PDF spans a larger area in state space and we need to collect more samples to get an accurate representation of the true PDF. Physically we can interpret this as a sign that there are more thermal fluctuations in the system.

Based on these plots we use a burn in time of 2500 MC-cycles for out next two simulations. Wanting to improve our results for the third simulation we then increase the burn in time further to 4000 MC-cycles. From the plots 3 and 4 it seems that the mean values haven't quite converged yet. However these mean values are calculated without discarding any samples, so waiting for the system to be fully converged means the walker has already collected a significant amount of samples from the high probability region. That being said, we probably could improve our results by increasing the burn in time even more to increase

our probability even further of starting our sampling in the bulk of the PDF.

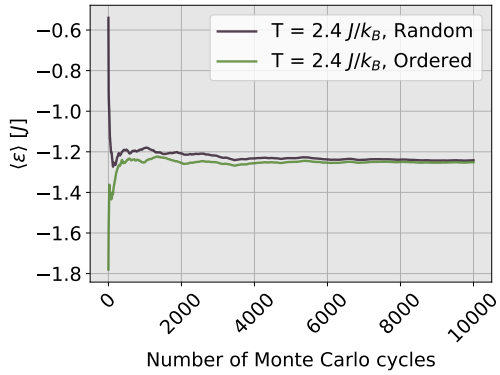

Figure 3: Expected energy over number of Monte Carlo cycles. $T = 2.4\frac{J}{k_B}$

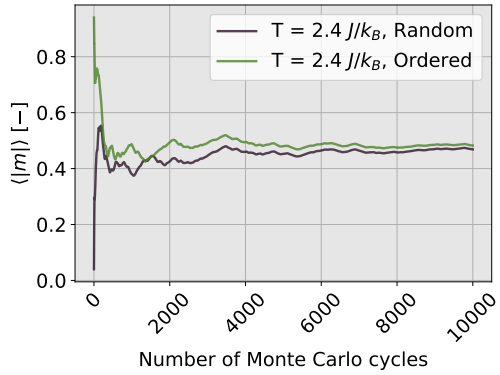

Figure 4: Expected energy over number of Monte Carlo cycles. $T = 2.4\frac{J}{k_B}$

4.3 Estimating the PDF

We estimate the full PDF for the mean energy per spin $\langle\epsilon\rangle$ of the 20×20 lattice at temperatures $T = 1J/k_B$ and $T = 2.4J/k_B$. After a burn in of 10000 cycles [2] we collect another 10^5 samples. The resulting distribution of mean energies is shown in figure 5. We can see that most of the states have a mean energy of $\langle\epsilon\rangle = -2.00J$. [3] In the majority of the samples the system is in the ground state with all the spins pointing in the same direction. When we flip one spin the energy increases by $\frac{\Delta E}{N} = \frac{8}{400}\text{J} = 0.02\text{J}$. On a rare occasion two spins flip simultaneously.

[2] This way we can simply keep running the simulations where we left off after studying the burn in section 4.2.
[3] The bins are artificially wide for visibility, the energies vary with increments of 0.02J.

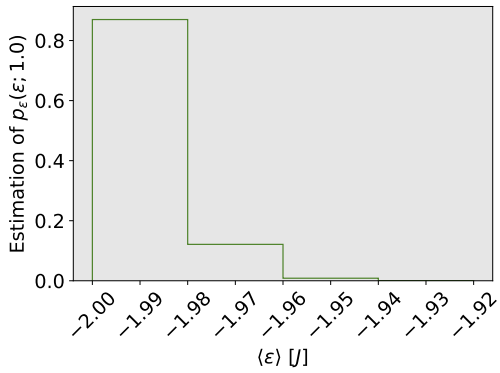

Figure 5: Estimation of PDF for expected energy per spin at a temperature of $T = 1.0.\frac{J}{k_B}$

At $T = 2.4J/k_B$ 6 we see that the PDF is distributed over a larger area. The bin size is chosen to be 0.01J, which is the minimal change in energy from flipping one spin. The mean value around 1.2 J as seen in figure 3 seems to match well with the energy distribution in figure 6. Due to more thermal fluctuations the PDF is has broadened and, as noted above, a larger area in state space is accessible with relatively high probability. This broadening is not linear with temperature. We expect this effect to be most prominent around the critical temperature as the system heats and transitions from an ordered phase to a disordered phase. At the peak of the curve there seems to be a discontinuity, we expect that this would smooth out if we were to collect more samples.

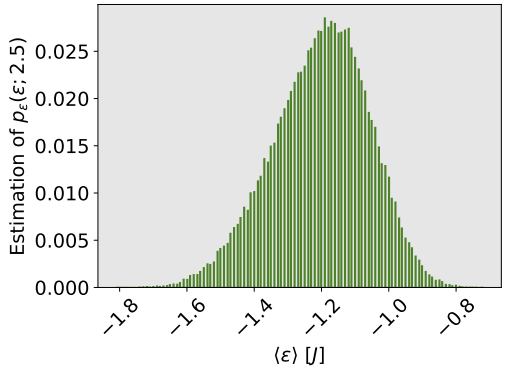

Figure 6: Estimation of PDF for expected energy per spin at a temperature of $T = 2.4.\frac{J}{k_B}$

4.4 Numerical quest for the critical temperature

To find the critical temperature of the system in the infinite limit we perform simulation of systems of increasing sizes. With lattice sized of 40×40, 60×60, 80×80 and 100×100, we use a burn in time of 2500 samples and run 10^6 cycles, initializing the system in a random state. We do three scans over temperature, first calculating $\langle\epsilon\rangle$, $\langle|m|\rangle$, C_V and χ for 10 temperatures between $T = 2.1\frac{J}{k_B}$ and $T = 2.4\frac{J}{k_B}$, afterwards increasing the temperature resolution.

The figures 7 show the combined results of our first, coarsest scan, and the our third scan, which had the finest resolution in temperature. As expected the energy per spin increase

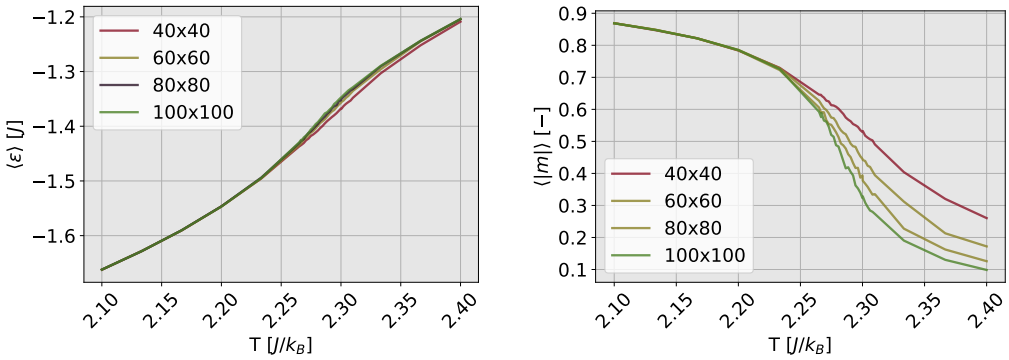

Figure 7: Mean energy and mean magnetization over temperatures.

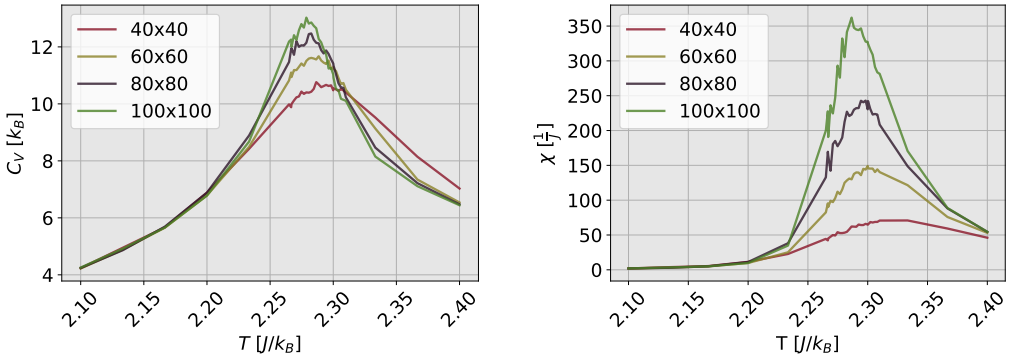

Figure 8: Specific heat capacity and magnetic susceptibility over temperatures.

with temperature, and the magnetization per spin falls as temperature increases. There is a slight difference between the energy increase of the different systems, the larger systems deviate slightly more from a straight line than the smallest one. We can see something similar in the magnetization, it falls off more drastically for larger systems. As we increase the system size towards infinity, we would expect a sudden drop off in magnetization at the critical temperature. From these plots, the critical temperature is not clearly distinguishable.

A quick way to understand this is to look at the heat capacity and magnetic susceptibility in 8. Heat capacity indicates how much energy is required to change temperature. If we look at it the other way, it also be interpreted as indicating how much the energy changes with temperature. The magnetic susceptibility can work as an indicator of the change in magnetization in a similar manner. We notice that the peak values for C_V are significantly smaller than the peak values of χ, which can explain why the change in magnetization is far more abrupt than the change in energy. In a physical system the critical temperature is found at the point where C_V and χ diverge. In our simulation of finite system sizes this corresponds to the top points of the graphs for C_V and χ. At the critical point all the spins are correlated and the covariance of the spins, i.e. the magnetic susceptibility will then increase with the number of spins in the system. The peak in χ therefore grows with system size, making the change in $\langle |m| \rangle$ more abrupt.

After the first scan we do another scan between $T = 2.6\frac{J}{k_B}$ and $T = 3.4\frac{J}{k_B}$. Since we are using a machine with 6 cores and we are running one thread per temperature, we realize that we can increase the number of temperatures points from 10 to 12 without significantly increasing the running time. Now all the cores will be busy until the end of the run. The results, coarse and fine grained combined, are shown in figure 7 and 8.

The critical temperature for our system is the point where C_V and χ diverges. The maximum points of our calculated C_V and χ are shown in table 2. As our error estimates in section 4.1 were on roughly a 1% relative error, we choose to give the results to three significant digits.

Lattice size	$T_C\ [J/k_B]$
40×40	2.32
60×60	2.29
80×80	2.29
100×100	2.28

Table 2: Values of T_C for different sized lattices.

As we move to larger lattice sizes the state space increases, at the same time we are increasing the step size in state space proportional to the lattice size. We have an error estimate for a 2×2 lattice, but we cannot be sure that the error will be of a similar magnitude for larger system sizes. A way of verifying our results is to compare our estimates for T_C to Onsagers analytical result 2.

Using the relation 3 we find an estimate for the critical temperature in the thermodynamic limit $T_C(L = \infty) \approx 2.25(5)\frac{J}{k_B}$.[4] This corresponds to the interception with the T-axis in figure 9. Compared to Onsagers analytical calculation 2 we find that our estimate has a relative error of 0.6%. Given that we have used a temperature resolution of $0.006\ \frac{J}{k_B}$ in the fine scan and that $T_C = 1\ \frac{J}{k_B}$ this level of accuracy seems to be as good as we can hope for. Given that the error for C_V and χ were of the order 1% we can also take this as an indication that the error is mainly dependent on the number of MC-cycles, which is the same as for the 2×2 system, and has a weak dependence on system size, if any. We cannot know this, however it is worth noting that the estimate for $T_C(L = \infty)$ is based on the simulation of

[4]The last digit, included in parenthesis, is on the same order as our temperature resolution, we cannot put much confidence in this. However it is included here to ease the comparison with the results from our third run.

four systems, not one. The estimate for $T_C(L = \infty)$ could be more accurate than the our estimate of T_C for any of the single lattices in isolation. Furthermore we don't need correct values of C_V and χ to locate T_C for the simulated systems, we only need for the peak of the curve to fall close to the true critical temperature for that system.

For our third and final run we used 24 points between $T = 2.265\frac{J}{k_B}$ and $T = 2.31\frac{J}{k_B}$. Using a burn in time of 4000 cycles and collecting 2×10^6 samples per temperature per lattice size. On this run the critical temperature for the 40×40-lattice dropped to $T_C \approx 2.30$, the other values in table 2 remain the same. Our estimate for the critical temperature in the thermodynamic limit came out as $T_C(L = \infty) \approx 2.27(7)\frac{J}{k_B}$. The relative error has now halved to 0.3%. We are probably approaching a point of diminishing returns. For it to make sense to use a finer temperature resolution we should use enough MC-cycles to be confident that our estimates of C_V and χ give the correct maximum point.

A more efficient way of improving our estimate could be to add a bigger lattice of say 120×120, rather than to increase the step size and number of MC-cycles even further. To halve the error, we had to quadruple the computation time, it is possible that adding another lattice could be more yielding.

Another effective way to improve our results could be to increase the burn in time. In the simulations presented here we discard the first 2500 samples in our second scan, and 4000 samples in the third scan. However our simulations of the 20×20-lattice show that the system has not quite converged yet after this number of samples, as seen in figure 4. It is possible that this would improve our accuracy somewhat, without drastically increasing computation time.

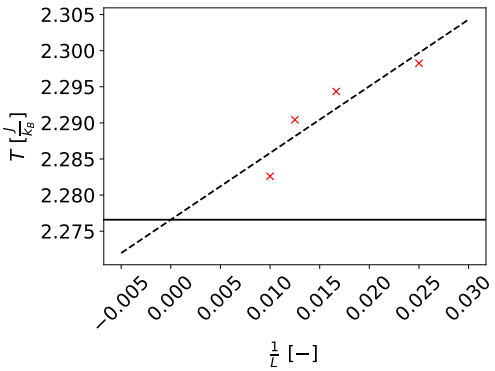

Figure 9: The four points indicate Tc for the four simulated systems. The point of intersection with $\frac{1}{L} = 0$ (T-axis) indicates T_C in the thermodynamic limit.

4.5 A note on the computational effects of parallelization

To shorten the runtime of the this simulation we've parallized the code with OpenMP. To demonstrate the effect of our parallelization, we have compared the runtime with and without parallelization. For 200 cycles and 10 temperatures the code ran for a total time of 37 seconds without parallelization. The parallelized code had a runtime of 6.2 seconds. To state that the runtime could roughly be reduced to the fraction of the number of cores seems right. This clearly show the effectiveness of parallelization when doing computational expensive simulations.

5 Conclusions

We have simulated spontaneous magnetization of a $2D$-lattice using the Ising model. In our first fine scan over temperature we found the critical temperature of our finite systems as presented in table 2. Increasing the resolution further the critical temperature of the smallest lattice, 40×40 dropped to $T_C = 2.30 J/k_B$, otherwise the critical temperatures remained the same to three significant digits. Using simulations of four different lattice sizes and the relation 3 we were able to estimate the critical temperature in the thermodynamic limit to be $T_C(L = \infty) = 2.25(5) J/k_B$, with a relative error of 0.6% when compared to Onsagers analytical result. Quadrupling the number of computations by doubling the temperature resolution and the number of MC-cycles per temperature we were able to obtain the result $T_C(L = \infty) = 2.27(7) J/k_B$, roughyly halving the relative error. In our study of the 20×20 system we were able to find the PDF for the mean energy $\langle \epsilon \rangle$ at the temperatures $T = 1 J/k_B$ and $T = 2.4 J/k_B$, we see that thermal fluctuations have a significant impact on the PDF at higher temperatures as the system has a tendency to deviate more from its mean state. The importance of throwing away the samples in the burn in phase of the MCMC run is stated as it effects the results accuracy. We have also indicated the significant effect code parallelization has on the run time of numerical simulations.

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