Studies of Phase Transitions in Magnetic Systems
FYS 3150 - Project 4

Johannes Kløve Kjernlie

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Abstract

The aim of this project is to investigate the behaviour of the Ising model in two dimensions. To compute the quantities of interest in the Ising model, we will implement the Metropolis Algorithm. Furthermore, the Ising model will experience a phase transition for a critical temperature, T_C, which we are interested in finding using numerical computations. The results yielded a good approximation for the exact critical temperature. Additionally, we derived the analytical expressions for a 2×2 lattice and compared the analytical values found for a given temperature with our numerically computed values. Also, here, our model was found to give sufficiently good approximations. In addition, MPI was used for parallelisation to enhance the computational efficiency of the program. Moreover, all the program code and benchmarks can be found at GitHub: `https://github.com/Kjernlie/FYS3150/tree/master/Project4`.

Contents

1 Introduction

In this project we want to study the Ising model in two dimensions. The Ising model is a mathematical model of ferromagnetism in statistical physics and is widely used for simulating phase transitions. Here, we will use the Metropolis algorithm for the simulations of the Ising model.

An introduction to the Ising model, Monte Carlo sampling, Markov Chains and the Metropolis algorithm will be given in Sec. 2.1.1, before we explain our implementation of the method briefly in Sec. 3. Further, in Sec. 4 we present the obtained results, and, finally, the author's conclusions are given in Sec. 5.

2 Theory

2.1 Ising model

2.1.1 Physical Background

Like previously mentioned the Ising model is a mathematical model of ferromagnetism in statistical physics. Ferromagnetism is the mechanism which makes certain materials permanent magnents, or attracted to attracted to magnets. Now, it is beneficial to introduce the idea of a canonical ensemble. An ensemble is a collection of microphysics systems, and a canonical ensemble is a statistical ensemble that represents the possible states of a mechanical system which is in thermal equilibrium with a heat bath at a constant temperature [4]. We introduce the Ising model to simulate the behaviour of magnetic moments in the framework of a canonical ensemble.

The Ising model is made up of discrete variables which represents magnetic dipole moments of atomic spins. These spins can be in one of two states, $+1$ $\uparrow$ or -1 $\downarrow$, and is arranged in a lattice where each spin can interact with its neighbours. For two- or higher-dimensional cases the Ising model can simulate phase transitions, and the two-dimensional square-lattice Ising model is one of the simplest statistical models to show a phase transition. This is also the model of interest for this project.

In its simplest form we can express the energy as

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

where $s_k = \pm 1$, N is the total number of spins, J is a coupling constant expressing the strength of the interaction between neigbouring spins, and $< kl >$ indicates that we sum over nearest neighbors only. $\mathcal{B}$ is an external magnetic field. Note that for $J > 0$ it is favourable for neighbouring spins to be aligned, since the this would lead to a lower energy [5]. This is a ferromagnetic interaction. For $J < 0$ we will get an antiferromagnetic interaction, while for $J = 0$ we have a noninteraction case.

In order to calculate relevant expectation values at a given temperature, we need a probability distribution

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

Here, $\beta = 1/kT$ is the inverse temperature, k the Boltzmann constant, E_i is the energy of a state i, and Z is a normalisation constant given by the partition function for the canonical ensemble

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

where the sum goes over all microstates, M.

Further, we are interested in certain thermodynamical quanitites when we are investigating the Ising model. The expected energy is given by

$$\langle E \rangle = \sum_{i=1}^{M} E_i P_i(\beta) = \frac{1}{Z} \sum_{i=1}^{M} E_i e^{-\beta E_i}, \tag{4}$$

with the corresponding variance

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

Using the variance of the energy we can find the specific heat at constant volume, which tells us how much the energy changes due to change in temperature. The specific heat is given by

$$C_V = \frac{1}{k_B T^2} \left(\langle E^2 \rangle - \langle E \rangle^2 \right). \tag{6}$$

Furthermore, we can find the expected magnetisation with

$$\langle \mathcal{M} \rangle = \sum_{i}^{M} \mathcal{M}_i P_i(\beta) = \frac{1}{Z} \sum_{i}^{M} \mathcal{M}_i e^{-\beta E_i}, \tag{7}$$

where $\mathcal{M}_i = \sum_{j=1}^{N} s_j$, that is, the sum over all spins for a given configuration i. And the corresponding variance is given by

$$\sigma_{\mathcal{M}}^2 = \langle \mathcal{M}^2 \rangle - \langle \mathcal{M} \rangle^2. \tag{8}$$

Now, we can find the magnetic susceptibility, χ, which indicates the ratio of magnetisation produced in a material to the magnetising force, and is expressed by

$$\chi = \frac{1}{k_B T} \left(\langle \mathcal{M}^2 \rangle - \langle \mathcal{M} \rangle^2 \right). \tag{9}$$

Additionally, using Ehrenfest's definition of the order of a phase transition, we can find a relationship between behaviour around the the critical point and various derivatives of the thermodynamical potential. Here, the thermodynamical potential is Helmholtz' free energy

$$F = \langle E \rangle - TS = -kTlnZ \tag{10}$$

so that $lnZ = -F/kT = -F\beta$. We can now express the expectation value for the energy as

$$\langle E \rangle = -\frac{\partial lnZ}{\partial \beta} = \frac{\partial(\beta F)}{\partial \beta}, \tag{11}$$

and the expectation value for the specific heat as

$$C_V = -\frac{1}{kT^2} \frac{\partial^2(\beta F)}{\partial \beta^2}. \tag{12}$$

2.1.2 Phase transition

We know that the Ising model in two dimensions with $\mathcal{B} = 0$ will have a phase transition for a given critical temperature, T_C. Below the T_C the Ising model exhibits a spontaneous magnetisation with $\langle \mathcal{M} \rangle \neq 0$, while above T_C the average magnetisation is zero. In other words we can say that the system will lose its ferromagnetic properties if the temperature is raised above T_C, i.e. the spins will align randomly, which makes the average magnetisation zero. This is called the paramagnetic phase.

Close to T_C the behaviour of several physical quantities can be characterised by a power law behaviour. For the Ising class of models, we have that

$$\langle M(T) \rangle \sim (T - T_C)^{\beta}, \tag{13}$$

$$C_V(T) \sim |T_C - T|^{\alpha}, \tag{14}$$

$$\chi(T) \sim |T_C - T|^{\gamma}, \tag{15}$$

with $\beta = 1/8$, $\alpha = 0$ and $\gamma = 7/4$.

Furthermore, we introduce the correlation length, which is expected to be of the order of the lattice spacing for $T >> T_C$. The correlation length will increase as the temperature approaches T_C, since the spins will become more correlated the closer we get to T_C. Actually, for a second-order phase transition, the correlation length will span the whole system. The divergent behaviour of the correlation ξ near T_C is given by

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

Moreover, we are always limited to a finite lattice. Thus, ξ will be proportional with the lattice size. We can relate the behaviour of finite lattices with an infinitely large lattice using so-called finite size scaling relations.

The critical temperature then scales as

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu}, \tag{17}$$

where a is a constant and ν defined in Eq. (16). By setting $T = T_C$ we obtain the mean magnetisaton

$$\langle \mathcal{M}(T) \rangle \sim (T - T_C)^{\beta} \rightarrow L^{-\beta/\nu}, \tag{18}$$

$$C_V(T) \sim |T_C - T|^{-\gamma} \rightarrow L^{\alpha/\nu}, \tag{19}$$

$$\chi(T) \sim |T_C - T|^{-\alpha} \rightarrow L^{\gamma/\nu}, \tag{20}$$

where a is a constant and ν as defined in Eq. (16).

2.1.3 Specialised case, 2×2 Ising model

In this project we will use the Ising model, without an externally applied magnetic field. The energy is then given by

$$E = -J \sum_{<kl>}^{N} s_k s_l. \tag{21}$$

Further, we assume that we have a ferromagnetic ordering, i.e. $J > 0$. Moreover, we will use periodic boundary conditions and the Metropolis algorithm only.

Here, we will have $2^4 = 16$ different configurations. Some configurations with their respective energies are presented here.

$$E = -8J \quad \begin{matrix}\uparrow & \uparrow \\ \uparrow & \uparrow\end{matrix} \qquad E = 0 \quad \begin{matrix}\uparrow & \uparrow \\ \uparrow & \downarrow\end{matrix} \qquad E = 0 \quad \begin{matrix}\downarrow & \downarrow \\ \uparrow & \downarrow\end{matrix} \qquad E = -8J \quad \begin{matrix}\downarrow & \downarrow \\ \downarrow & \downarrow\end{matrix}$$

From Eq. (21) we can see that we have a configuration energy of $E = -8J$ whenever all spins are parallel. If one single spin is anti-parallel to the rest we get a configuration energy of $E = 0$. For a system with two parallel spins and two anti-parallel spins we have a configuration energy of $E = 0$ or $E = 8J$. Furthermore, each energy state has a *degeneracy*, which tells us how many other configurations exist with the same energy state. In Tab (1) the configurations is listed with the respective energies and magnetisation.

Number spins up	Degeneracy	Energy	Magnetisation
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: Configurations for a 2×2 Ising model with energies and magnetisation.

2.1.4 Analytical solutions for a 2×2 Ising model

Here, we derive the closed form solutions of various physical quantities for a 2×2 Ising model. First, we find the partition function, Z

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

Further, the expectation value for the energy is

$$\begin{aligned} \langle E \rangle &= -\frac{\partial}{\partial \beta} \ln Z \\ &= -\frac{\partial}{\partial \beta} \ln(4\cosh(8\beta J) + 12) \\ &= \frac{-8J\sinh(8\beta J)}{\cosh(8\beta J) + 3}, \end{aligned}$$

and the the expectation value of the magnetic moment is

$$\begin{aligned}\langle \mathcal{M} \rangle &= \frac{1}{Z} \sum_{i=1}^{M} M_i e^{-\beta E_i} \\ &= \frac{1}{Z} \left(-4e^{8\beta J} - 8e^{0} + 8e^{0} + 4e^{8\beta J} \right) = 0.\end{aligned}$$

The mean absolute value of the magnetic moment is

$$\begin{aligned}\langle |\mathcal{M}| \rangle &= \frac{1}{Z} \left(4e^{8\beta J} + 8e^{0} + 8e^{0} + 4e^{8\beta J} \right) \\ &= \frac{2e^{8\beta J} + 4}{\cosh(8\beta J) + 3}.\end{aligned}$$

The expectation value for the specific heat, C_v is

$$\begin{aligned}C_V &= \frac{1}{kT^2} \frac{\partial^2}{\partial \beta^2} \ln Z \\ &= \frac{1}{kT^2} \frac{\partial}{\partial \beta} \left(\frac{8J \sinh(8\beta J)}{\cosh(8\beta J) + 3} \right) \\ &= \frac{1}{kT^2} \left(\frac{64J^2 \cosh(8\beta J)}{\cosh(8\beta J) + 3} - \frac{64J^2 \sinh^2(8\beta J)}{(\cosh(8\beta J) + 3)^2} \right).\end{aligned}$$

Lastly, we can find the susceptibility χ given by

$$\chi = \frac{1}{kT} \sigma^2_{\mathcal{M}},$$

where $\sigma^2_{\mathcal{M}}$ is the variance of the magnetic moment

$$\begin{aligned}\sigma^2_{\mathcal{M}} &= \langle \mathcal{M}^2 \rangle - \langle \mathcal{M} \rangle^2 \\ &= \frac{32}{Z} (e^{(}8\beta J) + 1) \\ &= \frac{8 \left(e^{8\beta J} + 1 \right)}{\cosh(8\beta J) + 3}.\end{aligned}$$

We can now find χ

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

The analytic results for $T = 1.0$ $[kT/J]$ are presented in Tab. (2).

2.2 The Monte Carlo method

Monte Carlo (MC) methods are a class of computational algorithms which use repeated random sampling to obtain numerical solutions. MC methods are

Quantity	Analytical value
$\langle E \rangle$	-1.99598
$\langle \lvert \mathcal{M} \rvert \rangle$	0.99866
C_V	0.03208
χ	3.99330

Table 2: Analytical values for 2×2 lattice.

widely used due to its simplicity and applicability to a broad range of problems. The MC method starts by using a sample method to draw a set of samples for the inputs, $\{\mathbf{x}^{(s)}\}_{s=1}^{N}$, where N is the number of samples. The samples are drawn from an input space $\Omega_{\mathbf{X}}$ defined by the joint probability density function of the inputs, $\rho_{\mathbf{X}}$. A set of outputs $\{x^{(s)}\}_{s=1}^{N}$ is found by evaluating the deterministic model $f(\mathbf{z})$ for each sample in $\{\mathbf{x}^{(s)}\}_{s=1}^{N}$.

Random sampling with the MC method gives an asymptotic approximation error of $\sigma_Y/\sqrt{N}$ [2]. This shows that the convergence rate is independent of the number of dimensions D, but might require very large Ns for the asymptotic error estimate to be valid. Thus, it could be challenging or infeasible to find accurate estimates for computationally expensive models. Nonetheless, we judge that the MC method will be feasible for our chosen problem.

2.3 Markov Chain Monte Carlo (MCMC)

In this project we need to find a way to obtain samples from the probability distribution expressed in Eq. (2). Alas, direct sampling can be difficult and this is where MCMC becomes very useful. The reason for this is that we can construct a reversible Markov chain with an equilibrium distribution equal to the target posterior distribution [3]. We explain the practical meaning of this statement in the following paragraphs. MCMC is a large field of research, and we will only give a short introduction in this report. For further interest, we recommend the work by Geyer, *Introduction to Markov Chain Monte Carlo* [3].

2.3.1 Markov Chains

A Markov chain is a specific type of stochastic process, which is an ordered collection of random variables. A stochastic process is given by

$$\big\{X_k : k \in K\big\}, \tag{22}$$

where K is the state space. The Markov chain is a sequence of random quantities X_k, each obtaining values in the state space K, with the following dependence condition on each state X_k

$$\begin{aligned} p(X_{k+1} = x_{k+1} | X_k = x_k, X_{k-1} = x_{k-1}, ..., X_0 = x_0) \\ = p(X_{k+1} = x_{k+1} | X_k = x_k). \end{aligned} \tag{23}$$

This condition says that the future state only depends on the current state, such that all past states are irrelevant. The "memorylessness" of a Markov chain is called the Markov property.

The joint distribution of a Markov chain is determined by the initial distribution which is the marginal distribution of X_1 and the transition probability distribution which is the conditional distribution of X_{k+1} given X_k. Under certain requirements, the Markov chain will converge to an equilibrium distribution. The essence of MCMC is to construct a Markov chain which fulfills these requirements and converges to the target posterior distribution. These requirements will be explained in the section below.

2.3.2 Requirements

The first requirement for the Markov chain is stationarity. A Markov chain is stationary if it is a stationary stochastic process, where a stochastic process is stationary if for any positive integer m the distribution of the m-tuple $(X_{k+1}, \ldots, X_{k+m})$ is independent of k. In a Markov chain we know that the conditional distribution of $(X_{k+2}, \ldots, X_{k+m})$ given X_{k+1} is independent of k. Thus, the Markov chain is stationary if and only if the marginal distribution of X_k is independent of k. If the Markov chain specified by an initial distribution and a transition probability is stationary, we say that the initial distribution is stationary, invariant or the equilibrium distribution. This is also indicated by saying that the initial distribution is preserved by the transition probability distribution [3].

Another important requirement is reversibility. A Markov chain is reversible if its transition probability is reversible with respect to its initial distribution. This is the case if the Markov chain $X_1, X_2, \ldots$ specified by the initial distribution and transition probability distribution has an exchangeable distribution of pairs (X_i, X_{i+1}). Hence, for any i and m the distributions of $(X_{i+1}, \ldots, X_{i+m})$ and $(X_{i+m}, \ldots, X_{i+1})$ are the same for a reversible Markov chain. Reversibility is important because all known methods for constructing transition probability mechanisms that preserve a specified equilibrium distribution are reversible [3].

2.4 The Metropolis-Hastings Algorithm

We mentioned in Sec. (2.3) that direct sampling from our probability distribution, given by Eq. (2) might be difficult. For our particular case, it is hard because you would have to compute the partition function, Z, for each state. Moreover, for the Ising model in two dimensions we have 2^N configurations, where $N = L \times L$ is the number of spins for a lattice of length L. Luckily, the Metropolis-Hasting Algorithm is a MCMC method that only considers ratios between probabilities such that we do not need to evaluate the partition function at all. For the interested reader *Introduction to Markov Chain Monte Carlo* by Geyer [3] is again recommended for a explanation of the Metropolis-Hastings Algorithm.

2.4.1 The Metropolis Algorithm

With the assumption of a symmetric proposal distribution, we get the Metropolis algorithm. The Metropolis algorithm for the Ising model, that we will implement in this project, is given in the following text box.

Metropolis Update for the Ising model

1. Start at an initial state with energy E_b using a random staring configuration.
2. Flip one spin only, before you compute the energy of this trial state E_t.
3. Calculate $\Delta E = E_t - E_b$.
4. Accept the new configuration if $\Delta E \leq 0$. Them, go to step 7.
5. $\delta E > 0$, calculate $w = e^{-(\beta \delta E)}$.
6. Compare w with a random number r. If
$$r \leq w, \tag{24}$$
accept the new configuration, else keep the old configuration.
7. Update various expectations values.
8. Repeat steps $(2) - (7)$ in order to obtain a sufficiently good representation of states.
9. Each time you go through the lattice, is one MC cycle. Lastly, you divide the various expectation values with the total number of MC cycles and the number of spins, to get the expectation values per spin.

3 Implementation

The Metropolis algorithm was implemented in the way outlined in Sec. (2.4.1). Further, I chose to use an object-oriented approach when writing the program in this project. The reason for this was mainly for my personal learning outcome. Still, I found the program structure to be good and easy to understand.

Also, I used the MPI (Message Passing Interface) library in $C++$ to parallelise the code. Using MPI I could run the code simultaneous on several processors making the program a lot more computationally efficient. Every time I wrote to file, I could use MPI to collect the data from each process, and write to one file.

The effect of MPI is demonstrated in the following text box.

```
\$ mpirun -n 1 ./main.x testing.dat 20 1000000 2.3 2.4 0.1
"""
Time = 52.9034 on number of processors: 1
"""

\$ mpirun -n 4 ./main.x testing.dat 20 250000 2.3 2.4 0.1
"""
Time = 18.3863 on number of processors: 4
"""
```

Here, the inputs after the executive is represented by *testing.dat*, which is the file the programs write out to, 20, which is the lattice size, 250000 or 1000000 is the number of MC cycles, 2.3 is the initial temperature, 2.4 is the final temperature and 0.1 is the temperature step. The number 1 or 4 represent the number of nodes (or processes) you want the program to run on. Therefore, running on 1 node with 1000000 MC samples, will yield the same result as running on 4 nodes with 250000 MC samples. Now, we see that running on several nodes is much more computational efficient with an execution time of 52.9034 seconds and 18.3863 seconds, for the running on 1 and 4 nodes, respectively.

4 Results

4.1 2×2 lattice

Here, we are interested in studying how our model approximates the analytical expressions derived in Appendix A for $T = 1.0$ $[kT/J]$. In Tab. (3), the approximate values for various numbers of Monte Carlo cycles is presented together with the analytical value. We see that that our model yields good results for large numbers of Monte Carlo samples. For 10^7 cycles, $\langle E \rangle$ and $\langle |\mathcal{M}| \rangle$ is very well approximated. It looks like the two other quantities are slower to converge, especially the specific heat, but at 10^7 all the quantities are sufficiently approximated.

Quantity	Analytical	10^4	10^5	10^6	10^7
$\langle E \rangle$	-1.99598	-1.99630	-1.99619	-1.99597	1.99600
$\langle \lvert\mathcal{M}\rvert \rangle$	0.99866	0.99883	0.99876	0.99867	0.99866
C_V	0.03208	0.02955	0.03058	0.03219	0.03191
χ	3.99330	3.96373	3.95243	3.98720	3.99296

Table 3: Values, given per spin, for 2×2 lattice.

4.2 20×20 lattice

In Fig. (1, 2, 3 and 4) the expectation values for the energy and mean magnetisation is plotted as functions of the number of MC samples, for $T = 1$ and $T = 2.4$. Additionally, we have plotted the expectation values for both random and ordered spin orientations as starting configurations.

We are interested in studying how many MC samples we need to get an equilibrium situation and can start calculating the expectation values for the quantities of interest. In Fig. (1) we see that the expectation values for both the energy and the mean magnetisation for $T = 1$ seem to stabilise around 35000 MC samples. For a random starting configuration in Fig. (2) it looks like the expectation values are stable already after 15000 MC samples.

For $T = 2.4$, and an ordered starting configuration, we see in Fig. (3) that the expectation values become stable after 130000 MC samples. Also, for a random starting configuration we see from Fig. 4 that the expectation values stabilize around 100000 MC samples. It is clear from all of the plots that the system stabilises faster for a random starting configuration. This makes sense because the random configuration will start closer to the most likely energy, and therefore, the system will stabilise faster. In the rest of the project we will use a random starting configuration in the simulations.

Furthermore, we are interested in seeing how the number of accepted configurations behaves as a function of temperature. In Fig. (5) we can see that the probability of a state being accepted is increasing with increasing temperature. Thus, it is clear that for increasing temperatures, the probability of any arbitrary state being close to the most likely state increases.

4.2.1 Probability distribution

Moreover, we are interested in analysing how the probability distributions for the expected energy looks for $T = 1$ and $T = 2.4$ in the 20×20 lattice. The probability distributions was found by counting the number of times a given energy appears in our computations. The results are presented in Fig (6) and (7) for $T = 1$ and $T = 2.4$, respectively. Interestingly, we have that the variance for the expected energy, σ_E^2, at $T = 1$ is much lower than the variance for $T = 2.4$, with $\sigma_E^2 = 13.20$ and $\sigma_E^2 = 3239.72$, respectively. This is related to the fact that an higher number of configurations was accepted for $T = 2.4$ than for $T = 1$, which we saw in Fig. (5).

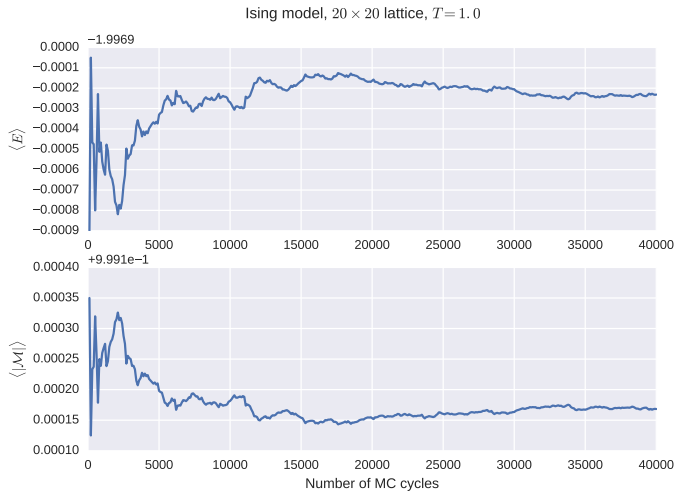

Figure 1: Figure showing expectation values of energy and mean magnetisation, both given per spin, for an increasing number of MC samples with $T = 1$. Here, the starting configuration was an ordered spin orientation.

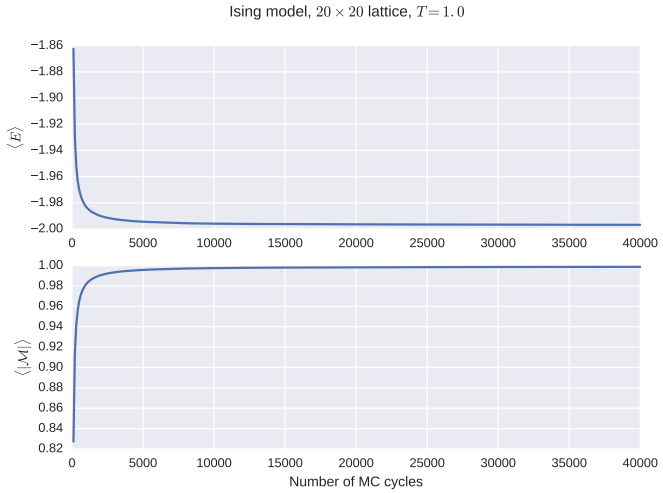

Figure 2: Figure showing expectation values of energy and mean magnetisation, both given per spin, for an increasing number of MC samples with $T = 1$. Here, the starting configuration was an random spin orientation.

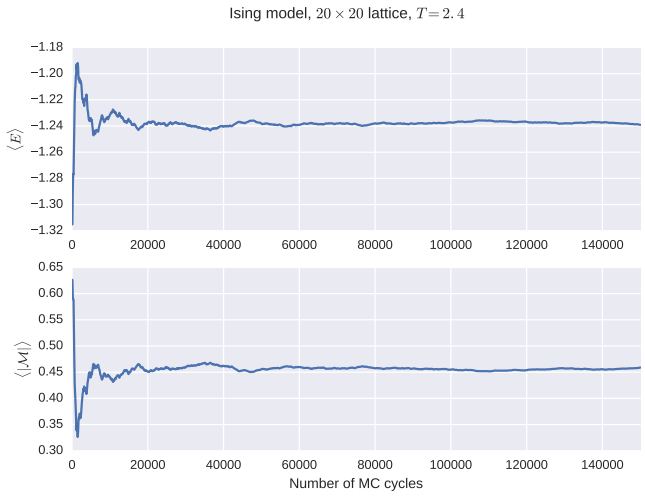

Figure 3: Figure showing expectation values of energy and mean magnetisation, both given per spin, for an increasing number of MC samples with $T = 2.4$. Here, the starting configuration was an ordered spin orientation.

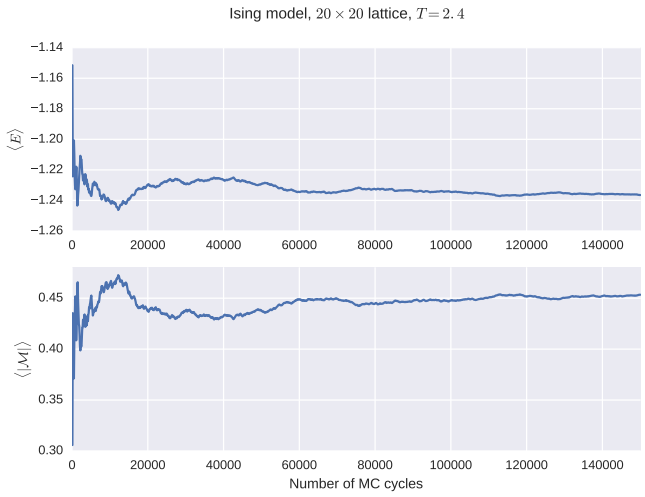

Figure 4: Figure showing expectation values of energy and mean magnetisation, both given per spin, for an increasing number of MC samples with $T = 2.4$. Here, the starting configuration was an random spin orientation.

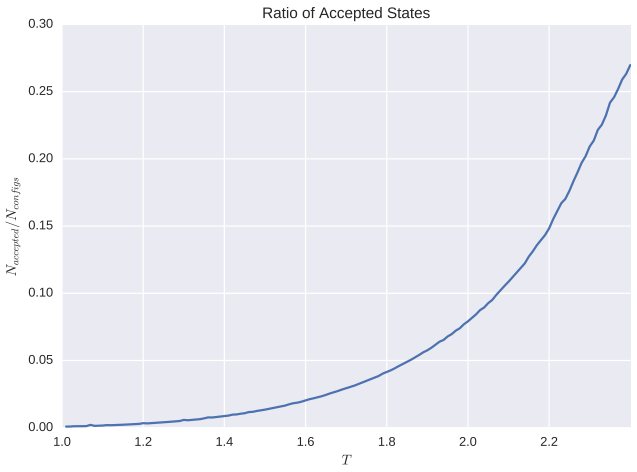

Figure 5: Figure showing the number of number of accepted configurations, $N_{accepted}$, divided with the total number of configurations, $N_configs$, plotted for increasing temperatures.

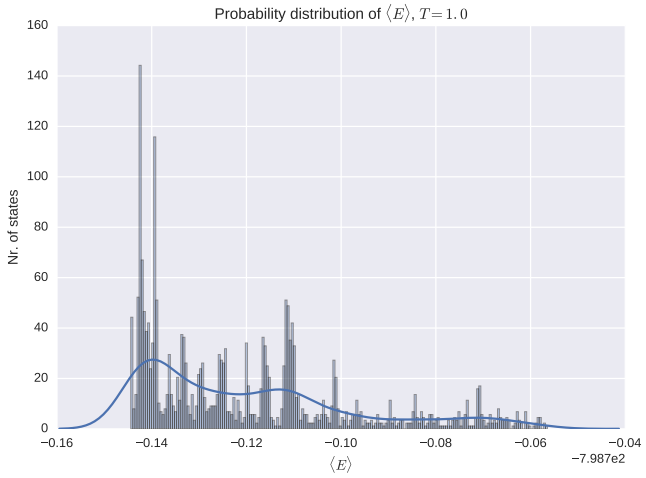

Figure 6: Histogram of expected energies for the system after the system has stabilised for $T = 1$. Here, 10^6 MC samples was used.

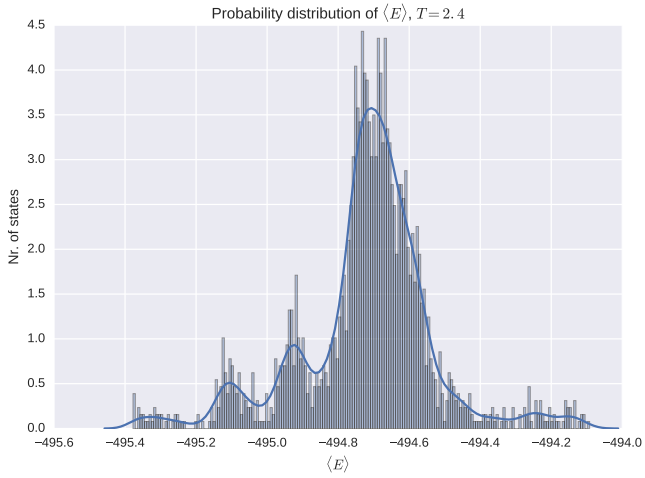

Figure 7: Histogram of expected energies for the system after the system has stabilised for $T = 2.4$. Here, 10^6 MC samples was used.

4.3 Phase transitions

Since we are interested in studying the phase transition in the Ising model, we want to look at the behaviour of $\langle E \rangle$, $\langle |M| \rangle$, C_V and χ close to the critical temperature. Therefore, since we from Lars Onsager that the exact result is $T_C = kT_C/J = 2/ln(1+\sqrt{2}) \approx 2.269$ with $\nu = 1$ [6], we calculate the quantities mentioned in the the temperature interval $[2.0, 2.3]$. This is plotted in Fig. (8), and here we see that both C_V and χ experience spikes in their values around ≈ 2.7. This is to be expected since we know that C_V and χ are discontinuous or diverge at the critical temperature, for an infinitely large lattice. For a finite lattice, we will instead see a broad maximum in C_V and χ close to the critical temperature, T_C, where this maximum will get sharper and sharper as the lattice size is increased [5]. Additionally, we see that χ and C_V is unstable for smaller temperatures, which suggest that we would need a larger number of MC samples to get an accurate representation.

Now, we want to use the scaling laws, derived in Sec. (2.1.2), to obtain the critical temperature. From Eq. (17), and reading of Fig. (8) we get

$$
\begin{aligned}
T_C(L = \infty) &= T_C(40) - a40^{-1} = 2.29 - \frac{a}{40}, \\
T_C(L = \infty) &= T_C(60) - a60^{-1} = 2.26 - \frac{a}{60}, \\
T_C(L = \infty) &= T_C(100) - a100^{-1} = 2.28 - \frac{a}{100}, \\
T_C(L = \infty) &= T_C(140) - a140^{-1} = 2.27 - \frac{a}{140}.
\end{aligned}
$$

Here, $\nu = 1$, and depending on the value of the constant a we can get a good

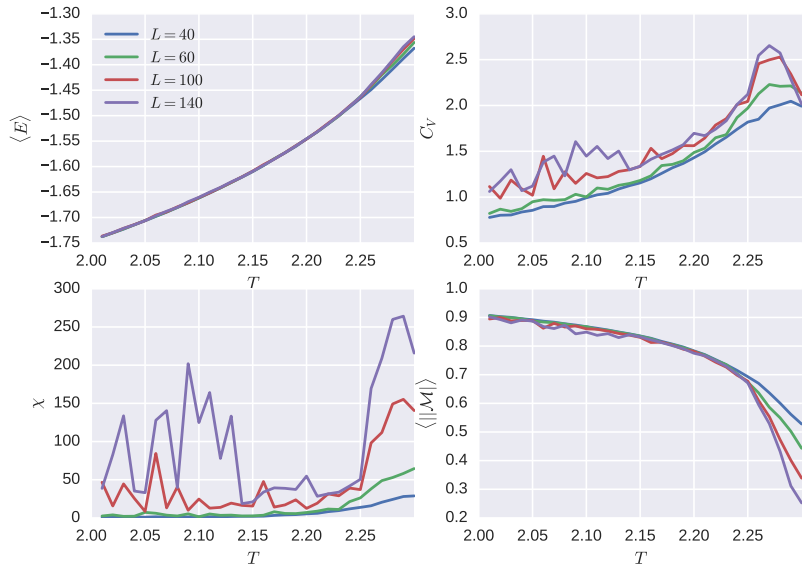

Figure 8: Figure showing how $\langle E \rangle$, C_V, χ and $\langle |\mathcal{M}| \rangle$ behaves as a function of temperature for increasing lattice sizes L. Here, the $L = 40$, $L = 60$ and $L = 100$ cases was found using 1×10^6 MC samples, while the $L = 140$ case was found using 2×10^6 MC samples. Furthermore, a temperature step size of $T_{step} = 0.01$ was used in all the computations. All the values are per spin.

results using this formula, close to the exact value $T_C \approx 2.269$.

5 Conclusions

In this project the Metropolis algorithm was implemented to simulate the Ising model for varying sizes of square finite lattices. We were interested in modeling the phase transition in the Ising model, and obtain the critical temperature, T_C. This was deemed successful as the model yielded results which closely approximated the exact value, $T_C = 2.269$. Also, for a 2×2 lattice we derived the analytical expressions for $\langle E \rangle$, $\langle |\mathcal{M}| \rangle$, C_V and χ, which our model managed to approximate well for $T = 1.0[kT/J]$.

5.1 Ideas for Further Work

Of course, it would be interesting to run a really large simulation with a huge number of MC samples, and a very small ΔT, to see if we could find better results. Also, it could be fun to look at the effect of flipping more than one spin

in an configuration. I would assume that this would lead to a faster stabilisation of the quantities of interest.

Furthermore, I would want to try to implement the generalised Polynomial Chaos (gPC) method as a substitute for the MC method. In the gPC method the output in a model is expanded into a series of orthogonal polynomials and expansion coefficients that are functions of the model's input. The expansion coefficients can be calculated with a much lower number of samples compared with the MC method, which makes the gPC method an excellent alternative to the MC method in many case [1, 7]. Note that I am not an expert in the gPC method, and can not immidiately say whether or not it is a good choice for the Ising model, but it would be very interesting to give it a try.

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