

# The Ising model and phase transitions in magnetic systems

Anna Lina Petruskeviciute Sjur

November 14, 2018

## Abstract

## 1 Introduction

expressed as

## 2 Methods

$$C_V = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_B T^2}, \quad (4)$$

### 2.1 Thermodynamic properties

while the susceptibility  $\chi$  is given by

In this report I will study different thermodynamic properties of a Canonical Ensemble in the form of a spin lattice. The probability distribution in such a system is given by the Boltzmann distribution,

$$\chi = \frac{\langle |M|^2 \rangle - \langle |M| \rangle^2}{k_B T}. \quad (5)$$

For a derivation of these expressions, see for example [2].

$$P_i(\beta) = \frac{e^{-\beta E_i}}{Z}, \quad (1)$$

where  $\beta = \frac{1}{k_B T}$ ,  $k_B$  is the Boltzmann constant, and  $E_i$  is the energy in a given microstate.  $Z$  is the partition function given by

$$Z = \sum_i e^{-\beta E_i}. \quad (2)$$

The expectation value to a given variable  $A$  is given by

$$\langle A \rangle = \frac{1}{Z} \sum_{i=1}^N D_i A_i e^{-\beta E_i} \quad (3)$$

where  $A_i$  is the value of the variable in question for the state  $i$ . Equation (3) gives a method for finding the expectation value of the energy  $E$  and mean magnetization  $|M|$ . Further, the specific heat at a constant volume  $C_V$  can be

### 2.2 The Ising model

The Ising model consists of variables  $s$  that can exist in two states, typically  $+1$  or  $-1$ . These variables represent magnetic dipole moments of atomic spin, and are ordered in a two dimensional lattice consisting of  $L \times L$  spins. Given that there is no external magnetic field, the energy of the system is modelled as

$$E = -J \sum_{\langle ij \rangle} s_i s_j, \quad (6)$$

where  $J$  is a coupling constant expressing the strength of the interaction between neighbouring spins. The symbol  $\langle ij \rangle$  means that the sum is over neighbouring spins. The magnetisation of the system is simply the sum of all the spins

$$M = \sum_i s_i. \quad (7)$$

For smaller systems, it is possible to calculate the expectation values analytically by finding and counting all the possible states. The different states for a  $2 \times 2$  lattice are listed in Table 1, and will be used together with equation (3) and (1) to test if the algorithm reaches the expectation values.

# spins up	D	E	M
4	1	-8J	4
3	4	0	2
2	4	0	0
2	2	8J	0
1	4	0	-2
0	1	-8J	-4

Table 1: The different states according to their energy and magnetization for a  $2 \times 2$  lattice.

FLAGG boundary conditions FLAGG

### 2.2.1 Phase transitions and critical temperature in the Ising model

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu} \quad (8)$$

$$T_C(L = \infty) = \frac{T_C(L_i)L_i - T_C(L_j)L_j}{L_i - L_j} \quad (9)$$

### 2.2.2 Metropolis' algorithm

One possible way of solving the Ising model is by using the so called Metropolis' algorithm. The key concept in this algorithm is to generate steps in a Markov chain, with a method for rejecting new steps. The Markov chain will eventually reach the most likely state. Algorithm 1 shows Metropolis' algorithm adapted for Ising's model, and is based on the algorithm found in [1]. For each spin in the lattice, a random spin is flipped. The energy difference is then computed, and the transition probability  $w$  is computed as

$$w = e^{-\beta\Delta E}. \quad (10)$$

In order to determine if the new state is accepted, the transition probability is compared with a number  $r$  given by a random number generator (RNG) with a uniform probability distribution. If  $w \geq r$ , the new state is accepted. The new state is also accepted if the new state has a lower energy. Each sweep over the lattice is called a Monte Carlo cycle (mcs). After a given number of mcs, the expectation values of the system will have reached equilibrium and the most likely configuration is reached. There can still be variations in  $E$  and  $|M|$ , but they will fluctuate around a given value. This is called the thermalisation time. In order to get good estimates for the expectation values, the sampling should start after the thermalization time is reached.

```

Initialise a state with energy  $E$ ;
for  $i = 1, \dots, mcs$  do
    foreach  $s$  do
        Flipp random spin;
        Calculate  $\Delta E$ ;
        if  $\Delta E \leq 0$  then
            Accept new state;
        else
            Calculate transition probability
                 $w$ ;
            Generate random number
                 $r \in [0, 1]$ ;
            if  $r \leq w$  then
                Accept new state;
            else
                Keep old state;
        Update expectation values;
    Calculate mean expectation values;

```

Algorithm 1: Metropolis' algorithm for solving The Ising model.

### 2.2.3 Probability distribution of the energies

One of the properties of the Ising model addressed in this report is the probability distribution of the energy states  $p(E)$ . In order to determine the distribution, the number of times each energy appears after the thermalization time is counted, and then divided by the total number of samples. This is done for temperatures  $1.0 k_B T/J$  and  $2.4 k_B T/J$ . This is compared with the variance of the energy, given as

$$\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2. \quad (11)$$

### 2.3 Implementation

Algorithm 1 can be calculation-heavy when using a large number of Monte Carlo cycles. In order to get a more efficient code, the calculations are parallelised. This is done using MPI. Each CPU is assigned only a fraction of the total number of  $mcs$ , and then all the expectation values are collected and the mean is calculated.

All programs are written in C++, using python3.6 to produce figures and tables.

## 3 Results

Figure 1 shows the expectation values for the energy and absolute magnetisation as a function of Monte Carlo sweeps with both an ordered and unordered initial configuration. Results for a low temperature 1.0 and a higher temperature 2.4, which is above the critical temperature, are shown. One can see that the expectation values stabilises almost immediately when an ordered starting configuration is chosen for the lower temperature. But when an unordered configuration is chosen, the values does not stabilise until about 25000  $mcs$ . As for the higher temperature, both an ordered

and unordered initial configuration gives a result that stabilises quite fast around a value, with some fluctuations. This happens after about 5000  $mcs$  for the energy, and after about 10000  $mcs$  for the magnetisation.

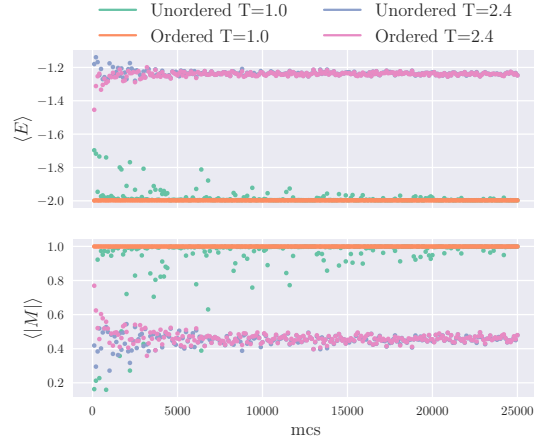


Figure 1: Plot over expectation values for energy  $E$  per spin and absolute magnetisation  $|M|$  per spin as a functions of Monte Carlo sweeps  $mcs$ . The expectation values are plotted for  $T = 1.0$  and  $T = 2.4$  with both an ordered and unordered initial state. Lattice size  $L = 20$  was used.

In Figure 2, the number of accepted configurations as a function of Monte Carlo cycles is shown. Again this is plotted for temperatures 1.0 and 2.4, with both an unordered and ordered initial configuration. FLAGG uteseende på grafene FLAGG

The probability distribution of  $E$  per spin is shown in Figure 3. For the temperature 1.0 the possible states are all close to -2.0, with two states highly more probable than the others. For the temperature 2.4, the distribution is closer to a normal distribution, with the most probable states around -1.2. The expectation value and variance of  $E$  for the same temperatures are shown in Table 2.

Figure 4 and 6 shows the expectation values for the energy and the absolute magnetisa-

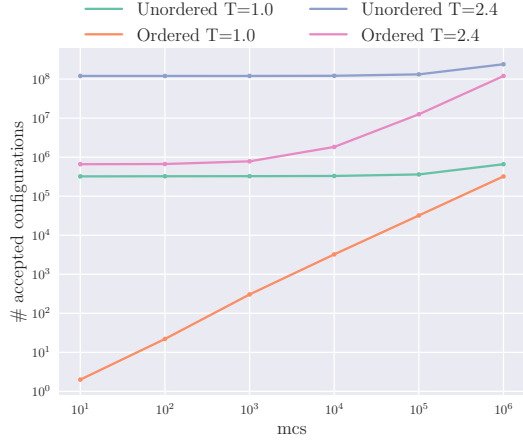


Figure 2: Plot over the number of accepted configurations as a function of Monte Carlo sweeps  $mcs$ . The number of accepted configurations are plotted for  $T = 1.0$  and  $T = 2.4$  with both an ordered and unordered initial state. Lattice size  $L = 20$  was used. The scale is logarithmic.

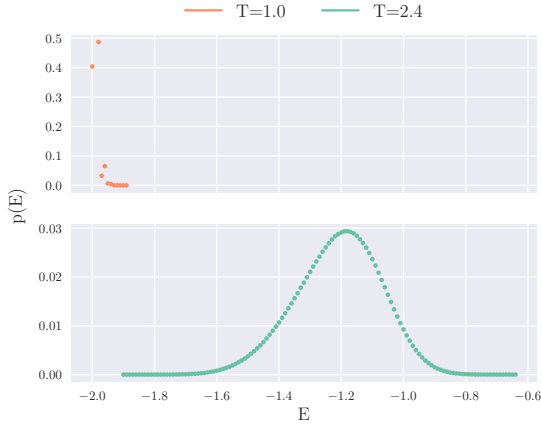


Figure 3: Plot over probabilities for a given energy  $E$  per spin. The top plot is for temperature  $T = 1.0$  while the bottom plot is for temperature  $T = 2.4$ .  $10^6$   $mcs$  were used. Lattice size  $L = 20$  was used.

T	$\langle E \rangle$	$\sigma^2$
1.0	-1.997	0.025
2.4	-1.237	8.116

Table 2: Table over the expectation value  $\langle E \rangle$  and variation  $\sigma^2$  of the energy per spin after  $10^6$   $mcs$  for temperatures  $T = 1.0$  and  $T = 2.4$ . Lattice size  $L = 20$  was used.

tion from  $T = 2.0$  to  $T = 2.3$ , while Figure 5 and 7 shows the specific heat and susceptibility for the same temperature interval. In all these plots results for lattices with size  $L = 40, 60, 80$  and 100 are shown.

In the energy plot, all expectation values are negative, and increases as temperature increase. For temperatures under 2.25, all the lattices gives the same results, but for higher temperatures, the values slightly diverge from each other.

A similar trend is found in the plot of the absolute magnetisation. The values for the different lattices are very similar until a temperature of about 2.20, and then diverge. Comparing the energy and magnetisation plots, the magnetisation values diverge more strongly from each other. All the magnetisation values are positive, and decrease as the temperature increases.

The plots over the specific heat and the susceptibility does also feature a divergent trend in the temperature interval 2.20 to 2.30. In addition, the plots are less smooth in this interval. The specific heat values increase with temperature until they reach a maxima between 2.25 and 2.30. The maximum values are slightly shifted towards lower temperatures as  $L$  increase. In the susceptibility plot, only the results for the lattice size  $L = 100$  has a maxima in this interval.

Figure 8 shows results for the specific heat in the temperature interval 2.26 to 2.30 with a higher resolution than Figure 5. In addition, a

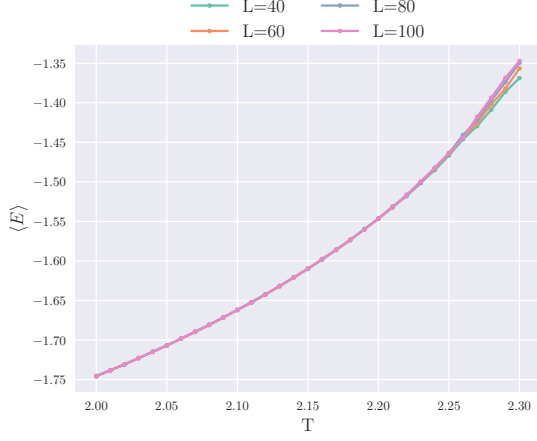


Figure 4: Plot over the expectation values for the energy per spin  $\langle E \rangle$  as a function of temperature  $T$  with step size  $10^{-3}$ . The results are from lattices with size  $L = 40, 60, 80$  and  $100$ .  $10^6$  *mcs* were used for each step.

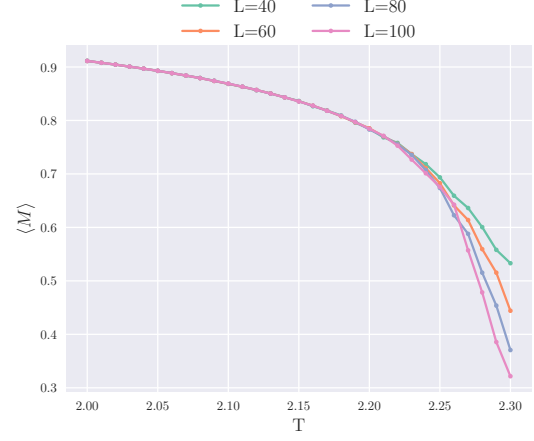


Figure 6: Plot over the expectation value for the absolute magnetisation per spin  $\langle |M| \rangle$  as a function of temperature  $T$  with step size  $10^{-3}$ . The results are from lattices with size  $L = 40, 60, 80$  and  $100$ .  $10^6$  *mcs* were used for each step.

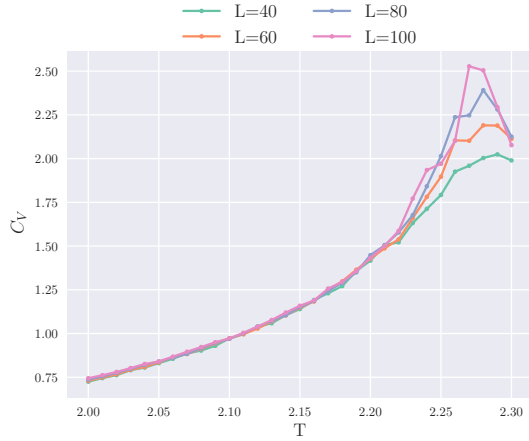


Figure 5: Plot over the expectation values for the specific heat per spin  $C_V$  as a function of temperature  $T$  with step size  $10^{-3}$ . The results are from lattices with size  $L = 40, 60, 80$  and  $100$ .  $10^6$  *mcs* were used for each step.

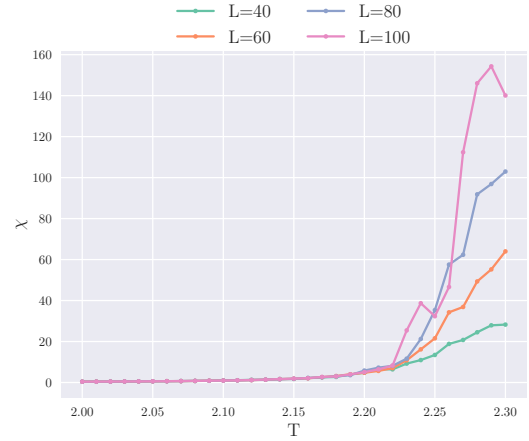


Figure 7: Plot over the expectation values for the susceptibility per spin  $\chi$  as a function of temperature  $T$  with step size  $10^{-3}$ . The results are from lattices with size  $L = 40, 60, 80$  and  $100$ .  $10^6$  *mcs* were used for each step.

running mean is shown.

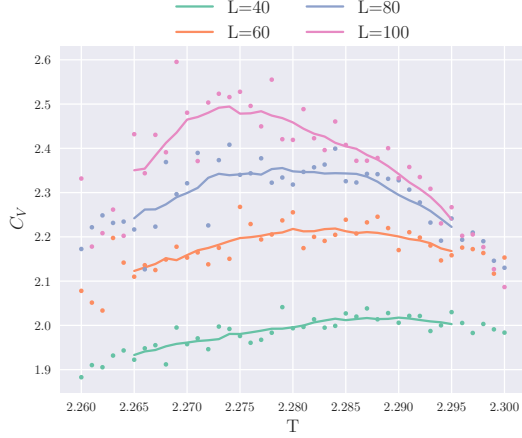


Figure 8: Plot over the expectation values for the specific heat per spin  $C_V$  as a function of temperature  $T$  with step size  $10^{-4}$ . The results are from lattices with size  $L = 40, 60, 80$  and  $100$ .  $10^6$  mcs were used for each step. The dots are the collected data, while the solid line is a running mean with a window size of 11.

$L_i$	$L_j$	LR	HR	HRRM
60	40	2.260	2.267	2.272
80	40	2.270	2.269	2.268
80	60	2.280	2.271	2.264
100	40	2.257	2.262	2.263
100	60	2.255	2.260	2.259
100	80	2.230	2.249	2.254
<b>Mean</b>		2.259	2.263	2.263
<b>STD</b>		0.015	0.007	0.006

## 4 Discussion

## References

- [1] Morten Hjorth-Jensen. Computational physics lecture notes fall 2015, aug 2015.
- [2] D.V. Schroeder. *An Introduction to Thermal Physics*. Addison Wesley, 1999.

Table 3: Critical temperature calculated using eq. 9 for different lattice sizes  $L$ . Results using low resolution values plotted in Figure 5 (LR), high resolution values (HR) and the running mean of the high resolution values (RMHR) plotted in Figure 8 are shown. In addition, the mean and standard deviation (STD) for each set of values are shown.

## Appendix