The Ising model and phase transitions in magnetic systems

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Abstract

1 Introduction

2 Methods

2.1 Thermodynamic properties

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,

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

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

$$Z = \sum_i e^{-\beta E_i}. \tag{2}$$

The expectation value to a given variable A is given by

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

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 expressed as

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

while the susceptibility χ is given by

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

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

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

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

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

$$M = \sum_i s_i. \tag{7}$$

For smaller systems, it is possibly to calculate the expectation values analytically by finding and counting all the possible states. The different states for a 2×2 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 2×2 lattice.

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2.2.1 Phase transitions and critical temperature in the Ising model

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

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

2.2.2 Metropolis' algorithm

One possibly way of solving the Ising model is by using the so called Metropolis' algorithm. The key concept in this algorithm is to generates steps in a Marcov 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

$$w = e^{-\beta \Delta E}. \tag{10}$$

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 an 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 an $|M|$, 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.

```
Initzialise a state with energy E;
for i = 1, ..., mcs do
    foreach s do
        Flipp random spin;
        Calculate ΔE;
        if ΔE ≤ 0 then
            Accept new state;
        else
            Calculate transition probability
             w;
            Generate random number
             r ∈ [0, 1];
            if r ≤ 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 termalization time is counted, and then divided by the total number of samples. This is done for temperatures 1.0 k_BT/J and 2.4 k_BT/J. This is compared with the variance of the energy, given as

$$\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2 . \tag{11}$$

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. 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.

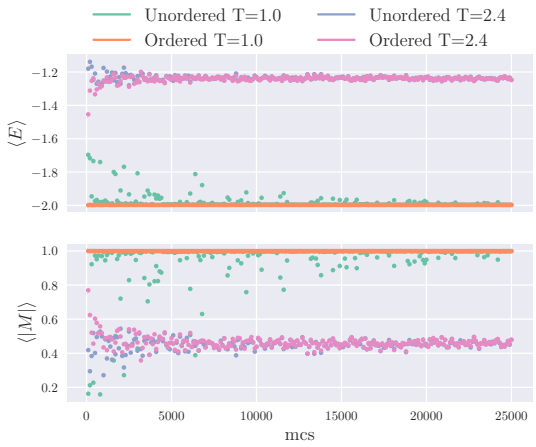

Figure 1: Plot over expectation values for energy E per spin and absolute magnetisation $|M|$ per spin as a functions of Monte Carlo sweeps *mcs*. The expectation values are plotted for $T = 1.0$ and $T = 2.4$ with both an ordered and unordered initial state.

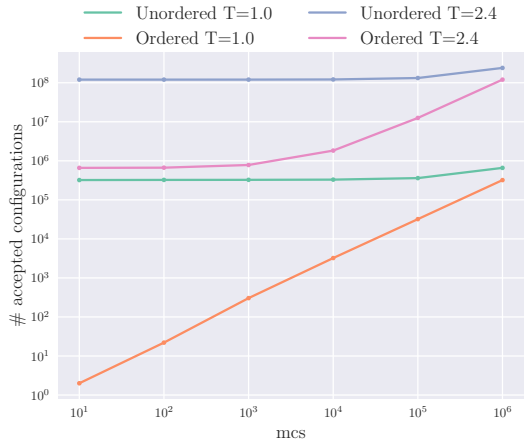

Figure 2: Plot over the number of accepted configurations as a function of Monte Carlo sweeps *mcs*. The number of accepted configurations are plotted for $T = 1.0$ and $T = 2.4$ with both an ordered and unordered initial state. The scale is logarithmic.

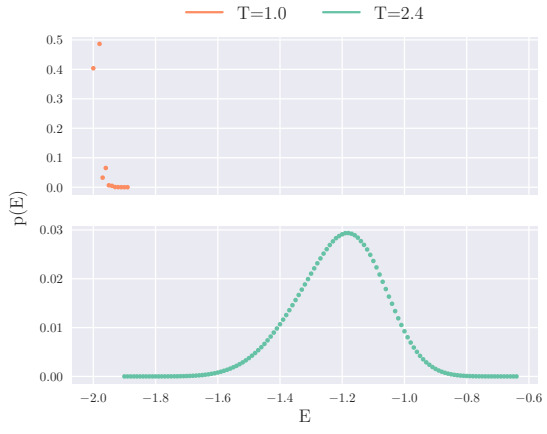

Figure 3: Plot over probabilities for a given energy E per spin. The top plot is for temperature $T = 1.0$ while the bottom plot is for temperature $T = 2.4$. 10^6 *mcs* were used.

T	$\langle E \rangle$	σ^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 σ^2 of the energy per spin after 10^6 *mcs* for temperatures $T = 1.0$ and $T = 2.4$.

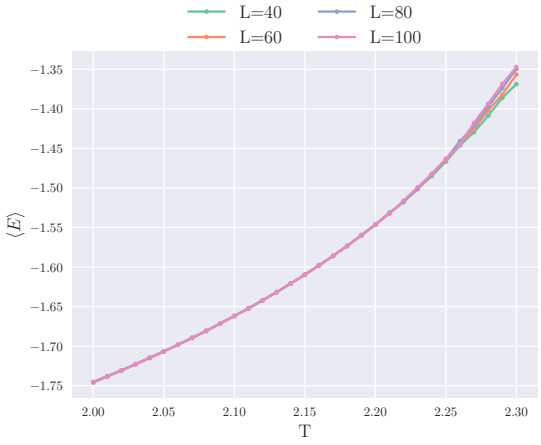

Figure 4: Plot over the expectation values for the energy per spin $\langle E \rangle$ as a function of temperature T with step size 10^{-3}. The results are from lattices with size $L = 40, 60, 80$ and 100. 10^6 *mcs* were used for each step.

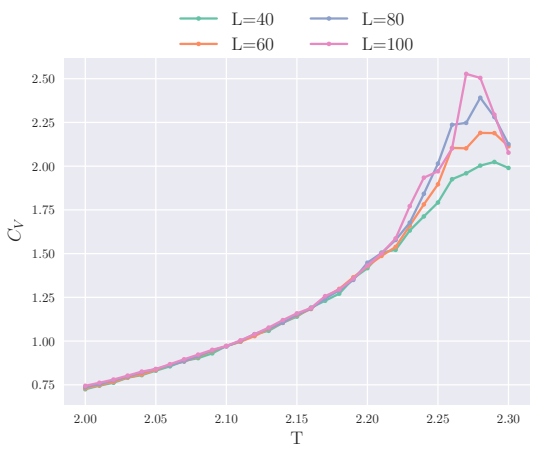

Figure 5: Plot over the expectation value for the absolute magnetisation per spin $\langle |M| \rangle$ as a function of temperature T with step size 10^{-3}. The results are from lattices with size $L = 40, 60, 80$ and 100. 10^6 *mcs* were used for each step.

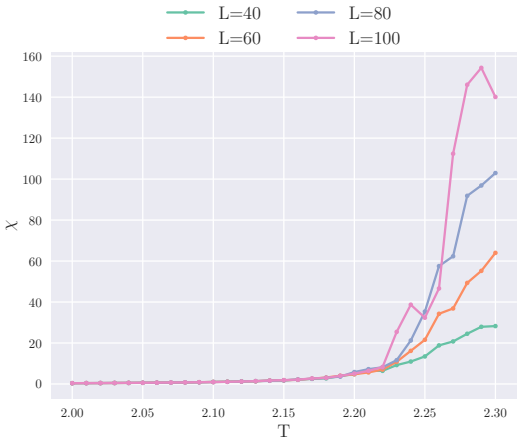

Figure 7: Plot over the expectation values for the susceptibility per spin χ as a function of temperature T with step size 10^{-3}.The results are from lattices with size $L = 40, 60, 80$ and 100. 10^6 *mcs* were used for each step.

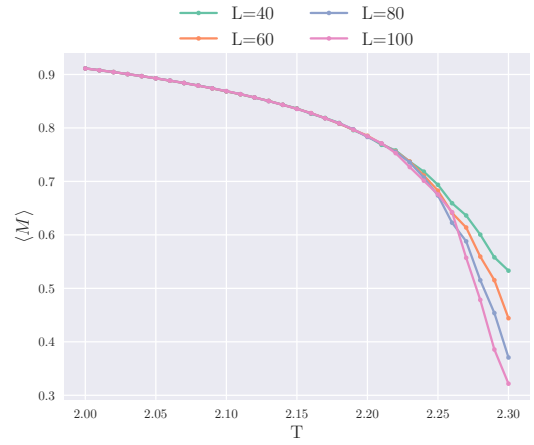

Figure 6: Plot over the expectation valuess for the specific heat per spin C_V as a function of temperature T with step size 10^{-3}. The results are from lattices with size $L = 40, 60, 80$ and 100. 10^6 *mcs* were used for each step.

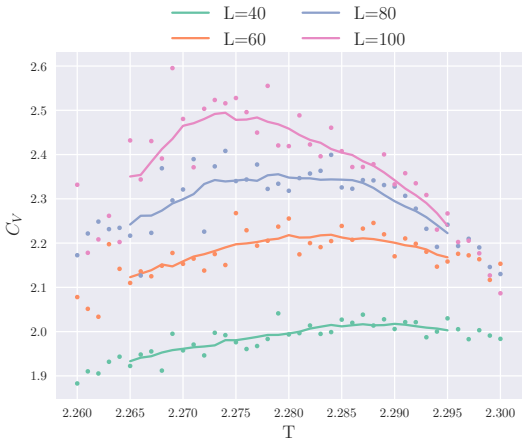

Figure 8: Plot over the expectation values for the specific heat per spin C_V as a function of temperature T with step size 10^{-4}.The results are from lattices with size $L = 40, 60, 80$ and 100. 10^6 *mcs* were used for each step. The dots are the collected data, while the solid line is a running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

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.

Appendix