The Ising model and phase transitions in magnetic systems

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November 12, 2018

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 is listed in Table 1, and will be used together with equation (3) and 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.

2.3 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

$$w = e^{-\beta \Delta E}. \tag{8}$$

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.

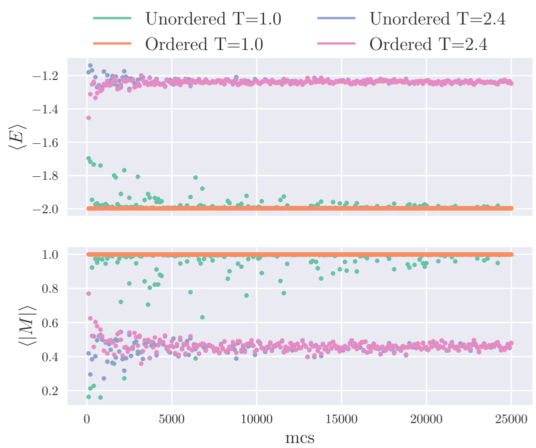

Figure 1:

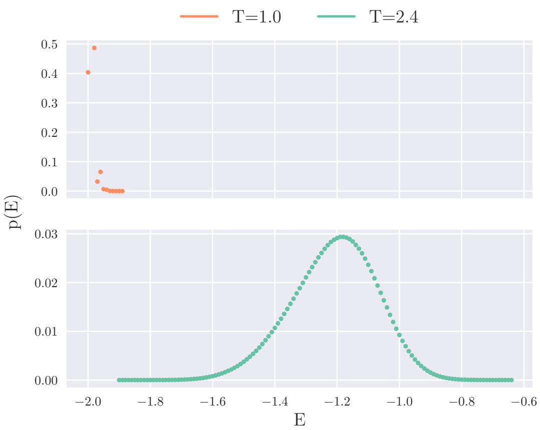

Figure 3:

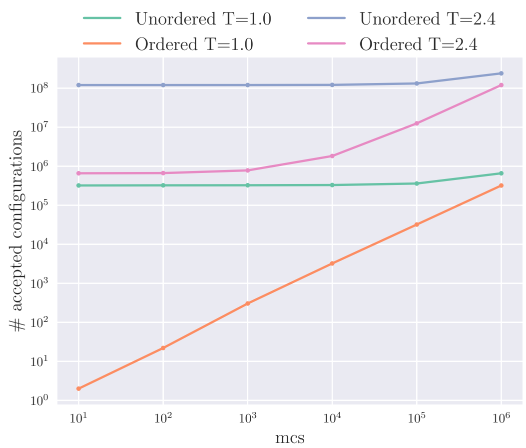

Figure 2:

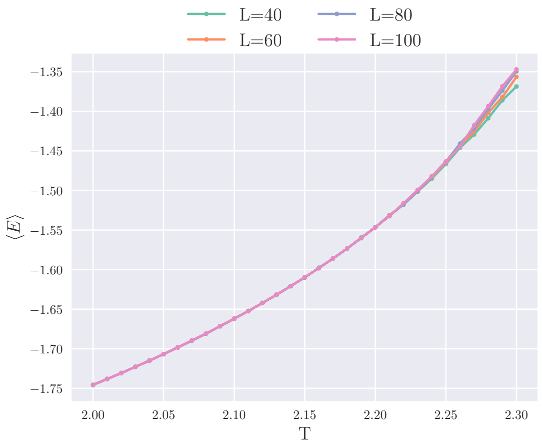

Figure 4:

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

Table 2:

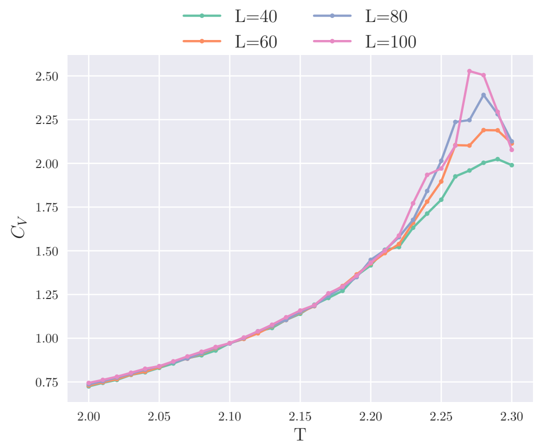

Figure 5:

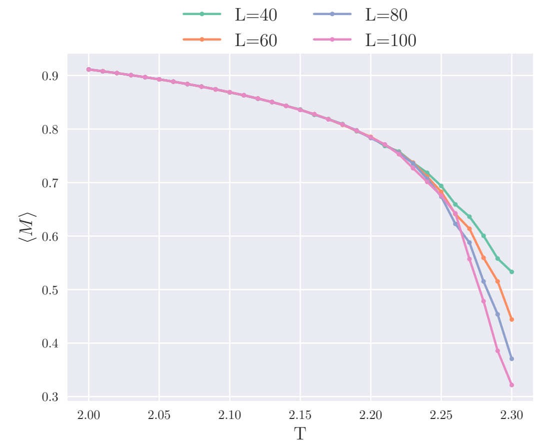

Figure 6:

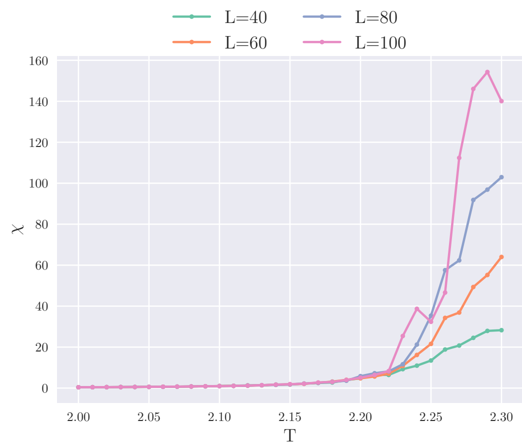

Figure 7:

2.4 Probability distribution

2.5 Programming technicalities

3 Results

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