

Project 4

FYS4150 Computational Physics

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Abstract

1 Introduction

The aim of this project is to do Monte Carlo simulations of magnetic systems described by the two-dimensional Ising model. The Ising model describes binary systems, that is a collection of objects with only two possible states each. Here we will take these two states to be spin-up and spin-down. In particular we will study phase transitions in such systems.

We will start by studying some analytical solutions to the Ising model by considering a 2×2 lattice. Then we will make a code that simulates the evolution of such systems for larger lattices. We will see how the system evolves depending on temperature and the initial state of the system, and we will finally study phase transitions, and extract the critical temperature.

In our simulations we will use the Metropolis algorithm for accepting or rejecting the Monte Carlo trials. We will also, as these simulations are quite time consuming, parallelize the code, so that we can distribute our simulation to multiple processors.

2 Theoretical framework

2.1 The Ising model

As mentioned in the introduction the Ising model describes a collection of objects, where each object can take two values, i.e. spin-up and spin-down, parametrized by $s = \pm 1$. We will consider a two-dimensional model with the spins organized in a square lattice with dimension L , so the total number of spins is given by $N = L \times L$. The two key quantities for describing our system will be energy and magnetization. The total energy of this system (with no external magnetic field) is given by

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

where J is a coupling constant and $\langle kl \rangle$ indicates that we sum over neighbouring spins only, i.e. one object is only "talking" to its closest neighbours. The total magnetization of the system is simply given by the sum over all spins:

$$M = \sum_k^N s_k. \quad (2)$$

A natural next step is to calculate expectation values within this theory, i.e. mean energy, $\langle E \rangle$, and mean magnetization $\langle M \rangle$. To be able to do so we need to introduce some concepts from statistical physics.

2.2 Elements from statistical physics

In order to calculate expectation values we need a probability distribution. In our case this is the Boltzmann distribution, given as

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

where $\beta = 1/k_B T$ (where k_B is Boltzmann's constant and T is temperature), E_i is the energy of state i and Z is the partition function. The partition function is given as

$$Z = \sum_{i=1}^n e^{-\beta E_i},$$

where the sum runs over all possible (micro)states of the system. The expectation value of some general quantity A can now be calculated as

$$\langle A \rangle = \sum_{i=1}^n A_i P_i(\beta) = \frac{1}{Z} \sum_{i=1}^n A_i e^{-\beta E_i},$$

and the variance of A is given as

$$\sigma_A^2 = \langle A^2 \rangle - \langle A \rangle^2.$$

By considering the variances of E and M we can also calculate specific heat, C_V , and susceptibility, χ , as

$$C_V = \frac{1}{k_B T^2} \sigma_E^2 \quad \text{and} \quad \chi = \frac{1}{k_B T} \sigma_M^2.$$

2.3 Analytical solutions

Using the above described framework we can study the Ising model for a 2×2 lattice analytically. This means that we have 4 objects which each can have $s = \pm 1$. Both in this and later analysis we will make use of so-called periodic boundary conditions, which means that we let the first and last spins in a lattice row be neighbours when summing up the energy.

We label the spins in the 2×2 lattice with $k \in \{1, 2, 3, 4\}$, and the energy is then given by

$$\begin{aligned} E &= -J(s_1 s_2 + s_2 s_1 + s_1 s_3 + s_3 s_1 + s_2 s_4 + s_4 s_2 + s_3 s_4 + s_4 s_3) \\ &= -2J(s_1 s_2 + s_1 s_3 + s_2 s_4 + s_3 s_4), \end{aligned}$$

and the magnetization as

$$M = s_1 + s_2 + s_3 + s_4.$$

Table 1 lists the possible values for these quantities for all possible spin configurations, along with the degeneracy for each spin configuration. Using this we find that the partition function is given as

$$Z = 12 + 2e^{8J\beta} + 2e^{-8J\beta} = 12 + 4 \cosh(8J\beta).$$

3 Code

4 Results

5 Summary and conclusions

Table 1: Degeneracy, energy and magnetization for the different spin configurations in the 2×2 lattice.

$\#$ spin-up	Degeneracy	E	M
4	1	$-8J$	4
3	4	0	2
2	2	$8J$	0
2	4	0	0
1	4	0	-2
0	1	$-8J$	-4