FYS4150 Project 4:
The Ising model in 2 dimensions

Marie Foss (# 56), Maria Hammerstrøm (# 59)

Abstract

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Github: *https://github.com/mariahammerstrom/Project4*

1 Introduction

The project deals with the Ising model in two dimensions, without an external magnetic field. The Ising model is a model to study phase transitions at finite temperature for magnetic systems. In its simplest form the **energy** for a specific microstate i is expressed as

$$E_i = -J \sum_{<kl>}^{N} s_k s_l, \tag{1}$$

with $s_k = \pm 1$, N is the total number of spins and J is a coupling constant expressing the strength of the interaction between neighboring spins. The symbol $< kl >$ indicates that we sum over nearest neighbors only. We will assume that we have a ferromagnetic ordering, meaning $J > 0$. We will use periodic boundary conditions and the Metropolis algorithm only.

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We will be using the **Boltzmann probability distribution** (PDF) defined as

$$w_i = \frac{1}{Z} e^{-\beta E_i}, \tag{2}$$

where $\beta = 1/kT$ with k the Boltzmann constant and T the temperature, and with Z as the **partition function** for the canonical ensemble defined as

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

summing over all micro states i. w_i expresses the probability of finding the system in a given microstate i.

The **magnetic moment** of a given microstate is

$$M_i = \sum_j s_j. \tag{4}$$

Some quantities we are interested in calculating, are the **expection values** for the energy $< E >$ and magnetic moment $< M >$:

$$\begin{aligned} < E > &= \frac{1}{Z} \sum_i E_i e^{-\beta E_i} \\ < M > &= \frac{1}{Z} \sum_i M_i e^{-\beta E_i}, \end{aligned} \tag{5}$$

as well as the variances for the energy σ_E^2 and for the magnetic moment σ_M^2:

$$\begin{aligned} \sigma_E^2 &=< E^2 > - < E >^2 \\ \sigma_M^2 &=< M^2 > - < M >^2, \end{aligned} \tag{6}$$

where

$$\sigma_E^2 = \frac{1}{Z} \sum_i E_i^2 e^{-\beta E_i} - \left[\frac{1}{Z} \sum_i E_i e^{-\beta E_i} \right]^2 \tag{7}$$

2 Methods

First we will assume that we only have two spins in each dimension, that is $L = 2$, where L is the lattice length. In this case, we can find a closed form expression for the partition function in Eq. (3) and the corresponding expectation values for E, $|\mathcal{M}|$, the specific heat C_V and the susceptibility χ as functions of T using periodic boundary conditions. **Periodic boundary conditions** means that the neighbor to the right of a given spin s_N in Eq. (1) takes the value of s_1. Similarly, the neighbor to the left of s_1 takes the value of s_N.

In the case $L = 2$ we can write Eq. (1) as:

$$E_i = -J\sum_{<kl>}^{N} s_k s_l = -J\sum_{k=1}^{2}\sum_{l=1}^{2} s_k s_l = -J(s_1 s_1 + s_1 s_2 + s_2 s_1 + s_2 s_2) \quad (8)$$

... EXPRESSIONS!

We write a code for the Ising model which computes the mean energy E, mean magnetization $|\mathcal{M}|$, the specific heat C_V and the susceptibility χ as functions of T using periodic boundary conditions for in the x and y directions. Using the Ising model in two dimensions, the number of configurations is given by 2^N with $N = L \times L$ number of spins for a lattice of length L.

We will use the **Metropolis algorithm**. The algorithm goes as follows:

- Generate a random configuration in the lattice to create an initial state with energy E_b.
- Change the initial configuration by flipping for example one spin only. Compute the energy of this state E_t.
- Calculate $\Delta E = E_t - E_b$.
- *The Metropolis test:* If $\Delta E \leq 0$ the new configuration is accepted, meaning the energy is lowered and we are moving towards the energy minimum at a given temperature. If $\Delta E > 0$, calculate $w = e^{-\beta \Delta E}$. If $w < r$ where r is a random number, accept the new configuration. If else, keep the old configuration.

3 Results

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Our numerical results from computing the mean energy E, mean magnetization $|\mathcal{M}|$, the specific heat C_V and the susceptibility χ as functions of T using periodic boundary conditions, can be compared with expressions given in Eq. (8) - (?) for a temperature $T = 1.0$ (in units of kT/J). This gives the following results:

Quantity	Closed form	Numerical
Mean energy E	-	-
Mean magnetization $|\mathcal{M}|$	-	-
Specific heat C_V	-	-
Susceptibility χ	-	-

The number of Monte Carlo cycles needed to achieve good agreement is XXX.

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4 Conclusions

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5 List of codes

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