

# Monte Carlo simulations

## The Ising Model and Phase transition

FYS3150: Computational Physics

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### I. INTRODUCTION

### II. THEORY

The Ising model is a binary system, where the objects at each lattice site can take one of two values, either spin up or spin down. The energy of the Ising model, with no external magnetic field can be expressed as

$$E = -J \sum_{\langle k, e \rangle} s_k s_e, \quad (1)$$

where we sum over the nearest neighbors interactions at each lattice site and  $s_i$  can take the values  $\pm 1$ , which represents either spin up or spin down, respectively.

#### A. Canonical Ensemble

In this article we will be working with an canonical ensemble, where the energy follows an expectation value at a given temperature. For us to calculate the expectation values such as the mean energy  $\langle E \rangle$ , we will be using a probability distribution, namely the Boltzmann distribution

$$P_i(\beta) = \frac{e^{-\beta E_i}}{Z} \quad (2)$$

where  $\beta = 1/k_B T$  being the inverse temperature,  $k_B$  is the Boltzmann constant,  $E_i$  is the energy at microstate  $i$  and  $Z$  is the partition function. We will in this article use natural units, that is  $k_B = J = 1$ .

The partition function  $Z$  is given as

$$Z = \sum_{i=1}^M e^{-\beta E_i}, \quad (3)$$

where we sum over all microstates  $M$ .

The expectation value of the energy can be calculated from the probability distribution  $P_i$  as

$$\langle E \rangle = \sum_{i=1}^M E_i P_i(\beta) = \frac{1}{Z} \sum_{i=1}^M E_i e^{-\beta E_i} \quad (4)$$

The corresponding variance is defined as

$$\begin{aligned} \sigma_E^2 &= \langle E^2 \rangle - \langle E \rangle^2 \\ &= \frac{1}{Z} \sum_{i=1}^M E_i^2 e^{-\beta E_i} - \left( \frac{1}{Z} \sum_{i=1}^M E_i e^{-\beta E_i} \right)^2 \end{aligned} \quad (5)$$

If we divide by  $k_B T^2$ , we obtain the specific heat

$$C_v = \frac{1}{k_B T^2} (\langle E^2 \rangle - \langle E \rangle^2). \quad (6)$$

In the same way we can evaluate the mean magnetization through

$$\langle \mathcal{M} \rangle = \sum_i^M \mathcal{M} P_i(\beta) = \frac{1}{Z} \sum_i^M \mathcal{M} e^{-\beta E_i} \quad (7)$$

and the corresponding variance

$$\begin{aligned} \sigma_{\mathcal{M}}^2 &= \langle \mathcal{M}^2 \rangle - \langle \mathcal{M} \rangle^2 \\ &= \frac{1}{Z} \sum_{i=1}^M \mathcal{M}_i^2 e^{-\beta E_i} - \left( \frac{1}{Z} \sum_{i=1}^M \mathcal{M}_i e^{-\beta E_i} \right)^2. \end{aligned} \quad (8)$$

This quantity defines the susceptibility  $\mathcal{X}$

$$\mathcal{X} = \frac{1}{k_B T} (\langle \mathcal{M}^2 \rangle - \langle \mathcal{M} \rangle^2). \quad (9)$$

### III. PHASE TRANSITION

#### A. Analytical Results

In 1944 Lars Onsager was the first to solve the Ising model analytically for a general lattice size  $L[1]$ . He found that the critical temperature of the system is

$$T_C = \frac{2J}{k_B \ln(1 + \sqrt{2})} \simeq 2.269 \dots \quad (10)$$

We will use the ideas from phase transition to try to estimate  $T_C$ , using larger lattice size.

However first we need a benchmark for our code, where we will use a 2x2 system with periodic boundary conditions to calculate numerical expectation values. The analytical expectation values and the partition function can be calculated through equations (4, 3, 7), and the

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\* <https://github.com/SigurdSundberg/FYS3150>

TABLE I: Display over the possible spin configurations for the 2x2 lattice. As well as listing the energy and magnetization of system.

$N_{\uparrow}$	Degeneracy	E	M	Configurations
4	1	-8J	4	$\begin{bmatrix} \uparrow & \uparrow \\ \uparrow & \uparrow \end{bmatrix}$
3	4	0	2	$\begin{bmatrix} \downarrow & \uparrow \\ \uparrow & \uparrow \end{bmatrix}$ $\begin{bmatrix} \uparrow & \downarrow \\ \uparrow & \uparrow \end{bmatrix}$ $\begin{bmatrix} \uparrow & \uparrow \\ \downarrow & \uparrow \end{bmatrix}$ $\begin{bmatrix} \uparrow & \uparrow \\ \uparrow & \downarrow \end{bmatrix}$
2	4	0	0	$\begin{bmatrix} \downarrow & \downarrow \\ \uparrow & \uparrow \end{bmatrix}$ $\begin{bmatrix} \uparrow & \uparrow \\ \downarrow & \downarrow \end{bmatrix}$ $\begin{bmatrix} \downarrow & \uparrow \\ \downarrow & \uparrow \end{bmatrix}$ $\begin{bmatrix} \uparrow & \downarrow \\ \uparrow & \downarrow \end{bmatrix}$
2	2	8J	0	$\begin{bmatrix} \downarrow & \downarrow \\ \downarrow & \downarrow \end{bmatrix}$ $\begin{bmatrix} \uparrow & \downarrow \\ \downarrow & \uparrow \end{bmatrix}$
1	4	0	-2	$\begin{bmatrix} \uparrow & \downarrow \\ \downarrow & \downarrow \end{bmatrix}$ $\begin{bmatrix} \downarrow & \uparrow \\ \downarrow & \downarrow \end{bmatrix}$ $\begin{bmatrix} \downarrow & \downarrow \\ \uparrow & \downarrow \end{bmatrix}$ $\begin{bmatrix} \downarrow & \downarrow \\ \downarrow & \uparrow \end{bmatrix}$
0	1	-8J	-4	$\begin{bmatrix} \downarrow & \downarrow \\ \downarrow & \downarrow \end{bmatrix}$

value displayed in table I. Likewise we can find values of  $E^2$  and  $M^2$ .

We find that

$$Z = 12 + 4 \cosh(8J\beta) \quad \beta = (k_B T)^{-1} \quad (11)$$

$$\langle E \rangle = -\frac{32J}{Z} \sinh(8J\beta) \quad (12)$$

$$\langle E^2 \rangle = \frac{256}{Z} \cosh(8J\beta) \quad (13)$$

$$\langle M \rangle = 0 \quad (14)$$

$$\langle M^2 \rangle = \frac{32}{Z} (e^{8J\beta} + 1) \quad (15)$$

$$\langle |M| \rangle = \frac{8}{Z} (e^{8J\beta} + 2) \quad (16)$$

From equation (6), the heat capacity of the system is

$$C_v = \frac{256}{Z k_B T^2} \left( \cosh(8J\beta) - \frac{4}{Z} \sinh^2(8J\beta) \right) \quad (17)$$

and we can find the susceptibility from equation (9), which can be expressed as

$$\chi = \frac{32\beta}{Z} (e^{8J\beta} + 1). \quad (18)$$

#### IV. ALGORITHMS

##### V. PERIODIC BOUNDARY CONDITIONS

When applying periodic boundary conditions we need a way to index ghosts points. In this project to represent our lattice we will use a matrix of size  $L \times L$ , thus needing to index points outside the scope of our lattice. The simple way of doing so would be to implement `if`-statements

to check whether we are indexing a ghost point or not. This is however slow and hard to optimize.

A second possibility for handling the ghost points would be to expand our matrix to a  $(L+2) \times (L+2)$  matrix, where we have the ability to index the ghosts points directly without the use of `if`-statements. However this runs into its own limitations, namely we would need to update the ghosts points whenever we change its corresponding value. In a 1-dimensional case this would lead to us having to update index 0 if we made a change to index  $n$ , for an array from 0 to  $n+1$ . This can be implemented using either `if`-statements or using properties of modulus operator.

A third method, which is the one used in this project, is using the modulus operator directly on a  $L \times L$  matrix. This is done by looking at the point of interest in the matrix and compute its neighboring indexes by the following equation

$$\text{neighbor} = (\text{current} + L + \text{position}) \% (L) \quad (19)$$

where current is the current matrix index,  $L$  is the dimensionality of the matrix and position is the index of the neighbor relative to current position. This equation handles both the ghost points and the normal points of the matrix and creates an efficient way for us to access all points of the matrix.

By implementing this as an inline function, we are able to, at compile time, to reduce the time used of our program.

#### VI. METROPOLIS-HASTINGS ALGORITHM

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**Algorithm 1:** Monte Carlo simulation with Metropolis sampling

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Pick T and  $L_i$ 
Compute  $E_i$  and  $M_i$ 
for  $i = 0; i < MC \text{ cycles}; i++$  do
    for  $j = 0; j < Total \text{ Spins}; j++$  do
        Sample a random index of the spin matrix
        Compute  $\Delta E$ 
        if  $\Delta E < 0$  or  $r < e^{-\beta \Delta E}$  then
            Accept the flip
            Update E and M
        end
        Update the mean values for E and M
    end
end
Normalize all computed values

```

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**VII. RESULTS****VIII. DISCUSSION****IX. CONCLUSION**

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- [1] Lars Onsager. Crystal statistics. i. a two-dimensional model with an order-disorder transition. *Phys. Rev.*, 65:117–149, Feb 1944.