

# Project 3

Anna Stray Rongve  
Knut Magnus Aasrud  
Amund Midtgard Raniseth

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## Abstract

## 1 Introduction

## 2 Theory

### 2.1 The problem

### 2.2 $2 \times 2$ lattice, analytical expressions

To get started we will find the analytical expression for the partition function and the corresponding expectation values for the energy  $E$ , the mean absolute value of the magnetic moment  $|M|$  (which we will refer to as magnetization), the specific heat  $C_V$  and the susceptibility  $\chi$  as function of  $T$  using periodic boundary conditions. These calculations will serve as benchmarks for our next steps.

#### Partition function, $Z$

The partition function in the canonical ensemble is defined as:

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

Where  $\beta = \frac{1}{k_B T}$  and  $E_i$  is the energy of the system in the microstate  $i$  and  $N$  is the respective microstate.

We therefore have to find  $E_i$  which is defined as:

$$E_i = -J \sum_{\langle kl \rangle}^N s_k s_l$$

Where  $\langle kl \rangle$  indicates that we sum only over the nearest neighbors and  $J$  is a constant for the bonding strenght. For our two dimensional system the equation

reads:

$$E_{i,2D} = -J \sum_i^N \sum_j^N (s_{i,j} s_{i,j+1} + s_{i,j} s_{i+1,j})$$

Four our two-spin-state system with two dimensions we get the following table if we use periodic boundary conditions:

Number of spins up	Degeneracy	Energy	Magnetization
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: Number of spins up, degeneracy, energy and magnetization of the two-dimensional benchmark scenario.

Where the magnetization is found by subtracting the number of spin downs from the number of spin up, or in other words the sum of the spins:

$$\mathcal{M} = \sum_{j=1}^N s_j$$

Getting back to the partition function, we insert all 16 of the  $E_i$  respectively.

$$Z = e^{-\beta(-8J)} + 2 \cdot e^{-\beta(8J)} + e^{-\beta(-8J)} = 2e^{-\beta 8J} + 2e^{\beta 8J}$$

### Energy expectation value, $\langle E \rangle$

The expectation value of the energy is defined as:

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

Where  $M$  is the sum over all microstates.  $P_i$  is the Boltzmann probability distribution which reads:

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

For our system, this is easily calculated by inserting the partition function and the microstate energy  $E_i$ .

$$\begin{aligned} \langle E \rangle &= \frac{1}{2e^{-\beta 8J} + 2e^{\beta 8J}} (2 \cdot -8J \cdot e^{\beta 8J} + 2 \cdot 8J \cdot e^{-\beta 8J}) \\ &= \frac{1}{2e^{-\beta 8J} + 2e^{\beta 8J}} (-16J e^{\beta 8J} + 16J e^{-\beta 8J}) \\ &= 8J \frac{1}{e^{-\beta 8J} + e^{\beta 8J}} (e^{-\beta 8J} - e^{\beta 8J}) \end{aligned}$$

**Magnetization,  $\mathcal{M}$**   
**Specific heat capacity,  $C_V$**   
**Susceptibility,  $\chi$**

#### **Analytical results:**

LISTING ALL THE ANALYTICAL RESULTS IN BEAUTIFUL MATH ALIGN

REF: <https://compphysics.github.io/ComputationalPhysics/doc/pub/statphys/pdf/statphys-print.pdf>

Which are all temperature dependent trough  $\beta = \frac{1}{k_B T}$ .

### **2.3 Ising model**

The Ising model is applied for the study of phase transistions at finite temperatures for magnetic systems. Energy is expressed as:

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

N is the number of spins and J is a constant expressing the interaction between neighboring spins. The sum is over the nearest neighbours only, indicated by  $\langle kl \rangle$  the above equation. For  $J \neq 0$  it is energetically favorable for neighboring spins to align. Leading to, at low temperatures, T, spontaneous magnetisation.

A probability distribution is needed in order to calculate the mean energy  $\langle E \rangle$  and magnetization  $\langle M \rangle$  at a given temperature. The distribution is given by:

$$P_i(\beta) = \frac{1}{M} \sum_{i=1}^M s_k s_l \exp -\beta E_i, \quad (2)$$

where M is all the microstates,  $P_i$  is the probability of having the system in a state/configuration i.

CONFIGURATIONS

## **3 Results**

## **4 Discussion**

## **5 Conclusion**