

# Project 3

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## 1 Theory

### 1.1 The problem

### 1.2 $2 \times 2$ 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

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:

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.