Project 3

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Abstract

1 Introduction

2 Theory

2.1 The problem

2.2 2×2 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 χ 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:

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

Where $< kl >$ 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.

3 Results

4 Discussion

5 Conclusion