Studies of phase transitions in magnetic systems

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I. INTRODUCTION

II. THEORY

Statistical terms

In this report we are going to use some basic statistical terms and expressions. For those not familiar with terms like standard deviation and mean value, they are covered below.

The expectation value or mean value, often written as $\langle A \rangle$, is the sum of all values A_i, divided by the total number N of values it can have:

$$\langle A \rangle = \frac{1}{N} \sum_{i}^{N} A_i$$

However, when given a probability distribution P_i, which describes the probability of having outcome A_i, one can also find the expectation value through

$$\langle A \rangle = \sum_{i}^{N} A_i P_i.$$

Variance or standard deviation (σ_A), is a measurement of the variation in a set of data A_i. The mathematical expression is given as

$$\sigma_A = \sqrt{\frac{1}{N-1} \sum_{i}^{N} (A_i - \langle A \rangle)^2} = \sqrt{\langle A^2 \rangle - \langle A \rangle^2},$$

where N is the total number of outcomes and $\langle A \rangle$ is the expectation value of A_i.

Canonical ensemble

The probability of finding a system in a given microstate is found through the canonical ensemble, given by equation (1) (see [2] chapter 13.2.2).

$$P_i(\beta) = \frac{\exp(-\beta E_i)}{Z}, \quad \beta = \frac{1}{k_B T} \tag{1}$$

Here $P_i(\beta)$ is the probability of finding the system with energy E_i and temperature T in Kelvin. k_B is Boltzmann constant and Z the partition function given by

$$Z = \sum_{i=1}^{M} \exp(-\beta E_i). \tag{2}$$

Here M is the total number of microstates.

The canonical ensemble and partition function is usually hard to find, however, when obtained we can use them to find many useful relations. Below we list the expressions (without derivation) we need in the report. Everything is from [2] chapter 13.2.2.

Mean energy $\langle E \rangle$ given as

$$\langle E \rangle = \frac{1}{Z} \sum_{i=1}^{M} E_i \exp(-\beta E_i). \tag{3}$$

Mean absolute value of the magnetic moment $\langle |M| \rangle$:

$$\langle |M| \rangle = \frac{1}{Z} \sum_{i=1}^{M} |M_i| \exp(-\beta E_i). \tag{4}$$

With this we can also find the susceptibility χ

$$\chi = \beta \sigma_M \tag{5}$$

Specific heat capacity at constant volume C_V is given by

$$C_V = \frac{\beta}{T} \sigma_E \tag{6}$$

Analytical expressions for 2x2 lattice

From [1] the energy in a 2D lattice with no external magnetic field is given by

$$E = -J \sum_{<kl>}^{N} s_k s_l, \tag{7}$$

where $s_k = \pm 1$ (representing the spin direction), N the total number of spins and J a coupling constant indicating the strength of the interaction between neighboring spins. The $< kl >$ means that we sum over the nearest neighbors. In this report we are only going to use periodic boundary conditions, meaning the edges are neighbors. For a square peace of (stretchy) paper, this would look like first folding it into a cylinder and then into a donut-shape.

Table I (from [2] table 13.4) shows the energy and magnetization of the 2D lattice for different spin configurations, as well as the multiplicity of each configuration. This can easily be derived with equation (7), and trying for all possible combinations. From this table we see that there are only five possible values for the energy differences ΔE:

- $\Delta E = \pm 16$ J for the difference between 8 J and -8 J (both ways)
- $\Delta E = \pm 8$ J for the difference between ± 8 J and 0 J (both ways)
- $\Delta E = 0$ J

With this we can find the partition function. Reading the values from table I and using equation (2) we find the partition function Z to be

$$\begin{aligned} Z &= \sum_{i=1}^{16} \exp(-\beta E_i) \\ &= 12 + 2\exp(8\beta) + 2\exp(-8\beta) \\ &= 12 + 4\cosh(8\beta). \end{aligned} \tag{8}$$

Number spins up	Degeneracy	Energy, [J]	Magnetization
4	1	-8	4
3	4	0	2
2	4	0	0
2	2	8	0
1	4	0	-2
0	1	-8	-4

Table I. Table showing the energy, multiplicity and magnetization of different configurations of spins in a 2×2 2D-lattice with periodic boundary conditions.

Now that we have the partition function and the canonical ensemble through equation (1), we can find a lot of useful values. With equations (3-6) we can find expected energy $\langle E \rangle$, mean absolute value of the magnetic moment $\langle |M| \rangle$, susceptibility χ and specific heat capacity at constant volume C_V.

III. METHODS

As presented in the Theory section (section II), we already know the energy differences in the lattice before we start the simulation. We can thus compute and store the different values of $e^{-\beta \Delta E}$ beforehand to avoid making these computations every time we update the energy.

A. Testing of algorithm

B. Boundary conditions

We are going to simulate a 2D lattice with periodic boundary conditions. This means that the neighbour to the right of s_N takes the value of s_0 and the neighbour to the left of s_0 takes the value of s_N.

IV. RESULTS

V. DISCUSSION

[1] Department of Physics, Univeristy of Oslo, Fall semester 2020, Computational Physics I FYS3150/FYS4150, Project 4.

[2] Morten Hjorth-Jensen, Computational Physics, Lecture Notes Fall 2015, August 2015, https://github.com/CompPhysics/ComputationalPhysics/blob/master/doc/Lectures/lectures2015.pdf.