Studies of phase transitions in magnetic systems

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CONTENTS

I. INTRODUCTION

For our studies we have used c++ for heavy computation, python for visualization and bash for automation. All the code along with instructions on how to run it, can be cloned from our GitHub repository here[1].

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

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[1] github.com/sigurdru/FYS3150/tree/master/Project3

constant and Z the partition function given by

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

Where 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 will need in the report. Everything is from [2] chapter 13.2.2.

The mean energy $\langle E \rangle$ given as

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

and the mean square energy ($\langle E^2 \rangle$) is calculated by

$$\langle E^2 \rangle = \frac{1}{Z} \sum_{i=1}^M E_i^2 \exp(-\beta E_i). \tag{4}$$

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

$$\langle |M| \rangle = \frac{1}{Z} \sum_{i=1}^M |M_i| \exp(-\beta E_i), \tag{5}$$

and mean square magnetic moment ($\langle M^2 \rangle$) by

$$\langle M^2 \rangle = \frac{1}{Z} \sum_{i=1}^M M_i^2 \exp(-\beta E_i). \tag{6}$$

With this we can also find the susceptibility χ

$$\chi = \beta \sigma_M, \quad \sigma_M = \sqrt{\langle M^2 \rangle - \langle |M| \rangle} \tag{7}$$

Where σ_M is the variance of $|M|$. We evaluate the absolute value of M because that gives nicer plots. Specific heat capacity at constant volume C_V is given by

$$C_V = \frac{\beta}{T} \sigma_E, \quad \sigma_E = \sqrt{\langle E^2 \rangle - \langle E \rangle} \tag{8}$$

σ_E is the variance of E.

Two dimensional lattice

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

$$E = -J \sum_{<kl>}^N s_k s_l, \tag{9}$$

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.

III.   METHODS

In this report we are only going to use periodic bound-
ary 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.

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.

A.   Units

We scale our units in order to have easier numbers to
work with. We scale our units with J and the Boltzmann
constant k_B, such that temperature has a dimensionless
unit of kT/J.

B.   Testing of algorithm

In order to make sure our algorithm is running cor-
rectly, we want to test it. We do this by comparing it to
analytical results, namely a 2x2 lattice.

By using equation (9) and testing all 16 different com-
binations for a 2D lattice, we have made a table (see I)
that shows all the possible energies and magnetizations,
as well as the multiplicity of each configuration (marked
as degeneracy). With this we can find the analytical term

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 magneti-
zation of different configurations of spins in a 2×2 2D-lattice
with periodic boundary conditions.

of the partition function (Z). Reading the values from
table I and using equation (2) we get:

$$Z = \sum_{i=1}^{16} \exp(-\beta E_i)$$
$$= 12 + 2\exp(8\beta) + 2\exp(-8\beta)$$
$$= 12 + 4\cosh(8\beta). \tag{10}$$

With the partition function and the canonical ensemble
through equation (1), we can find a lot of useful values.
With equations (3-8) we can find expected energy $\langle E \rangle$,
mean absolute value of the magnetic moment $\langle |M| \rangle$, sus-
ceptibility χ and specific heat capacity at constant vol-
ume C_V. The calculations are done in the appendix VI B.

IV.   RESULTS

V.   DISCUSSION

VI.   APPENDIX

A.   Algorithm specific optimization

In order to make our algorithm run faster, we do some
optimization. We list the optimizations we implemented
here, to make our code easier to understand and as a
guide for anyone who wants to do something similar.

Through table I, we already know the possible energy
differences (ΔE) in the lattice before we start the simu-
lation.

- $\Delta E = \pm 16$ 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

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.

As mentioned above, we are going to use periodic
boundary conditions. The easiest, but slow way of im-
plementing this, is with if-tests. However we did it with
a simple function (in c++),

```cpp
int PeriodicBoundary(int i, int limit, int add) {
    return (i+limit+add) % (limit);
}
```

that takes the current index you are evaluating (`i`), the
total size (`limit`) and the amount you want to go forward
and backward (`add`). Then we sum all the arguments and
take the rest, reassuring us we always arrive at the right
index, or if we are at the edge, wrap back around.

B. Calculations of 2x2 lattice

Inserting the values from table I into equations (1) and (3-8) we get

$$\langle E \rangle = \frac{1}{Z} \left(-8Je^{8\beta J} + 2 \cdot 8Je^{-8\beta J} - 8Je^{8\beta J} \right)$$

$$= \frac{-32J}{Z} \cosh(8\beta J)$$

$$\langle E^2 \rangle = \frac{1}{Z} \left((-8J)^2 e^{8\beta J} + 2 \cdot (8J)^2 e^{-8\beta J} (-8J)^2 e^{8\beta J} \right)$$

$$= \frac{256J^2}{Z} \cosh(8\beta J)$$

$$\langle |M| \rangle = \frac{1}{Z} \left(4e^{8\beta J} + 4 \cdot 2e^0 + 4 \cdot 2e^0 + 4e^{8\beta J} \right)$$

$$= \frac{8}{Z} \left(2 + e^{8\beta J} \right)$$

$$\langle M^2 \rangle = \frac{1}{Z} \left(4^2 e^{8\beta J} + 4 \cdot 2^2 e^0 + 4 \cdot 2^2 e^0 + 4^2 e^{8\beta J} \right)$$

$$= \frac{32}{Z} \left(1 + e^{8\beta J} \right)$$

$$\chi = \frac{32\beta J^2}{Z} \left(1 + e^{8\beta J} \right) - \frac{64\beta}{Z^2} \left(2 + e^{8\beta J} \right)^2$$

$$C_V = \frac{1024\beta J^2}{TZ^2} \left(3 \cosh(8\beta J) + 1 \right)$$

[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.