Project 4

For the course FYS3150

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November 20, 2019
Week 43 - ?

TING Å GJØRE

- a) ferdig
- b) code is ran, discuss results
- c) code is ran, discuss results (see RESULTS.txt)
- d) code is ran, see probability-distribution.py (input energy/L20.....txt)
- e) currently running, need plotting-program and timing analysis!
- f) TRENGER ALT

legge Cv og susc utledning i appendix eller ha det i teori??

Abstract

In this numerical project we have simulated some solid-state properties using the two-dimensional Ising model. The system was comprised of flippings spins, and they simulated energies, heat capacity, magnetization and susceptibility. The results were FORTELL NOE OM RESULTATENE

Contents

1 Introduction

The simulation consisted of a 2-dimensional lattice with spins pointing up or down. They

2 Theory

2.1 Analytical solution for 2×2 lattice

The energies in this lattice is given by the set $E_i = \{-8J, -4J, 0, 4J, 8J\}$.

2.1.1 Partition function

The partition function is given by the equation below.

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

The sum runs from 1 to M, which is 16 because of the 2×2 lattice. This applies to every sum calculated which are related to the specific heat and susceptibility.

The partition function is derived in the appendix, see A.1.1. From the appendix it is found that the partition function for this system is given by

$$Z = 4\cosh(8\beta J) + 12 \tag{2}$$

2.1.2 Energy and magnetization

The expectation value of the energy is

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

This analytical expression is derived in the appendix in section A.1.2. Here it is found that the energy is given by

$$\langle E \rangle = -\frac{32J}{Z} \sinh(8\beta J) \tag{4}$$

The expectation value of the magnetization is

$$\langle \mathcal{M} \rangle = \frac{1}{Z} \sum_{i=1}^{M} \mathcal{M}_i e^{-\beta E_i} \tag{5}$$

This equation is derived in the appendix, see section A.1.3. Here it is found that the expectation value of the magnetization is

$$\langle \mathcal{M} \rangle = 0 \tag{6}$$

Because this becomes zero, we will look at the mean magnetization. The contributions of the spins to the mean magnetization will not cancel eachother out, and the mean magnetization should not be zero. **riktig???**

The expectation value of the mean magnetization is

$$\langle |\mathcal{M}| \rangle = \frac{1}{Z} \sum_{i=1}^{M} |\mathcal{M}_i| e^{-\beta E_i} \tag{7}$$

It is derived in the appendix in section A.1.3. The analytical expression is the following

$$\langle|\mathcal{M}|\rangle = \frac{8}{Z}\left(e^{\beta 8J} + 2\right) \tag{8}$$

2.1.3 Specific heat

The specific heat is given by the equation

$$C_V = \frac{1}{k_B T^2}\left(\langle E^2\rangle - \langle E\rangle^2\right) \tag{9}$$

Therefore the expectation value of the energy squared has to be calculated. See the section A.1.2.

Now the specific heat can be calculated.

$$C_V = \frac{1}{k_B T^2}\left(\langle E^2\rangle - \langle E\rangle^2\right) = \frac{1}{k_B T^2}\left(\frac{256J^2}{Z}\cosh(8\beta J) - \left(-\frac{32J}{Z}\sinh(8\beta J)\right)^2\right)$$

The analytical expression for the specific heat is

$$C_V = \frac{1}{k_B T^2}\left(\frac{256J^2}{Z}\cosh(8\beta J) - \left(-\frac{32J}{Z}\sinh(8\beta J)\right)^2\right) \tag{10}$$

2.1.4 Susceptibility

The susceptibility is given by

$$\chi = \frac{1}{k_B T}\left(\langle \mathcal{M}^2\rangle - \langle \mathcal{M}\rangle^2\right) \tag{11}$$

The expectation value of the magnetization squared therefore has to be calculated, see the section A.1.3.

Now calculating the susceptibility of the system.

$$\begin{aligned}
\chi &= \frac{1}{k_B T}\left(\langle \mathcal{M}^2\rangle - \langle \mathcal{M}\rangle^2\right) \\
&= \frac{1}{k_B T}\left[\frac{32}{Z}\left(e^{8\beta J} + 1\right) - 0^2\right] \\
&= \frac{1}{k_B T}\frac{32}{Z}\left(e^{8\beta J} + 1\right)
\end{aligned}$$

The analytical expression for the susceptibility is therefore

$$\chi = \frac{1}{k_B T}\frac{32}{Z}\left(e^{8\beta J} + 1\right) \tag{12}$$

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3 Method

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4 Results

`.txt`-files for all the raw data generated by the projects are up on our GitHub.

4.1 2x2-lattice

When comparing the analytical results for the 2x2-lattice to the numerical simulation we found the following. See Table (1).

Table 1: 2x2 - Analytical vs numerical values (output/L2_n1000_T1.0_ord0.txt)

	Analytical	numerical at T=1.0
<E>	ALEXANDRA	-1.998
Cv	ALEXANDRA	0.015984
χ	ALEXANDRA	0.000999
<|M|>	ALEXANDRA	0.9995

Running the 2x2-simulation the following data arised. See figures (1), (2).

4.2 20x20-lattice

4.2.1 Probability distributions

4.3 Critical Temperature

Table 2: Critical temperature for simulations

L	T_c
40	VALUE
60	VALUE
80	VALUE
100	VALUE

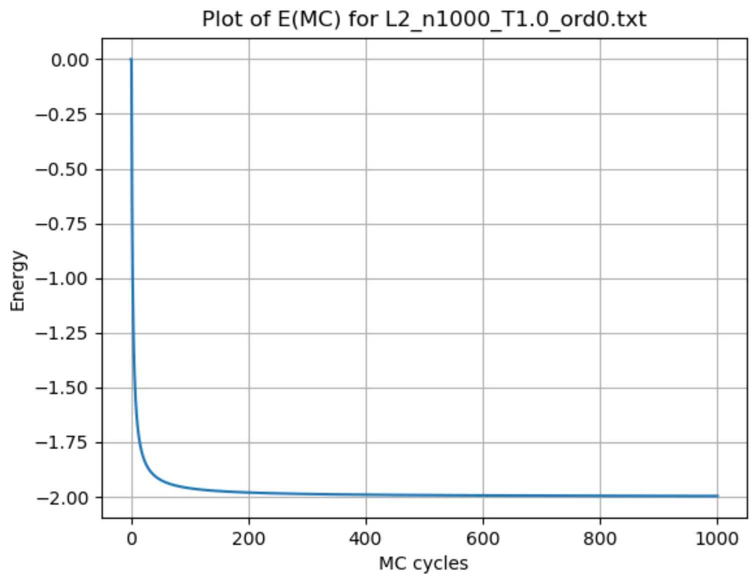

Figure 1: Energy-plot as function of MC-cycles. 2x2, MC1000, T=1.0, unordered spin

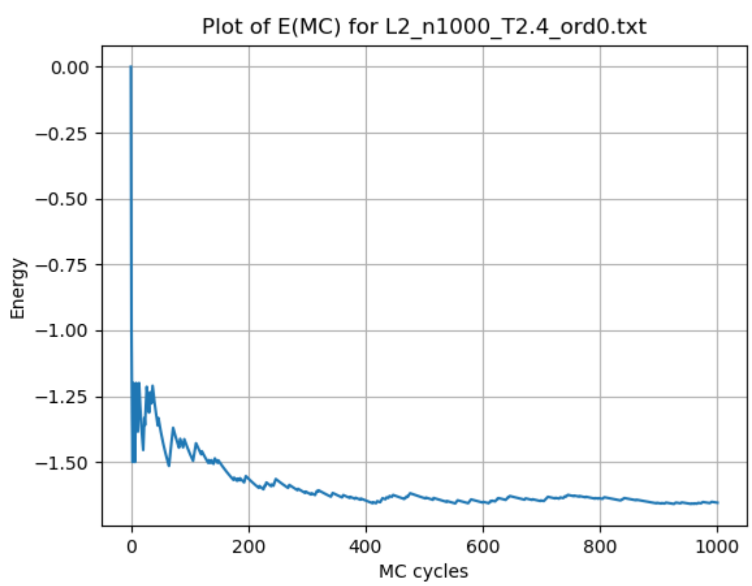

Figure 2: Energy-plot as function of MC-cycles. 2x2, MC1000, T=2.4, unordered spin

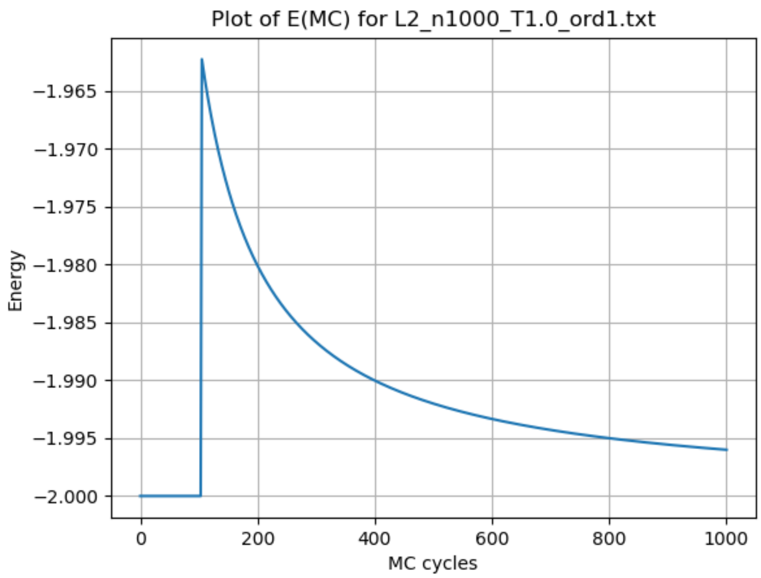

Figure 3: Energy-plot as function of MC-cycles. 2x2, MC1000, T=1.0, ordered spin

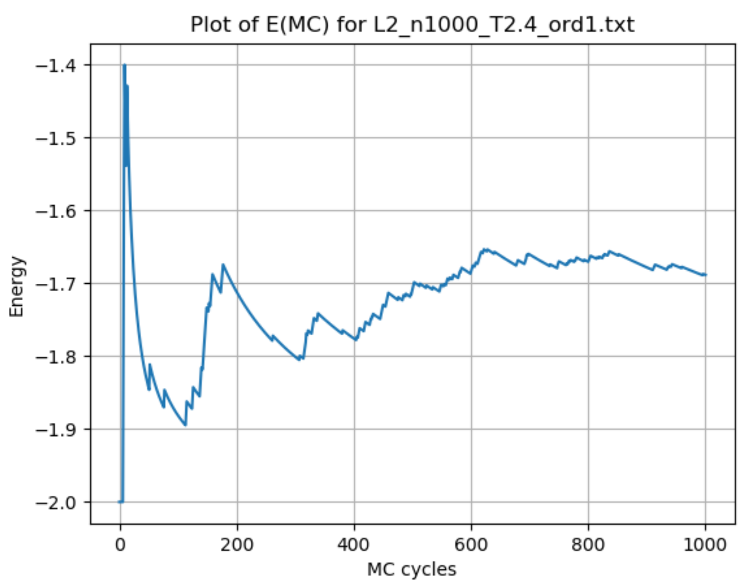

Figure 4: Energy-plot as function of MC-cycles. 2x2, MC1000, T=2.4, ordered spin

5 Discussion

Comparing the 2x2-lattice's numerical values with the analytical ones we see there is a major discrepancy. See table (1). This is quite unnerving. However, after many hours of debugging and re-checking analytical expressions, no reason was found, and as such the results have been left like that. The reason for this error could be from numerical errors, truncation errors hidden somewhere, faulty expressions or other similar explanations.
For 4c) see RESULTS.txt
For 4d) Jeg prøvde SÅ HARDT å fikse et plot av sannsynlighetsfordelingen, men det ble f*cked Se koden for hva jeg har gjort og prøv å finne ut av det. I PDF-en for Project 4 står det vi skal sammenligne med variansen.. prøv å fikse i koden prøvde jeg å bruke variansen som filter, men tror ikke vi kan det. Samtidig må vi kutte ut all dataen som lages før latticen når equilibrium.
For 4e) ALEXANDRA
For 4f) ERIK

6 Conclusion and perspective

7 References

[1] Morten H. Jensen (2019), Project 4, Departement of Physics, University of Oslo, Norway

[2] Erik B. Grammeltvedt, Alexandra Jahr Kolstad, Erlend T. North (2019), GitHub, Students of Departement of Physics, University of Oslo, Norway

[3] Morten H. Jensen (2015), Lecture slides for FYS3150, Department of Physics, University of Oslo, Norway

[4] Onsager (1944), "A Two-Dimensional Model with an Order-Disorder Transition", American Physical Society

A Appendix - endre navn senere?

A.1 Derivation of analytical formulae

To derive the analytical formulae we need to know the hyperbolic functions cosh and sinh, and their correlation to the exponential function.

They are as follows

$$2\cosh(x) = e^{x} + e^{-x}$$
$$2\sinh(x) = e^{x} - e^{-x}$$

A.1.1 Derivation of the partition function

The partition function is introduced in section 2.1.1.

Deriving the equation.

$$
\begin{aligned}
Z &= \sum_{i=1}^{M} e^{-\beta E_i} = \sum_{i=1}^{16} e^{-\beta E_i} \\
&= 1 \cdot e^{-\beta(-8J)} + 4 \cdot e^{-\beta(0J)} + 2 \cdot e^{-\beta(8J)} + 4 \cdot e^{-\beta(0J)} + 4 \cdot e^{-\beta(0J)} + 1 \cdot e^{-\beta(-8J)} \\
&= e^{8\ \beta J} + 4 + 2 \cdot e^{-8\beta J} + 4 + 4 + e^{8\beta J} \\
&= 2e^{8\beta J} + 2e^{-8\beta J} + 12 \\
&= 2\left(e^{8\beta J} + e^{-8\beta J}\right) + 12 \\
&= 2\left(2\cosh(8\beta J)\right) + 12 \\
&= 4\cosh(8\beta J) + 12
\end{aligned}
$$

A.1.2 Derivation of the expectation values of the energies

The expectation value of the energy is introduced in section 2.1.2.

Deriving the equation.

$$
\begin{aligned}
\langle E \rangle &= \frac{1}{Z} \sum_{i=1}^{M} E_i e^{-\beta E_i} \\
&= \frac{1}{Z}\left[1 \cdot (-8J)e^{-\beta(-8J)} + 4 \cdot 0 + 2 \cdot (8J)e^{-\beta(8J)} + 4 \cdot 0 + 1 \cdot (-8J)e^{-\beta(-8J)}\right] \\
&= \frac{1}{Z}\left[-8Je^{\beta 8J} + 2 \cdot 8Je^{-\beta 8J} - 8Je^{\beta 8J}\right] \\
&= \frac{2}{Z}\left[-8Je^{\beta 8J} + 8Je^{-\beta 8J}\right] \\
&= -\frac{16J}{Z}\left(e^{8\beta J} - e^{-8\beta J}\right) \\
&= -\frac{16J}{Z}(2\sinh(8\beta J)) \\
&= -\frac{32J}{Z}\sinh(8\beta J)
\end{aligned}
$$

The expectation value of the energy squared is introduced in section 2.1.3.

Deriving the equation.

$$
\begin{aligned}
\langle E^2 \rangle &= \frac{1}{Z} \sum_{i=1}^{M} E_i^2 e^{-\beta E_i} \\
&= \frac{1}{Z} \left[1 \cdot (-8J)^2 e^{-\beta(-8J)} + 4 \cdot 0 + 2 \cdot (8J)^2 e^{-\beta(8J)} + 4 \cdot 0 + 1 \cdot (-8J)^2 e^{-\beta(-8J)} \right] \\
&= \frac{1}{Z} \left[64J^2 e^{\beta 8J} + 2 \cdot 64J^2 e^{-\beta 8J} + 64J^2 e^{\beta 8J} \right] \\
&= \frac{2 \cdot 64J^2}{Z} \left[e^{\beta 8J} + e^{-\beta 8J} \right] \\
&= \frac{128J^2}{Z} (2\cosh(8\beta J)) \\
&= \frac{256J^2}{Z} \cosh(8\beta J)
\end{aligned}
$$

A.1.3 Derivation of the expectation values of the magnetizations

The expectation value of the magnetization is introduced in section 2.1.2.

Deriving the equation.

$$
\begin{aligned}
\langle \mathcal{M} \rangle &= \frac{1}{Z} \sum_{i=1}^{M} \mathcal{M}_i e^{-\beta E_i} \\
&= \frac{1}{Z} \left[1 \cdot 4e^{-\beta(-8J)} + 4 \cdot 2e^{-\beta(0J)} + 2 \cdot 0 + 4 \cdot 0 + 4 \cdot (-2)e^{-\beta(0J)} + 1 \cdot (-4)e^{-\beta(-8J)} \right] \\
&= \frac{1}{Z} \left[4e^{\beta 8J} + 8 - 8 - 4e^{\beta 8J} \right] \\
&= \frac{1}{Z} \cdot 0 \\
&= 0
\end{aligned}
$$

The expectation value of the mean magnetization is introduced in section 2.1.2.

Deriving the equation.

$$
\begin{aligned}
\langle |\mathcal{M}| \rangle &= \frac{1}{Z} \sum_{i=1}^{M} |\mathcal{M}_i| e^{-\beta E_i} \\
&= \frac{1}{Z} \left[1 \cdot |4| e^{-\beta(-8J)} + 4 \cdot |2| e^{-\beta(0J)} + 2 \cdot |0| + 4 \cdot |0| + 4 \cdot |-2| e^{-\beta(0J)} + 1 \cdot |-4| e^{-\beta(-8J)} \right] \\
&= \frac{1}{Z} \left[4e^{\beta 8J} + 8 + 8 + 4e^{\beta 8J} \right] \\
&= \frac{1}{Z} \cdot 4 \left[2e^{\beta 8J} + 4 \right] \\
&= \frac{8}{Z} \left(e^{\beta 8J} + 2 \right)
\end{aligned}
$$

The expectation value of the magnetization squared is introduced in section 2.1.4.

Deriving the equation.

$$
\begin{aligned}
\langle \mathcal{M}^2 \rangle &= \frac{1}{Z} \sum_{i=1}^{M} \mathcal{M}_i^2 e^{-\beta E_i} \\
&= \frac{1}{Z} \left[1 \cdot 4^2 e^{-\beta(-8J)} + 4 \cdot 2^2 e^{-\beta(0J)} + 2 \cdot 0 + 4 \cdot 0 + 4 \cdot (-2)^2 e^{-\beta(0J)} + 1 \cdot (-4)^2 e^{-\beta(-8J)} \right] \\
&= \frac{1}{Z} \left[16 e^{\beta 8J} + 16 + 16 + 16 e^{\beta 8J} \right] \\
&= \frac{1}{Z} \left[2 e^{8\beta J} + 2 \right] \\
&= \frac{32}{Z} \left(e^{8\beta J} + 1 \right)
\end{aligned}
$$

A.2 Extracting the critical temperature

In order to find the critical temperature we will use [1]'s Eq. (3). It is shown below:

$$T_c(L) - T_c(L = \infty) = aL^{-1/\nu}$$

where $\nu = 1$. This gives

$$T_c(L) - T_c(L = \infty) = \frac{a}{L}$$

In order to find a we subtract the equation with different L-values.

$$T_c(L_{100}) - T_c(L = \infty) = \frac{a}{L_{100}}$$

$$T_c(L_{80}) - T_c(L = \infty) = \frac{a}{L_{80}}$$

Subtracting gives

$$T_c(L_{100}) - T_c(L_{80}) = \frac{a}{L_{100} - L_{80}}$$

$$(T_c(L_{100}) - T_c(L_{80})) \cdot (L_{100} - L_{80}) = a$$