Project 4
For the course FYS3150

Erik Grammeltvedt, Erlend Tiberg North and Alexandra Jahr Kolstad

November 1, 2019
Week 43 - ?

TING Å GJØRE

- a) ferdig
- b) alt
- c) alt
- d) alt
- e) alt
- f) alt

Abstract

Contents

1 Introduction

2 Theory

2.1 Analytical solution for 2×2 lattice

The energies in this study 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. To calculate the partition function we need to know that

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

Calculating the partition function.

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

The partition function for this system is therefore given by $Z = 4\cosh(8\beta J) + 12$.

2.1.2 Energy and mean magnetization

The expectation value of the energy is

$$
\langle E \rangle = \frac{1}{Z} \sum_{i=1}^{M} E_i e^{-\beta E_i} \tag{2}
$$

In addition we need to know that

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

The expectation value of the energy is

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

The expectation value of the mean magnetization is

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

For this system it is

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

2.1.3 Specific heat

The specific heat is given by the equation

$$C_V = \frac{1}{k_B T^2}\left(\langle E^2\rangle - \langle E\rangle^2\right) \tag{4}$$

Therefore the expectation value of the energy squared has to be calculated.

$$
\begin{aligned}
\langle E^2\rangle &= \frac{1}{Z}\sum_{i=1}^{M} E_i^2 e^{-\beta E_i} \\
&= \frac{1}{Z}\left[1\cdot(-8J)^2 e^{-\beta(-8J)} + 4\cdot 0 + 2\cdot(8J)^2 e^{-\beta(8J)} + 4\cdot 0 + 1\cdot(-8J)^2 e^{-\beta(-8J)}\right] \\
&= \frac{1}{Z}\left[16J^2 e^{\beta 8J} + 2\cdot 16J^2 e^{-\beta 8J} + 16J^2 e^{\beta 8J}\right] \\
&= \frac{2\cdot 16J^2}{Z}\left[e^{\beta 8J} + e^{-\beta 8J}\right] \\
&= \frac{32J^2}{Z}(2\cosh(8\beta J)) \\
&= \frac{64J^2}{Z}\cosh(8\beta J)
\end{aligned}
$$

Now the specific heat can be calculated.

$$C_V = \frac{1}{k_B T^2}\left(\langle E^2\rangle - \langle E\rangle^2\right) = \frac{1}{k_B T^2}\left(\frac{64J^2}{Z}\cosh(8\beta J) - \left(-\frac{32J}{Z}\sinh(8\beta J)\right)^2\right)$$

2.1.4 Susceptibility

The susceptibility is given by

$$\chi = \frac{1}{k_B T^2}\left(\langle M^2\rangle - \langle M\rangle^2\right) \tag{5}$$

The expectation value of the mean magnetization squared therefore has to be calculated.

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

Now calculating the susceptibility of the system.

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

3 Method

4 Results

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

5 Discussion

6 Conclusion and perspective

7 Appendix

8 References

[1] Morten H. Jensen (2019), Project 3, 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] Weisstein, Eric W. "Laguerre Polynomial.", From MathWorld–A Wolfram Web Resource.