

Project 4

For the course FYS3150

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Abstract

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1 Introduction

2 Theory

2.1 Analytical solution for 2×2 lattice

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

$$\langle E \rangle = -7.98393$$

$$\langle E^2 \rangle = 15.96786$$

$$C_V = (15.96 - (-7.98)^2) = -47.77528 \quad \text{????????}$$

$$\langle M \rangle = 0 \quad \text{????????????????}$$

$$\langle M^2 \rangle = 15.97322$$

$$\chi = (15.97322 - (0)^2) = 15.97322$$

2.1.1 Partition function

The partition function is given by the equation below.

$$Z = \sum_{i=1}^M e^{-\beta E_i} \quad (1)$$

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.

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

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

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

In addition we need to know that

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

The expectation value of the energy is

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

The expectation value of the mean magnetization is

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

For this system it is

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

2.1.3 Specific heat

The specific heat is given by the equation

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

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

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

Now the specific heat can be calculated.

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

2.1.4 Susceptibility

The susceptibility is given by

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

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

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

Now calculating the susceptibility of the system.

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

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 Department 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.