

Project 3

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Abstract

1 Introduction

2 Theory

2.1 The problem

WRITE a bit about the system we want to solve! What is it?

2.2 2×2 lattice, analytical expressions

To get started we will find the analytical expression for the partition function and the corresponding expectation values for the energy E , the mean absolute value of the magnetic moment $|M|$ (which we will refer to as magnetization), the specific heat C_V and the susceptibility χ as function of T using periodic boundary conditions. These calculations will serve as benchmarks for our next steps.

Partition function, Z

The partition function in the canonical ensemble is defined as:

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

Where $\beta = \frac{1}{k_B T}$ and E_i is the energy of the system in the microstate i and M is the number of microstates ($= 2^N$ if N is number of electrons).

We therefore have to find E_i which is defined as:

$$E_i = -J \sum_{\langle kl \rangle}^N s_k s_l$$

Where $\langle kl \rangle$ indicates that we sum only over the nearest neighbors and J is a constant for the bonding strenght. For our two dimensional system the equation reads:

$$E_{i,2D} = -J \sum_i^N \sum_j^N (s_{i,j} s_{i,j+1} + s_{i,j} s_{i+1,j})$$

Four our two-spin-state system with two dimensions we get the following table if we use periodic boundary conditions:

Number of spins up	Degeneracy	Energy	Magnetization
4	1	-8J	4
3	4	0	2
2	4	0	0
2	2	8J	0
1	4	0	-2
0	1	-8J	-4

Table 1: Number of spins up, degeneracy, energy and magnetization of the two-dimensional benchmark scenario.

Where the magnetization is found by subtracting the number of spin downs from the number of spin up, or in other words the sum of the spins:

$$\mathcal{M} = \sum_{j=1}^N s_j$$

Getting back to the partition function, we insert all 16 of the E_i respectively. For the degeneracies, we just multiply one iteration of the respective E_i with the amount of degeneracies. When the energy E_i is zero, we will just add one to the sum since $e^0 = 1$. Thus we get the following:

$$Z = e^{-\beta(-8J)} + 2 \cdot e^{-\beta(8J)} + e^{-\beta(-8J)} + 12 = 2e^{-\beta 8J} + 2e^{\beta 8J} + 12$$

Energy expectation value, $\langle E \rangle$

The expectation value of the energy is defined as:

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

Where M is the sum over all microstates. P_i is the Boltzmann probability distribution which reads:

$$P_i(\beta) = \frac{e^{\beta E_i}}{Z}$$

For our system, this is easily calculated by inserting the partition function and the microstate energy E_i .

$$\begin{aligned}
\langle E \rangle &= \frac{1}{2e^{-\beta 8J} + 2e^{\beta 8J} + 12} (2 \cdot -8J \cdot e^{\beta 8J} + 2 \cdot 8J \cdot e^{-\beta 8J}) \\
&= \frac{1}{2e^{-\beta 8J} + 2e^{\beta 8J} + 12} (-16J e^{\beta 8J} + 16J e^{-\beta 8J}) \\
&= 8J \frac{1}{e^{-\beta 8J} + e^{\beta 8J} + 6} (e^{-\beta 8J} - e^{\beta 8J})
\end{aligned}$$

Since the variance of the mean energy (σ_E) is needed for the heat capacity later, we will calculate this here.

$$\begin{aligned}
\sigma_E^2 &= \langle E^2 \rangle - \langle E \rangle^2 = \frac{1}{Z} \sum E_i^2 e^{-\beta E_i} - \left(\frac{1}{Z} \sum E_i e^{-\beta E_i} \right)^2 \\
&= \frac{1}{2e^{-\beta 8J} + 2e^{\beta 8J} + 12} (2 \cdot (-8J)^2 \cdot e^{\beta 8J} + 2 \cdot (8J)^2 \cdot e^{-\beta 8J}) \\
&\quad - \left(8J \frac{1}{e^{-\beta 8J} + e^{\beta 8J} + 6} (e^{-\beta 8J} - e^{\beta 8J}) \right)^2
\end{aligned}$$

To simplify calculations, we define $a = e^{\beta 8J}$ and $b = e^{-\beta 8J}$. These terms will be precalculated in the program code.

$$\begin{aligned}
&= \frac{1}{2b + 2a + 12} (2 \cdot (-8J)^2 a + 2 \cdot (8J)^2 b) - \left(8J \frac{1}{a + b + 6} (b - a) \right)^2 \\
&= 64J^2 \left(\frac{1}{a + b + 6} (a + b) \right) - \left(\frac{1}{a + b + 6} (b - a) \right)^2 \\
&= 64J^2 \frac{1}{a + b + 6} \left((a + b) - \frac{1}{a + b + 6} (b - a)^2 \right) \\
&= 64J^2 \left(\frac{1}{a + b + 6} \right)^2 ((a + b + 6)(a + b) - (b - a)^2) \\
&= 64J^2 \left(\frac{1}{a + b + 6} \right)^2 (a^2 + ab + ba + b^2 + 6a + 6b - (b^2 - 2ab + a^2)) \\
&= 64J^2 \left(\frac{1}{a + b + 6} \right)^2 (a^2 + ab + ba + b^2 + 6a + 6b - b^2 + 2ab - a^2) \\
&= 64J^2 \left(\frac{1}{a + b + 6} \right)^2 (6a + 6b + 4ab)
\end{aligned}$$

If we now insert the terms for a and b we get the following:

$$\sigma_E^2 = 64J^2 \left(\frac{1}{e^{-\beta 8J} + e^{\beta 8J} + 6} \right)^2 (4 + 6(e^{-\beta 8J} + e^{\beta 8J}))$$

Magnetization, \mathcal{M}

In the canonical ensemble the absolute mean magnetization can be described as

$$\langle \mathcal{M} \rangle = \sum_i^M |\mathcal{M}_i| P_i(\beta) = \frac{1}{Z} \sum_i^M |\mathcal{M}_i| e^{-\beta E_i}$$

We can now simply insert the magnetization and the energies for each respective microstate. This is found in table 2.

$$\begin{aligned} \langle \mathcal{M} \rangle &= \frac{1}{2e^{-\beta 8J} + 2e^{\beta 8J} + 12} \left(1 \cdot 4e^{-\beta(-8J)} + 4 \cdot 2e^{-\beta \cdot 0} + 4 \cdot 0e^{-\beta \cdot 0} \right. \\ &\quad \left. + 2 \cdot 0e^{-\beta 8J} + 4 \cdot |-2|e^{-\beta \cdot 0} + 1 \cdot |-4|e^{-\beta(-8J)} \right) \\ &= \frac{1}{2e^{-\beta 8J} + 2e^{\beta 8J} + 12} (4e^{\beta 8J} + 8e^{-\beta \cdot 0} + 8e^{-\beta \cdot 0} + 4e^{\beta 8J}) \\ &= \frac{1}{2e^{-\beta 8J} + 2e^{\beta 8J} + 12} (4e^{\beta 8J} + 4e^{\beta 8J} + 8 + 8) \\ &= \frac{1}{2e^{-\beta 8J} + 2e^{\beta 8J} + 12} (8e^{\beta 8J} + 16) \\ &= 4 \frac{1}{e^{-\beta 8J} + e^{\beta 8J} + 6} (e^{\beta 8J} + 2) \end{aligned}$$

Since the variance of the mean magnetization (σ_M) is needed for the susceptibility later, we will calculate this here. ney

$$\begin{aligned}
\sigma_{\mathcal{M}}^2 &= \langle \mathcal{M}^2 \rangle - \langle \mathcal{M} \rangle^2 = \frac{1}{Z} \sum |\mathcal{M}|^2 e^{-\beta E_i} - \left(\frac{1}{Z} \sum |\mathcal{M}| e^{-\beta E_i} \right)^2 \\
&= \frac{1}{2e^{-\beta 8J} + 2e^{\beta 8J} + 12} \left(1 \cdot 4^2 e^{-\beta(-8J)} + 4 \cdot 2^2 e^{-\beta \cdot 0} + 4 \cdot 0^2 e^{-\beta \cdot 0} \right. \\
&\quad \left. + 2 \cdot 0^2 e^{-\beta 8J} + 4 \cdot |-2|^2 e^{-\beta \cdot 0} + 1 \cdot |-4|^2 e^{-\beta(-8J)} \right) \\
&\quad - \left(4 \frac{1}{e^{-\beta 8J} + e^{\beta 8J} + 6} (e^{\beta 8J} + 2) \right)^2 \\
&= \frac{1}{2e^{-\beta 8J} + 2e^{\beta 8J} + 12} (16e^{\beta 8J} + 16 + 16 + 16e^{\beta 8J}) \\
&\quad - \left(4 \frac{1}{e^{-\beta 8J} + e^{\beta 8J} + 6} (e^{\beta 8J} + 2) \right)^2 \\
&= 16 \frac{1}{e^{-\beta 8J} + e^{\beta 8J} + 6} (e^{\beta 8J} + 1) \\
&\quad - 16 \left(\frac{1}{e^{-\beta 8J} + e^{\beta 8J} + 6} \right)^2 (e^{\beta 8J} + 2)^2
\end{aligned}$$

Specific heat capacity, C_V

The specific heat capacity is defined as

$$C_V = \frac{\sigma_E^2}{k_B T^2}$$

Inserting the value σ_E^2 we get

$$C_V = \frac{\left(64J^2 \left(\frac{1}{e^{-\beta 8J} + e^{\beta 8J} + 6} \right)^2 (4 + 6(e^{-\beta 8J} + e^{\beta 8J})) \right)^2}{k_B T^2}$$

Susceptibility, χ

The susceptibility is defined as

$$\chi = \frac{\sigma_{\mathcal{M}}^2}{k_B T^2}$$

Inserting the value $\sigma_{\mathcal{M}}^2$ we get

$$\chi = \frac{16 \frac{1}{e^{-\beta 8J} + e^{\beta 8J} + 6} (e^{\beta 8J} + 1) - 16 \left(\frac{1}{e^{-\beta 8J} + e^{\beta 8J} + 6} \right)^2 (e^{\beta 8J} + 2)^2}{k_B T^2}$$

Note that these four characteristics are temperature dependent through $\beta = \frac{1}{k_B T}$.
Ref [1].

2.3 Ising model

The Ising model is applied for the study of phase transistions at finite temperatures for magnetic systems. Energy is expressed as:

$$E = -J \sum_{\langle kl \rangle}^N s_k s_l \quad s_k = \pm 1 \quad (1)$$

N is the number of spins and J is a constant expressing the interaction between neighboring spins. The sum is over the nearest neighbours only, indicated by $\langle kl \rangle$ the above equation. For $J \leq 0$ it is energetically favorable for neighboring spins to align. Leading to, at low temperatures, T, spontaneous magnetisation.

A probability distribution is needed in order to calculate the mean energy $\langle E \rangle$ and magnetization $\langle M \rangle$ at a given temperature. The distribution is given by:

$$P_i(\beta) = \frac{1}{Z} \exp(-\beta E_i), \quad (2)$$

where M is all the microstates, P_i is the probability of having the system in a state/configuration i.

CONFIGURATIONS

3 Results

3.1 2×2 lattice, analytical expressions

If we scale the value of β from $1/k_B T$ to $1/J$ (Scaling factor kT/J) in the analytical expression from section 2.2, we will get a good benchmark for computer computations to come. These values are listed in table 2 below.

Mean energy, $\langle E \rangle$:	$-7.9839J$
Mean absolute magnetization, $\langle M \rangle$:	3.9893
Specific heat capacity, C_V :	0.0165
Susceptibility, χ :	0.0160

Table 2: Material characteristics benchmark for a 2×2 lattice

4 Discussion

5 Conclusion

References

- [1] Morten Hjorth-jensen. *Computational Physics Lectures: Statistical physics and the Ising Model*. 2019.