Project 3

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Abstract

1 Introduction

2 Theory

2.1 The problem

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:

$$E_i = -J \sum_{<kl>}^{N} s_k s_l$$

Where $< kl >$ 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 respecitve 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.

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

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

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

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

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

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

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

Magnetization, $\mathcal{M}$
In the canonical ensemble the 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 1.

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

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

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

Specific heat capacity, C_V
The specific heat capacity is defined as

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

Insering the value σ_E^2 we get

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

Susceptibility, χ
The susceptibilitys is defined as

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

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

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

Note that these four characteristics are temperature dependent trough $\beta = \frac{1}{k_B T}$. 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:

$$E = -J\sum_{<kl>}^{N} s_k s_l \qquad s_k = \pm 1 \tag{1}$$

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 ¡kl¿ the above equation. For J ¿ 0 it is energetically favorable for neighboring spins to align. Leading to, at low temperatures, T, spontanious magnetisation.

A probability distribution is neede in order to calculate the mean energy ¡E¿ and magnetization ¡M¿ at a given temperature. The distribution is given by:

$$P_i(\beta) = \sum_{i=1}^{M} s_k s_l \exp -\beta E_i, \tag{2}$$

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

CONFIGURATIONS

3 Results

4 Discussion

5 Conclusion

References

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