Project 3

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November 14, 2019

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:

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

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:

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

$$Z = 4cosh(\beta 8J) + 12$$

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.

$$
\begin{aligned}
\langle E \rangle &= \frac{1}{2e^{-\beta 8J} + 2e^{\beta 8J} + 12}\left(2 \cdot -8J \cdot e^{\beta 8J} + 2 \cdot 8J \cdot e^{-\beta 8J}\right) \\
&= \frac{1}{2e^{-\beta 8J} + 2e^{\beta 8J} + 12}\left(-16Je^{\beta 8J} + 16Je^{-\beta 8J}\right) \\
&= 8J\frac{1}{e^{-\beta 8J} + e^{\beta 8J} + 6}\left(e^{-\beta 8J} - e^{\beta 8J}\right) \\
&= -8J\frac{sinh(\beta 8J)}{cosh(\beta 8J) + 3}
\end{aligned}
$$

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

$$
\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2 = \frac{1}{Z}\sum E_i^2 e^{-\beta E_i} - \left(\frac{1}{Z}\sum E_i e^{-\beta E_i}\right)^2
$$

$$
\begin{aligned}
&= \frac{1}{2e^{-\beta 8J} + 2e^{\beta 8J} + 12}\left(2 \cdot (-8J)^2 \cdot e^{\beta 8J} + 2 \cdot (8J)^2 \cdot e^{-\beta 8J}\right) \\
&\qquad - \left(-8J\frac{sinh(\beta 8J)}{cosh(\beta 8J) + 3}\right)^2
\end{aligned}
$$

$$
\begin{aligned}
&= 128J^2\frac{2cosh(\beta 8J)}{4cosh(\beta 8J) + 12} - \left(-8J\frac{sinh(\beta 8J)}{cosh(\beta 8J) + 3}\right)^2 \\
&= 64J^2\frac{cosh(\beta 8J)}{cosh(\beta 8J) + 3} - \left(-8J\frac{sinh(\beta 8J)}{cosh(\beta 8J) + 3}\right)^2
\end{aligned}
$$

$$
\sigma_E^2 = 64J^2\left(\frac{cosh(\beta 8J)}{cosh(\beta 8J) + 3} - \left(\frac{sinh(\beta 8J)}{cosh(\beta 8J) + 3}\right)^2\right)
$$

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 **??**.

$$
\begin{aligned}
\langle|\mathcal{M}|\rangle &= \frac{1}{4cosh(\beta 8J)+12}\left(4\cdot e^{\beta 8J}+4\cdot 2\cdot e^{0}+4\cdot|-2|\cdot e^{0}+|-4|\cdot e^{\beta 8J}\right)\\
&= \frac{1}{cosh(\beta 8J)+3}\left(e^{\beta 8J}+2+2+e^{\beta 8J}\right)\\
&= \frac{1}{cosh(\beta 8J)+3}\left(2e^{\beta 8J}+4\right)\\
&= \frac{2e^{\beta 8J}+4}{cosh(\beta 8J)+3}
\end{aligned}
$$

Since the variance of the mean magnetization (σ_M) is needed for the susceptibility later, we will calculate this here. For this we will need $\langle\mathcal{M}^2\rangle$, and the regular mean absolute $\langle\mathcal{M}\rangle$.

$$
\begin{aligned}
\langle\mathcal{M}\rangle &= \frac{1}{4cosh(\beta 8J)+12}\left(4\cdot e^{\beta 8J}+4\cdot 2\cdot e^{0}+4\cdot -2\cdot e^{0}+-4\cdot e^{\beta 8J}\right)\\
&= \frac{1}{cosh(\beta 8J)+3}\left(4e^{\beta 8J}-4e^{\beta 8J}+8-8\right)\\
&= \frac{1}{cosh(\beta 8J)+3}(0)\\
\langle\mathcal{M}\rangle &= 0
\end{aligned}
$$

$$
\begin{aligned}
\langle\mathcal{M}^2\rangle &= \frac{1}{Z}\sum|\mathcal{M}_\rangle|^2 e^{-\beta E_i}\\
&= \frac{1}{4cosh(\beta 8J)+12}\left(4^2\cdot e^{\beta 8J}+4\cdot 2^2\cdot e^{0}+4\cdot|-2|^2\cdot e^{0}+|-4|^2\cdot e^{\beta 8J}\right)\\
&= \frac{1}{4cosh(\beta 8J)+12}\left(16\cdot e^{\beta 8J}+16\cdot e^{0}+16\cdot e^{0}+16\cdot e^{\beta 8J}\right)\\
&= \frac{4}{cosh(\beta 8J)+3}\left(2e^{\beta 8J}+2\right)\\
\langle\mathcal{M}^2\rangle &= \frac{8e^{\beta 8J}+8}{cosh(\beta 8J)+3}
\end{aligned}
$$

And we get the variance:

$$
\begin{aligned}
\sigma_{\mathcal{M}}^2 &= \langle\mathcal{M}^2\rangle-\langle\mathcal{M}\rangle^2\\
&= \frac{8e^{\beta 8J}+8}{cosh(\beta 8J)+3}-(0)^2\\
\sigma_{\mathcal{M}}^2 &= \frac{8e^{\beta 8J}+8}{cosh(\beta 8J)+3}
\end{aligned}
$$

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

$$C_V = \frac{1}{k_B T^2} 64J^2 \left(\frac{cosh(\beta 8J)}{cosh(\beta 8J) + 3} - \left(\frac{-sinh(\beta 8J)}{cosh(\beta 8J) + 3} \right)^2 \right)$$

This is the main function we will be comparing to the values from our computations later.

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

$$\chi = \frac{1}{k_B T^2} \frac{8e^{\beta 8J} + 8}{cosh(\beta 8J) + 3}$$

Note that these four characteristics are temperature dependent trough $\beta = \frac{1}{k_B T}$. Ref [**Mortenstatphys2019**].

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 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:

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

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

We are also utilizing the Metropolis algorithm which basically checks if we can get a lower energy for the system if we flip a spin, and if that is the case, it flips the spin.
The pseudocode looks as follows:

```
for Temperature;

   for MonteCarlo Cycle;

      -Metropolis algorithm
      -Sum all values

   end for MonteCarlo loop

   -Divide values by MC cycles
   -Output values

end for Temperature loop
```

2.4 Analyzing the probability distribution

We will also compute the probability of the energy, $P(E)$ for the system with $L = 20$ with the temperatures $T = 1, 2.4$. This is computed by counting the number of times a given energy appears in our computation. The computation will start at a number of Monte Carlo cycles of which we know that the system is stable. We will also compare the results with the computed variance energy σ_E^2 and discuss the behavior.

3 Results

3.1 2×2 lattice, analytical expressoins

If we scale the value of β from $1/k_B T$ to $1/J$ (Scaling factor $k_B T/J$) in the analytical expression from section **??**, we will get a good benchmark for computer computations to come. These values are listed in table **??** below. Note that all values are divided by four, since we want the values per bond, and not for the entire lattice.

Mean energy, $\langle E \rangle$:	-1.9960
Mean absolute magnetization, $\langle |\mathcal{M}| \rangle$:	0.9987
Specific heat capacity, C_V:	0.0321
Susceptibility, χ:	3.9933

Table 2: Benchmark for material characteristics per bond for a 2×2 lattice

3.2 Ising model: simulation over temperature

We ran the program for different amounts of Monte Carlo cycles and plottet the error (analytical - simulated) in figure **??** below. It seems we want to use around 10^7 MC cycles or more to get a good simulation.

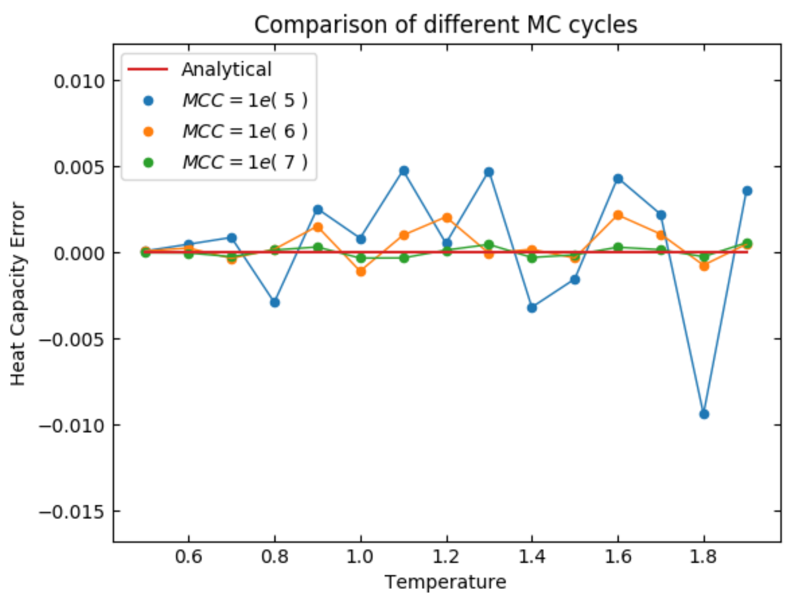

Figure 1: Shows the accuracy of different amount of MC cycles over temperature.

4 Discussion

5 Conclusion