The ising model

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1 Introduction

2 Method

The analytical expressions

We have the normalization constant Z which defines the partition function:

$$Z(\beta) = \sum_s e^{(-\beta E_s)} \quad (1)$$

With $\beta = 1/k_B T$, where T is temperature and k_B is Boltzmann's constant. We can use this partition function to find the probability P_s of finding a system in a state s:

$$P_s = \frac{e^{-(\beta E_s)}}{Z} \quad (2)$$

Where E_s is the energy in a given state. We have that the mean energy E_m is given by:

$$E_m = \sum_s \frac{E_s e^{-(\beta * E_s)}}{Z} \quad (3)$$

The mean energy can be used to find the energy variance σ_E^2:

$$\begin{aligned}\sigma_E^2 &= \langle E^2 \rangle - \langle E \rangle^2 \\ &= \sum_s \frac{E_s^2 e^{-(\beta * E_s)}}{Z} - \left(\sum_s \frac{E_s e^{-(\beta * E_s)}}{Z} \right)^2\end{aligned} \quad (4)$$

This variance can give us the heat capacity C_v of the system:

$$C_v = \frac{1}{kT} \sigma_E^2 \quad (5)$$

We have that the mean magnetization $\langle M \rangle$ is given by:

$$\langle M \rangle = \sum_s^M M_s P_s(\beta) = \frac{1}{Z} \sum_s^M M_s e^{-(\beta E_s)} \quad (6)$$

Where M_s is the different magnetizations. We have that the corresponding magnetic variance is given by:

$$\begin{aligned}\sigma_M^2 &= \langle M^2 \rangle - \langle M \rangle^2 \\ &= \frac{1}{Z} \sum_s^M M_s^2 e^{-(\beta E_s)}\end{aligned} \quad (7)$$

We can use the magnetic variance to find the susceptibility χ:

$$\chi = \frac{1}{k_B T} \sigma_M^2 \quad (8)$$

Specific case for a 2 X 2 lattice

We can use our analytical expressions in conjunction with some periodic boundary conditions. We assume two spins in each dimension L=2. If we draw up each lattice with the different spin orientations we can find the degeneracy, energy and magnetization for each state. These values can be used to find the analytical expressions with periodic boundary conditions.

Metropolis algorithm

The metropolis algorithm only considers ratios between probabilities, which means that we do not need to calculate the partition function at all when we are using the algorithm.

3 Results

Table 1: Energy and magnetization given number of up spins.

$N_{\text{spins up}}$	Degeneracy	E	M
4	1	-8 J	4
3	4	0	2
2	4	0	0
2	2	8 J	0
1	4	0	-2
0	1	-8 J	-4

In Table 1 we have the energy and magnetization given the number of up spins.

Specific case for a 2 X 2 lattice

We have that the partition function for our specific 2×2 lattice case is given by:

$$Z = 4\cosh(8J\beta) + 12 \tag{9}$$

The energy is given by:

$$E_m = -8\left(\frac{\sinh(8J\beta)}{\cosh(8J\beta) + 4}\right) \tag{10}$$

The magnetization is given by:

$$\langle M \rangle = \frac{\cosh(8J\beta) + 4}{\cosh(8J\beta) + 3} \tag{11}$$

The calculations are given in appendix X.

4 Discussion

5 Concluding remarks

A Calculations

The partition function for the 2×2 lattice is given by equation 1:

$$\begin{aligned} Z &= 2e^{8J\beta} + 2e^{-8J\beta} + 12e^{0} \\ &= 4\cosh{(8J\beta)} + 12 \end{aligned} \tag{12}$$

This expression combined with equation 3 gives the energy:

$$\begin{aligned} E_m &= \frac{2 \times 8Je^{-8J\beta} - 2 \times 8Je^{8J\beta}}{Z} \\ &= \frac{-16J(e^{8J\beta} - e^{-8J\beta})}{Z} \\ &= \frac{-32\sinh{(8J\beta)}}{4\cosh{(8J\beta)} + 12} \\ &= -8\left(\frac{\sinh{(8J\beta)}}{\cosh{(8J\beta)} + 3}\right) \end{aligned} \tag{13}$$

We find the mean magnetization by using equation 6:

$$\begin{aligned} \langle M \rangle &= 4 \times P(-8J) + 4 \times 2 \times P(0) + 4 \times 0 \\ &+ 2 \times 0 + 4 \times 2 \times P(0) + 4 \times 1 \times P(-8) \\ &= 4\left(\frac{e^{-8J\beta}}{4\cosh{(8J\beta)} + 12}\right) + 16\left(\frac{e^{-0J\beta}}{4\cosh{(8J\beta)} + 12}\right) + 4\left(\frac{e^{8J\beta}}{4\cosh{(8J\beta)} + 12}\right) \\ &= \frac{4(e^{-8J\beta} + e^{8J\beta}) + 16}{4\cosh{(8J\beta)} + 12} = \frac{4\cosh{(8J\beta)} + 16}{4\cosh{(8J\beta)} + 12} = \frac{\cosh{(8J\beta)} + 4}{\cosh{(8J\beta)} + 3} \end{aligned} \tag{14}$$

References

[1] kilder