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:

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

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:

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

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

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

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

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

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

$$C_v = \frac{1}{kT} \sigma_E^2 \tag{5}$$

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

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

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

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

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

$$\chi = \frac{1}{k_B T} \sigma_M^2 \tag{8}$$

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. We have five different spin orientations if we are studying the spin structures in Figure 1. The energy differences ΔE in such a structure is given by:

$$\Delta E = E_2 - E_1 = 2J s_l^1 \sum_{<k>}^N s_k \tag{9}$$

where E_2 is the energy after, E_1 the energy before and the sum runs over the nearest neighbors k of spin l. We can also find the difference in magnetization ΔM by only flipping the spin in the middle (dot in Figure 1):

$$\Delta M = M_2 - M_1 = \pm 2 \tag{10}$$

Where M_2 is the magnetization after and M_1 is the magnetization before we flip the spin. We can see that the change in magnetization is always $\Delta M = \pm 2$, given that we only have spin configurations L=$\pm$1. These expressions are only valid as long as we have zero magnetic field.

Metropolis algorithm

We wish to find the energy differences and the change in magnetization as we run through our simulation. It is beneficial to find the energy differences before we do the metropolis sampling. Since we are only flipping one spin at a time, it is possible to find and store all the energy differences in an array as $e^{\beta \Delta E}$. This saves a lot of time, as we don't have to evaluate the exponentials in the Monte Carlo sampling.

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 [1].

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

$$Z = 4\cosh(8J\beta) + 12 \tag{11}$$

We have that the partition function for our specific 2×2 lattice case is given by equation 11.

$$E_m = -8\left(\frac{\sinh(8J\beta)}{\cosh(8J\beta) + 4}\right) \tag{12}$$

The mean energy is given by equation 12.

$$C_v = \frac{1}{kT}\Bigg(4cosh(8\beta) + 12 \\ - \left(\frac{-8\sinh(8J\beta)}{\cosh(8J\beta) + 3}\right)^2\Bigg) \tag{13}$$

The heat capacity is given by equation 13.

$$\langle M \rangle = 0 \tag{14}$$

The mean magnetization is given by equation 14.

$$\chi = \frac{1}{kT}\left(\frac{32e^{8\beta} + 128}{4cosh + 12}\right) \tag{15}$$

The susceptibility is given by equation 15. All the calculations are given in appendix B.

In the 2×2 lattice case there are only five possible values for the energy difference. These are given in section 23 in appendix B.

4 Discussion

5 Concluding remarks

A Appendix

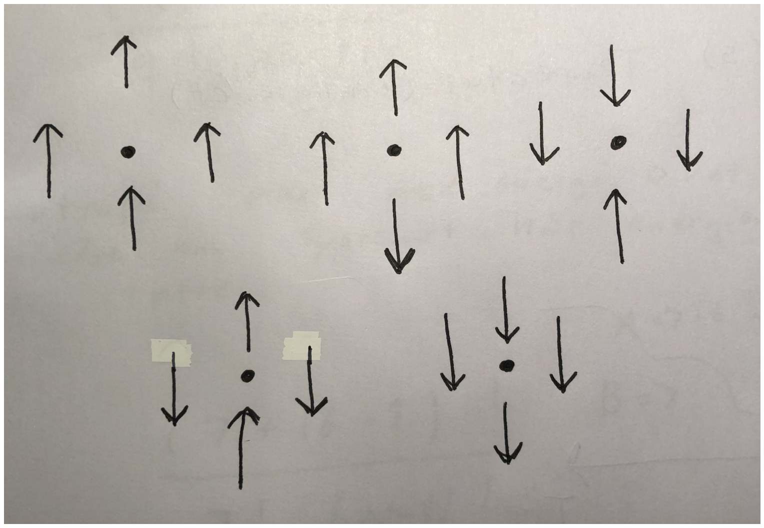

Figure 1: The different spin orientations.

B Appendix

Analytical expression

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

$$\begin{aligned} Z &= 2e^{8J\beta} + 2e^{-8J\beta} + 12e^{0} \\ &= 4\cosh(8J\beta) + 12 \end{aligned} \tag{16}$$

This expression combined with equation 3 gives the energy:

$$\begin{aligned} E_m &= \frac{2 \times 8Je^{-8J\beta} - 2 \times 8Je^{8J\beta}}{Z} \\ &= \frac{-16J(e^{8J\beta} - e^{-8J\beta})}{Z} \\ &= \frac{-32\sinh(8J\beta)}{4\cosh(8J\beta) + 12} \\ &= -8\left(\frac{\sinh(8J\beta)}{\cosh(8J\beta) + 3}\right) \end{aligned} \tag{17}$$

We also have a variance $< \sigma_E^2 >$ which we find by using equation 4:

$$\begin{aligned} < \sigma_E^2 > &= \left(\frac{2 \times (-8)^2 e^{-(-8\beta)} + 2 \times (8)^2 e^{-(8\beta)}}{Z}\right) - E_m^2 \\ &= \frac{128(e^{8\beta} + e^{-8\beta})}{Z} - E_m^2 = \frac{256\cosh(8\beta)}{4cosh(8\beta) + 12} - \left(\frac{-8\sinh(8J\beta)}{\cosh(8J\beta) + 3}\right)^2 \end{aligned} \tag{18}$$

Which gives us the heat capacity C_v by using equation 5:

$$C_v = \frac{1}{kT}\left(4cosh(8\beta) + 12 - \left(\frac{-8\sinh{(8J\beta)}}{\cosh{(8J\beta)}+3}\right)^2\right) \tag{19}$$

We find the mean magnetization by using equation 6:

$$\begin{aligned}\langle M\rangle &= 1\times 4\times P(-8) + 4\times 2\times P(0) + 4\times 0 \\ &+ 2\times 0 + 4\times(-2)\times P(0) + 1\times(-4)\times P(-8) \\ &= 4\left(\frac{e^{-8J\beta}}{4\cosh{(8J\beta)}+12}\right) - 4\left(\frac{e^{-8J\beta}}{4\cosh{(8J\beta)}+12}\right) \\ &= 0\end{aligned} \tag{20}$$

We also have a variance $<\sigma_M^2>$ which we find by using equation 7:

$$\begin{aligned}<\sigma_M^2> &= \frac{1}{Z}\left(4^2e^{-(-8\beta)} + 8^2e^0 + (-8)^2e^0 + (-4)^2e^{-(-8\beta)}\right) \\ &= \frac{16e^{8\beta}+64+64+6e^{8\beta}}{Z} = \frac{32e^{8\beta}+128}{4cosh+12}\end{aligned} \tag{21}$$

Which gives us the susceptibility χ by using equation 8:

$$\chi = \frac{1}{kT}\left(\frac{32e^{8\beta}+128}{4cosh+12}\right) \tag{22}$$

Boundary conditions and Boltzmanns distribution

We assume that the original position of the middle spin in Figure 1 is up (the middle spin is the dot). We find the energy differences by using equation 10:

$$\begin{aligned}\Delta E_1 &= 4-(-4) = 8 \\ \Delta E_2 &= 2-(-2) = 4 \\ \Delta E_3 &= -2-(2) = -4 \\ \Delta E_4 &= 0-0 = 0 \\ \Delta E_5 &= -4-(4) = -8\end{aligned} \tag{23}$$

We can see that we obtain five different energy differences as we flip the spin from up to down in the middle of the structures in Figure 1.

References

[1] Jensen, M.H., 2015, Computational Physics Lecture Notes Fall 2015