

FYS4150: Project 4

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1 Introduction

The aim of this project is to study the Ising model in two dimensions.

2 The Ising model (ch. 13)

The Ising model describes phase transitions in two dimensions. At a given critical temperature the model exhibits a phase transition from one magnetic moment (spin) to a phase with zero magnetization. Without an externally applied field, this is described as

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

where $s_k = \pm 1$, N is the total number of spins and J is a coupling constant.

3 The Metropolis algorithm (ch. 12)

4 2x2 lattice

We consider a 2×2 -lattice, meaning $L = 2$. The spins have 16 configurations. The probability distribution is given by

$$P_i(\beta) = \frac{e^{-\beta E_i}}{Z} \quad (2)$$

Number of spins pointing up	Degeneracy	Energy
0	1	-8J
1	4	0
2	6	8J
3	4	0
4	1	-8J

Figure 1: Possible energies for a 2×2 -lattice of spin particles.

where $\beta = \frac{1}{kT}$ is the inverse temperature, k is the Boltzmann constant, E_i is the energy of a state i . The partition function is

$$Z = \sum_{i=1}^M e^{-\beta E_i} \quad (3)$$

This function is difficult to compute since we need all states. The Metropolis algorithm only considers *ratios* between probabilities, so we don't need to calculate this (luckily!)

$$\text{Metropolis} \rightarrow \frac{P_s}{P_t} = \frac{e^{-(\beta E_s)}}{e^{-(\beta E_k)}} = e^{-\beta(E_s - E_k)} = e^{-\beta \Delta E}$$

The partition function in our case is

$$\begin{aligned} Z(\beta) &= \sum_{i=1}^M e^{-(\beta E_i)} \\ &= 2e^{-\beta \cdot (-8J)} + 8e^{-\beta \cdot 0} + 6e^{-\beta \cdot 8J} \\ &= 8 + 2e^{8\beta J} + 6e^{-8\beta J} \end{aligned}$$

The energy expectation value

$$\begin{aligned} \langle E \rangle &= -\frac{\partial \ln Z}{\partial \beta} = -\frac{\partial \ln Z}{\partial Z} \frac{\partial Z}{\partial \beta} = -\frac{1}{Z} \frac{\partial Z}{\partial \beta} \\ &= -\frac{1}{8 + 2e^{8\beta J} + 6e^{-8\beta J}} (8J \cdot 2e^{8\beta J} - 8J \cdot 6e^{-8\beta J}) \\ &= 8J \frac{e^{8\beta J} - 3e^{-8\beta J}}{4 + e^{8\beta J} + 3e^{-8\beta J}} \end{aligned}$$

with the corresponding variance

$$\begin{aligned}
\sigma^2 &= \langle E^2 \rangle - \langle E \rangle^2 = \frac{1}{Z} \sum_{i=1}^M E_i^2 e^{-\beta E_i} - \left(\frac{1}{Z} \sum_{i=1}^M E_i e^{-\beta E_i} \right)^2 \\
\sigma^2 &= 64J^2 \frac{e^{8\beta J} - 3e^{-8\beta J}}{4 + e^{8\beta J} + 3e^{-8\beta J}} - \left(8J \frac{e^{8\beta J} - 3e^{-8\beta J}}{4 + e^{8\beta J} + 3e^{-8\beta J}} \right)^2 \\
&= 64J^2 \frac{e^{8\beta J} - 3e^{-8\beta J}}{4 + e^{8\beta J} + 3e^{-8\beta J}} - 64J^2 \left(\frac{e^{16\beta J} - 6 \cdot e^{8\beta J} e^{-8\beta J} + 9e^{-16\beta J}}{(4 + e^{8\beta J} + 3e^{-8\beta J})^2} \right) \\
&= \frac{64J^2}{(4 + e^{8\beta J} + 3e^{-8\beta J})^2} \left[(e^{8\beta J} - 3e^{-8\beta J})(4 + e^{8\beta J} + 3e^{-8\beta J}) - e^{16\beta J} - 6 + 9e^{-16\beta J} \right] \\
&= \frac{64J^2}{(4 + e^{8\beta J} + 3e^{-8\beta J})^2} \left[4e^{8\beta J} - 12e^{-8\beta J} - 6 \right]
\end{aligned}$$

The specific heat capacity

$$C_V = \frac{1}{k_B T^2} (\langle E^2 \rangle - \langle E \rangle^2) \quad (4)$$

$$C_V = \frac{64J^2}{k_B T^2} \frac{4e^{8\beta J} - 12e^{-8\beta J} - 6}{(4 + e^{8\beta J} + 3e^{-8\beta J})^2}$$

The mean absolute value of the magnetic moment (mean magnetization)

$$\langle \mathcal{M} \rangle = \frac{1}{Z} \sum_i^M \mathcal{M}_i e^{-\beta E_i} \quad (5)$$

$$\langle \mathcal{M} \rangle = \frac{1}{Z} (-4e^{8\beta J} - 2 \cdot 4e^0 + 0 \cdot e^{-8\beta J} + 2 \cdot 4e^0 + 4e^{8\beta J}) = 0$$

The susceptibility

$$\chi = \frac{1}{k_B T} (\langle \mathcal{M}^2 \rangle - \langle \mathcal{M} \rangle^2) \quad (6)$$

$$\begin{aligned}
\chi &= \frac{1}{k_B T} \frac{1}{Z} \sum_i^M \mathcal{M}_i^2 e^{-\beta E_i} \\
&= \frac{1}{k_B T} \frac{1}{Z} (16e^{8\beta J} + 4 \cdot 4e^0 + 0 \cdot e^{-8\beta J} + 4 \cdot 4e^0 + 16e^{8\beta J}) \\
&= \frac{16}{k_B T} \frac{e^{8\beta J} + 1}{4 + e^{8\beta J} + 3e^{-8\beta J}}
\end{aligned}$$

The analytical values are found in table (4).

Z	$\langle E \rangle$	$\langle \mathcal{M} \rangle$	C_V	χ
5969.92	7.99	0	0.0856	0.00268

Figure 2: Analytical values of the expectation values. Here $J = 1$, $k = 1$, $T = 1.0$ K.

5 Sources