FYS4150: Project 4

Ingrid A V Holm

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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 pahse 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

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

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 conifgurations. The domain here is $\{-4, -2, 0, 2, 4\}$ with the probability distribution function $\{\frac{1}{16}, \frac{4}{16}, \frac{8}{16}, \frac{4}{16}, \frac{1}{16}\}$. Probability distribution

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

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

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

For four spins we have 16 different configurations. If we choose periodic boundary conditions the energies are given by the expression

$$E = -J \sum_{j=1}^{N} s_j s_{j+1} \tag{4}$$

$$E = -J(s_1 s_2 + s_2 s_3 + s_3 s_4 + s_4 s_1)$$

The energies are then

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

The probability of finding the system in a state s is given by

$$P_s = \frac{e^{-(\beta E_s)}}{Z} \tag{5}$$

Where Z is the partition function, given by (why is this??)

$$Z(\beta) = \sum_{s} e^{-(\beta E_s)} \tag{6}$$

This fuction 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 energies are then

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

The partition function in our case is

$$\begin{aligned}
Z(\beta) &= \sum_s e^{-(\beta E_s)} \\
&= 2e^{-\beta\cdot(-8J)} + 8e^{-\beta\cdot 0} + 6e^{-\beta\cdot 8J} \\
&= 8 + 2e^{8\beta J} + 6e^{-8\beta J} \\
&= 2(e^{8\beta J} + e^{-8\beta J}) + 4(2 + e^{-8\beta J}) \\
&= 2\cosh(8\beta J) + 4(2 + e^{-8\beta J})
\end{aligned}$$

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

$$\sigma^2 = \langle E^2 \rangle - \langle E \rangle^2 = \frac{1}{Z}\sum_{i=1}^{M} E_i^2 e^{-\beta E_i} - \left(\frac{1}{Z}\sum_{i=1}^{M} E_i e^{-\beta E_i}\right)^2$$

$$
\begin{aligned}
\sigma^2 &= 64J^2 \frac{e^{8\beta J} - 3e^{-8\beta J}}{4 + e^{8\beta J} + 3e^{-8\beta J}} - \big(8J \frac{e^{8\beta J} - 3e^{-8\beta J}}{4 + e^{8\beta J} + 3e^{-8\beta J}}\big)^2 \\
&= 64J^2 \frac{e^{8\beta J} - 3e^{-8\beta J}}{4 + e^{8\beta J} + 3e^{-8\beta J}} - 64J^2 \big(\frac{e^{16\beta J} - 6 \cdot e^{8\beta J} e^{-8\beta J} + 9e^{-16\beta J}}{(4 + e^{8\beta J} + 3e^{-8\beta J})^2}\big) \\
&= \frac{64J^2}{(4 + e^{8\beta J} + 3e^{-8\beta J})^2} \Big[(e^{8\beta J} - 3e^{-8\beta J})(4 + e^{8\beta J} + 3e^{-8\beta J}) - e^{16\beta J} - 6 + 9e^{-16\beta J}\Big] \\
&= \frac{64J^2}{(4 + e^{8\beta J} + 3e^{-8\beta J})^2} \Big[4e^{8\beta J} - 12e^{-8\beta J} - 6\Big]
\end{aligned}
$$

The specific heat capacity

$$
C_V = \frac{1}{k_B T^2} (\langle E^2 \rangle - \langle E \rangle^2) \tag{7}
$$

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

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

$$
\langle \mathcal{M} \rangle = \frac{1}{Z} \sum_i^M \mathcal{M}_i e^{-\beta E_i} \tag{8}
$$

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

The susceptibility

$$
\chi = \frac{1}{k_B T} (\langle \mathcal{M}^2 \rangle - \langle \mathcal{M} \rangle^2) \tag{9}
$$

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

5 Sources