UNIVERSITY OF OSLO

COMPUTATIONAL PHYSICS

Project 4

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Abstract

[1]

[1] FiXme Note: write abstract

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CHAPTER

1 INTRODUCTION

Awesome introduction!!!!!

CHAPTER

2 METHOD

Write awesome introduction

The source codes for the algorithms described in this chapter can be found in the Github folder `https://`. [1]

2.1 Nature of the problem

This problem also have a nature!!

2.1.1 Determining Quantities

For the canonical ensemble with probability distribution given by the Boltzmann distribution

$$P_i(\beta) = \frac{e^{-\beta E_i}}{Z} \tag{2.1}$$

with $\beta = 1/k_B T$, in which k_B is Boltzmann's constant and T is the temperature of the system, E_i being the energy of the i'th microstate, and Z being the partition function given by

$$Z = \sum_{i=1}^{M} e^{-\beta E_i} \tag{2.2}$$

for a system with M microstates. For each microstate i in a spin system with N spins $s_i = \pm 1$, the energy E_i and magnetization $\mathscr{M}_i$ are given as [2]

$$E_i = -J \sum_{<kl>}^{N} s_k s_l \qquad \text{and} \qquad \mathscr{M}_i = \sum_{j=1}^{N} s_j \tag{2.3}$$

in which $< kl >$ means that the sum is over nearest neighbours, only. The expectation value of the energy, is then given as

$$\langle E \rangle = \sum_{i=1}^{M} E_i P_i(\beta) = \frac{1}{Z} \sum_{i=1}^{M} E_i e^{-\beta E_i} \tag{2.4}$$

[1] FiXme Note: fix lines!
[2] FiXme Note: what is J ?!

whilst the expectation value of the magnetization, can be determined by

$$\langle \mathscr{M} \rangle = \sum_{i=1}^{M} \mathscr{M}_i P_i(\beta) = \frac{1}{Z} \sum_{i=1}^{M} \mathscr{M}_i e^{-\beta E_i} \tag{2.5}$$

From the variance of E and $\mathscr{M}$, the specific heat C_v and susceptibility χ can be found, respectively. That is

$$C_v = \frac{1}{k_B T^2} \left\langle \langle E^2 \rangle - \langle E \rangle^2 \right\rangle \qquad \text{and} \qquad \chi = \frac{1}{k_B T} \left\langle \langle \mathscr{M}^2 \rangle - \langle \mathscr{M} \rangle^2 \right\rangle \tag{2.6}$$

2.1.2 Closed Form Expressions of Quantities for the General 2×2 Spin Case

The system consisting of 2×2 spins has in total $2^4 = 16$ spin configurations. These 16 configurations are given in Fig. 2.1 below.

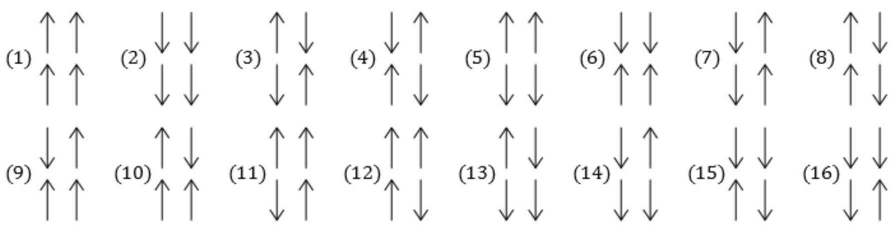

Figure 2.1. The 16 different spin configurations for the 2 dimensional case with 2 spins in each dimension. An arrow pointing upwards represents spin up with the spin value $s_{up} = +1$, whilst an arrow pointing downwards represent spin down with the spin value $s_{down} = -1$. The corresponding energies and magnetizations of each of the micro states can be found in Tab. 2.1.

The energy and magnetization for each of the 16 microstates are given in Tab. 2.1 and are calculated from Eq. (2.3). As an example, the energy and magnetization of the ninth microstate, given in Fig. 2.1 as the state with one spin down and three spin up, is calculates here:

$$\begin{aligned} E_9 &= -J \sum_{<kl>}^{2\times 2} s_k s_l \\ &= -J[((-1)\cdot 1 + (-1)\cdot 1) + (1\cdot(-1) + 1\cdot 1) + (1\cdot(-1) + 1\cdot 1) + (1\cdot 1 + 1\cdot 1)] \\ &= 0 \end{aligned}$$

and

$$\mathscr{M}_9 = \sum_{j=1}^{2\times 2} s_j = (-1) + 1 + 1 + 1 = 2$$

Table 2.1. Energy and magnetization of each of the spin configurations given in Fig. 2.1.

Configuration	Energy	Magnetization
(1)	$-8J$	4
(2)	$-8J$	-4
(3) – (4)	$8J$	0
(5) – (8)	0	0
(9) – (12)	0	2
(13) – (16)	0	-2

Hence the partition function Z defined in Eq. (2.2) for this 2×2 spin system becomes

$$Z = 12 + 2\left(e^{8\beta J} + e^{-8\beta J}\right) = 12 + 4\cosh(8\beta J) \tag{2.7}$$

In the last equation sign, Euler's identity [3] and the definition of $\cosh\theta$ is used. With this partition function and the energy and magnetization for each of the 16 microstates given in Tab. 2.1, the expectation value of the energy and the magnetization becomes

$$\langle E\rangle = \frac{1}{Z}(-16Je^{8\beta J} + 16Je^{-8\beta J}) = \frac{16J}{Z}(e^{-8\beta J} - e^{8\beta J}) \tag{2.8}$$

and

$$\langle \mathscr{M}\rangle = \frac{1}{Z}(4e^{8\beta J} - 4e^{8\beta J} + 2 - 2) = 0 \tag{2.9}$$

However, the expectation value of the absolute value of the magnetization differ from zero. That is

$$\langle |\mathscr{M}|\rangle = \frac{1}{Z}\left(|4|e^{8\beta J} + |-4|e^{8\beta J} + |2| + |-2|\right) = \frac{1}{Z}(8e^{8\beta J} + 4) \tag{2.10}$$

To compute the specific heat C_v and the susceptibility, the quantities $\left\langle E^2\right\rangle$ and $\left\langle \mathscr{M}^2\right\rangle$ must be known. For this 2×2 spin case they become

$$\left\langle E^2\right\rangle = \frac{1}{Z}\sum_{i=1}^{16} E_i^2 e^{-\beta E_i} = \frac{128J^2}{Z}(e^{8\beta J} + e^{-8\beta J}) \tag{2.11}$$

and

$$\left\langle \mathscr{M}^2\right\rangle = \frac{1}{Z}\sum_{i=1}^{16} \mathscr{M}_i^2 e^{\beta E_i} = \frac{32}{Z}(e^{8\beta J} + 1) \tag{2.12}$$

The specific heat C_v and the susceptibility χ can now be determined by the expressions in Eq. (2.6), and after some joggling with the results gained by Eq. (2.8), (2.9), (2.11) and (2.12), it is evident that

$$C_v = \frac{128J^2}{Zk_BT^2}\left[e^{8\beta J} + e^{-8\beta J} - \frac{2e^{-16\beta J} + 2e^{16\beta J} + 4}{Z}\right] \tag{2.13}$$

[4] and

$$\chi = \frac{1}{k_BTZ}\left[32(e^{8\beta J} + 1) - \frac{1}{Z}\left(8e^{8\beta J} + 4\right)^2\right] \tag{2.14}$$

[3] FiXme Note: ok?
[4] FiXme Note: check that this is correct

2.1.3 Closed Form Solutions for the 2×2 case with $T = 1.0$

[5] In this project, the temperature is given in the units of $[k_B T/J] = [1/\beta J]$. To distinguish this from the temperature T in the ordinary unit of Kelvin [6], the considered temperature is, in this section, written as $\tilde{T}$. In [7], the c++ code for computing the expectation value of the energy and the magnetization and the specific heat and susceptibility of the 2×2 spin case with temperature $\tilde{T} = 1.0$ is introduced. The section is dedicated to find the closed form solutions for these quantities for this situation with the purpose of testing the code introduced in the mentioned section. [8]

With $\tilde{T} = 1/\beta J = 1.0$, the partition function in Eq. (2.7) gives the value

$$Z = 12 + 4\cosh(8) \approx 6000 \tag{2.15}$$

The expectation value of the magnetization is surely still zero, whilst the expectation value of the absolute value of the magnetization becomes

$$\langle \mathscr{M} \rangle = \frac{1}{Z}(8e^8 + 4) \approx 3.9926 \tag{2.16}$$

With the temperature given in units of $[k_B T/J]$, the formulas for determining the expectation value of the energy and the specific heat and susceptibility, given in the previous section, must be slightly modified to give a value. E.g. the expectation value of the energy given by Eq. (2.8) will have to be divided by J, giving the computed expectation value in the unit of $[E/J]$. For a temperature of $\tilde{T} = 1.0$, the computed expectation value of the energy is then

$$\langle \tilde{E} \rangle = \frac{\langle E \rangle}{J} = \frac{16}{Z}(e^{-8} - e^8) \approx -7.9839 \tag{2.17}$$

This is approximately the same as the lowest energy state of the system (see Tab. 2.1), which is also what was to be expected for low temperatures. To find C_v and χ, Eq. (2.13) and (2.14) are considered, and with a temperature $\tilde{T} = 1.0$, they give the values

$$\tilde{C}_v = \frac{C_v}{J} \approx 0.12830 \qquad \text{and} \qquad \tilde{\chi} = \chi J \approx 0.03209$$

[9] The values of the quantities gained in this section for the 2×2 spin case with $\tilde{T} = 1.0$ in units of $[k_B T/J] = [1/\beta J]$ are collected in the table below.

Table 2.2. Various quantity values for the 2×2 spin case with temperature $\tilde{T} = 1.0$ in units of $[k_B T/J] = [1/\beta J]$.

$\langle \tilde{E} \rangle$	$\langle \mathscr{M} \rangle$	$\langle \lvert \mathscr{M} \rvert \rangle$	$\tilde{C}_v$	$\tilde{\chi}$
-7.9839	0	3.9926	0.12830	0.03209

[10]

[5] FiXme Note: introduce value of partition function
[6] FiXme Note: ok??
[7] FiXme Note: ref, to section for 2x2 case
[8] FiXme Note: any ideas to improving this section??
[9] FiXme Note: check results, especially χ
[10] FiXme Note: fix χ

CHAPTER

3 RESULTS AND DISCUSSION

write awesome introduction!

The results from running the codes bla bla bla can be found in the GitHub folder `https://`. [1]

[1] FiXme Note: fix lines!

CHAPTER

4 CONCLUSION

Conclude!!!!

BIBLIOGRAPHY