

FYS3150 Project 4

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Abstract

1 Introduction

2 Theory

3 Results

3.1 Example: Analytical expression for the 2×2 case

For a 2×2 lattice, the thermodynamic quantities can be found analytically without too much work. To find the partition function, we need to write out all possible microstates and calculate their energies. Using the periodic boundary conditions, we get

Microstate	Energy	Magnetization
$\begin{array}{cccc} & \downarrow & \downarrow & \\ \downarrow & \downarrow & \downarrow & \downarrow \\ \downarrow & \downarrow & \downarrow & \downarrow \\ & \downarrow & \downarrow & \end{array}$	$E = -8J$	$M = -4$
$\begin{array}{cccc} & \downarrow & \uparrow & \\ \downarrow & \downarrow & \downarrow & \downarrow \\ \uparrow & \downarrow & \uparrow & \downarrow \\ & \downarrow & \downarrow & \end{array}$	$E = 0$	$M = -2$
$\begin{array}{cccc} & \uparrow & \downarrow & \\ \downarrow & \downarrow & \downarrow & \downarrow \\ \downarrow & \uparrow & \downarrow & \uparrow \\ & \downarrow & \downarrow & \end{array}$	$E = 0$	$M = -2$
$\begin{array}{cccc} & \uparrow & \uparrow & \\ \downarrow & \downarrow & \downarrow & \downarrow \\ \uparrow & \uparrow & \uparrow & \uparrow \\ & \downarrow & \downarrow & \end{array}$	$E = 0$	$M = 0$
$\begin{array}{cccc} & \downarrow & \downarrow & \\ \uparrow & \downarrow & \uparrow & \downarrow \\ \downarrow & \downarrow & \downarrow & \downarrow \\ & \downarrow & \uparrow & \end{array}$	$E = 0$	$M = -2$
$\begin{array}{cccc} & \downarrow & \uparrow & \\ \uparrow & \downarrow & \uparrow & \downarrow \\ \uparrow & \downarrow & \uparrow & \downarrow \\ & \downarrow & \uparrow & \end{array}$	$E = 0$	$M = 0$
$\begin{array}{cccc} & \uparrow & \downarrow & \\ \uparrow & \downarrow & \uparrow & \downarrow \\ \downarrow & \uparrow & \downarrow & \uparrow \\ & \downarrow & \uparrow & \end{array}$	$E = 8J$	$M = 0$
$\begin{array}{cccc} & \uparrow & \uparrow & \\ \uparrow & \downarrow & \uparrow & \downarrow \\ \uparrow & \uparrow & \uparrow & \uparrow \\ & \downarrow & \uparrow & \end{array}$	$E = 0$	$M = 2$
$\begin{array}{cccc} & \downarrow & \downarrow & \\ \downarrow & \uparrow & \downarrow & \uparrow \\ \downarrow & \downarrow & \downarrow & \downarrow \\ & \uparrow & \downarrow & \end{array}$	$E = 0$	$M = -2$
$\begin{array}{cccc} & \downarrow & \uparrow & \\ \downarrow & \uparrow & \downarrow & \uparrow \\ \uparrow & \downarrow & \uparrow & \downarrow \\ & \uparrow & \downarrow & \end{array}$	$E = 8J$	$M = 0$

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$ \begin{array}{cccc} & \uparrow & \downarrow & \\ \downarrow & \uparrow & \downarrow & \uparrow \\ \downarrow & \uparrow & \downarrow & \uparrow \\ & \uparrow & \downarrow & \end{array} $	$E = 0$	$M = 0$
$ \begin{array}{cccc} & \uparrow & \uparrow & \\ \downarrow & \uparrow & \downarrow & \uparrow \\ \uparrow & \uparrow & \uparrow & \uparrow \\ & \uparrow & \downarrow & \end{array} $	$E = 0$	$M = 2$
$ \begin{array}{cccc} & \downarrow & \downarrow & \\ \uparrow & \uparrow & \uparrow & \uparrow \\ \downarrow & \downarrow & \downarrow & \downarrow \\ & \uparrow & \uparrow & \end{array} $	$E = 0$	$M = 0$
$ \begin{array}{cccc} & \downarrow & \uparrow & \\ \uparrow & \uparrow & \uparrow & \uparrow \\ \uparrow & \downarrow & \uparrow & \downarrow \\ & \uparrow & \uparrow & \end{array} $	$E = 0$	$M = 2$
$ \begin{array}{cccc} & \uparrow & \downarrow & \\ \uparrow & \uparrow & \uparrow & \uparrow \\ \downarrow & \uparrow & \downarrow & \uparrow \\ & \uparrow & \uparrow & \end{array} $	$E = 0$	$M = 2$
$ \begin{array}{cccc} & \uparrow & \uparrow & \\ \uparrow & \uparrow & \uparrow & \uparrow \\ \uparrow & \uparrow & \uparrow & \uparrow \\ & \uparrow & \uparrow & \end{array} $	$E = -8J$	$M = 4$

To summarise, we have

Number of \uparrow	Multiplicity	Energy	Magnetisation
4	1	$-8J$	4
3	4	0	2
2	2	$8J$	0
2	4	0	0
1	4	0	-2
0	1	$-8J$	-4

Summing over all microstates, we get the partition function

$$Z = \sum_{\text{all microstates}} e^{-\beta E_i} = 2e^{8J\beta} + 2e^{-8J\beta} + 12$$

The expectation value of the energy can then be found from

$$\begin{aligned} \langle E \rangle &= -\frac{\partial \ln(Z)}{\partial \beta} = -\frac{\partial}{\partial \beta} \left(\ln(2e^{8J\beta} + 2e^{-8J\beta} + 12) \right) \\ &= -\frac{1}{2e^{8J\beta} + 2e^{-8J\beta} + 12} \left(16Je^{8J\beta} - 16Je^{-8J\beta} \right) \\ &= -\frac{8J(e^{8J\beta} - e^{-8J\beta})}{e^{8J\beta} + e^{-8J\beta} + 6} \end{aligned}$$

yielding the heat capacity

$$\begin{aligned} C_V &= \frac{\partial}{\partial T} (\langle E \rangle) = \frac{\partial \beta}{\partial T} \frac{\partial}{\partial \beta} (\langle E \rangle) = -\frac{1}{kT^2} \frac{\partial}{\partial \beta} (\langle E \rangle) \\ &= -\frac{1}{kT^2} \frac{\partial}{\partial \beta} \left(-\frac{8J(e^{8J\beta} - e^{-8J\beta})}{e^{8J\beta} + e^{-8J\beta} + 6} \right) \\ &= \frac{8J}{kT^2} \frac{8J(e^{8J\beta} + e^{-8J\beta})(e^{8J\beta} + e^{-8J\beta} + 6) - (e^{8J\beta} - e^{-8J\beta})8J(e^{8J\beta} - e^{-8J\beta})}{(e^{8J\beta} + e^{-8J\beta} + 6)^2} \\ &= \frac{64J^2}{kT^2} \frac{6(e^{8J\beta} + e^{-8J\beta}) + (e^{8J\beta} + e^{-8J\beta})^2 - (e^{8J\beta} - e^{-8J\beta})^2}{(e^{8J\beta} + e^{-8J\beta} + 6)^2} \\ &= \frac{64J^2}{kT^2} \frac{6(e^{8J\beta} + e^{-8J\beta}) + e^{16J\beta} + 2 + e^{-16J\beta} - (e^{16J\beta} - 2 + e^{-16J\beta})}{(e^{8J\beta} + e^{-8J\beta} + 6)^2} \\ &= \frac{64J^2}{kT^2} \frac{6(e^{8J\beta} + e^{-8J\beta}) + 4}{(e^{8J\beta} + e^{-8J\beta} + 6)^2} \end{aligned}$$

To find the various quantities connected to magnetization, we use the general formula

$$\langle A \rangle = \frac{1}{Z} \sum_{\text{all microstates}} A_i e^{-\beta E_i}$$

Mean magnetic moment(s):

$$\begin{aligned} \langle M \rangle &= \frac{1}{2e^{8J\beta} + 2e^{-8J\beta} + 12} \left(-4e^{8J\beta} + 4 \cdot (-2) + 0 + 0 + 4 \cdot 2 + 4e^{8J\beta} \right) = 0 \\ \langle M^2 \rangle &= \frac{1}{2e^{8J\beta} + 2e^{-8J\beta} + 12} \left((-4)^2 e^{8J\beta} + 4 \cdot (-2)^2 + 0 + 0 + 4 \cdot 2^2 + 4^2 e^{8J\beta} \right) \\ &= \frac{32(e^{8J\beta} + 1)}{2e^{8J\beta} + 2e^{-8J\beta} + 12} = \frac{16(e^{8J\beta} + 1)}{e^{8J\beta} + e^{-8J\beta} + 6} \\ \langle |M| \rangle &= \frac{1}{2e^{8J\beta} + 2e^{-8J\beta} + 12} \left(|-4|e^{8J\beta} + 4 \cdot |-2| + 0 + 0 + 4 \cdot 2 + 4e^{8J\beta} \right) \end{aligned}$$

$$= \frac{8(e^{8J\beta} + 2)}{2e^{8J\beta} + 2e^{-8J\beta} + 12} = \frac{4(e^{8J\beta} + 2)}{e^{8J\beta} + e^{-8J\beta} + 6}$$

Magnetic susceptibility:

$$\chi = \beta \left(\langle M^2 \rangle - \langle M \rangle^2 \right) = \frac{16\beta(e^{8J\beta} + 1)}{e^{8J\beta} + e^{-8J\beta} + 6}$$

3.2 Comparison with numerical results

With $J = 1$ and $\beta = 1$, the above expressions give

$$\begin{aligned} \langle E \rangle &= -7.9839 & C_V &= 0.128329 \\ \langle |M| \rangle &= 3.99464 & \chi &= 15.9732 \end{aligned}$$

Running 100 000 Monte Carlo cycles with the same parameters gives figure 1 on the following page.

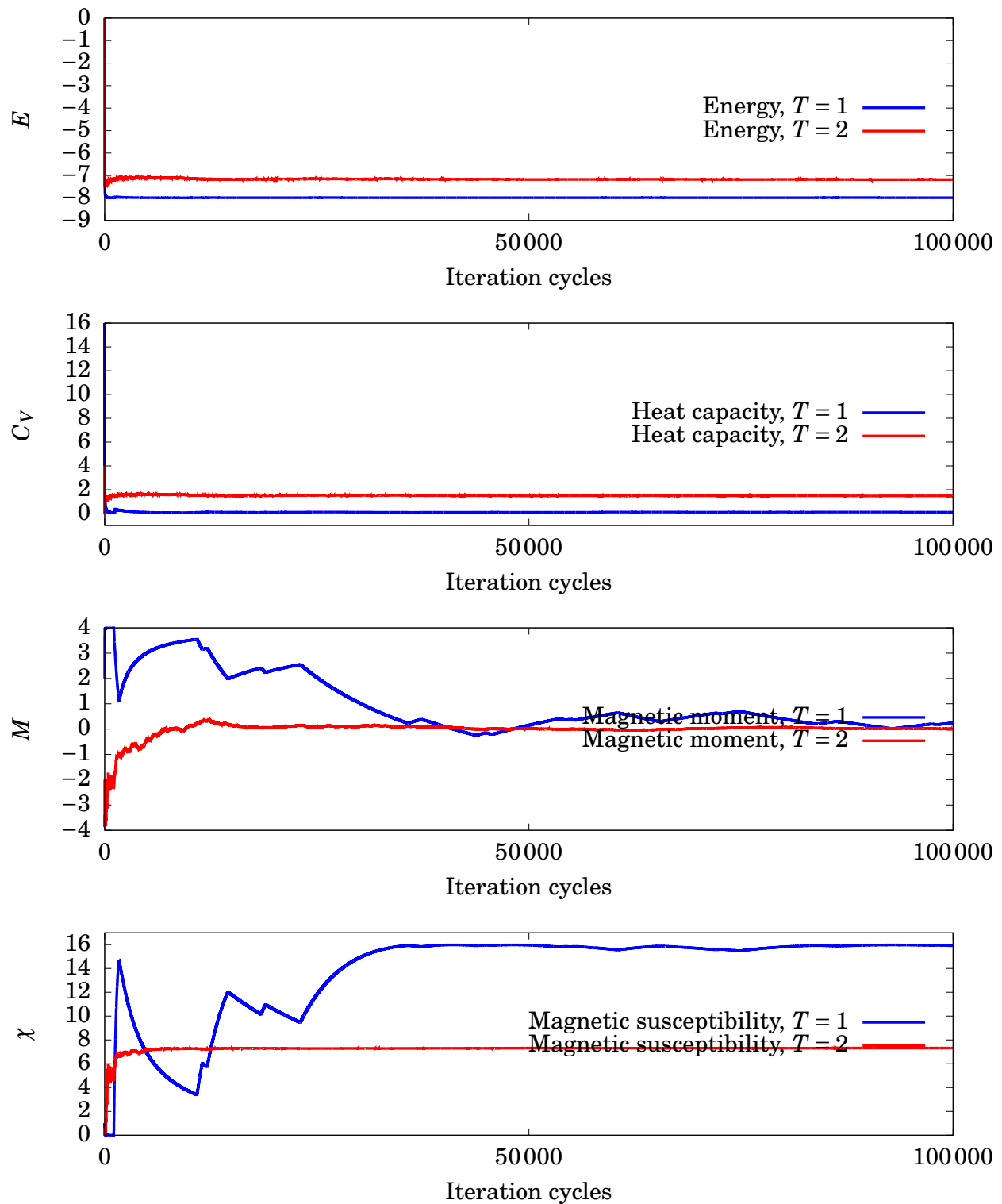


Figure 1: Numerical results from 100 000 Monte Carlo cycles.

These results fit fairly well with the numbers calculated above, but we see from the graphs that the values for the heat capacity and magnetic susceptibility have yet to settle down completely. Running with 10 000 000 Monte Carlo cycles yields

10000000 1 -7.984 63.872 -0.101365 15.9734 3.9947 0.12775 15.9631

where the numbers are i , T , $\langle E \rangle$, $\langle E^2 \rangle$, $\langle M \rangle$, $\langle M^2 \rangle$, $\langle |M| \rangle$, C_V and χ . The results fit very well with the analytical results.