

Project 4 FYS4150

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Abstract

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1 Introduction

2 Theory

Boltzman Markow chain - convergence

L=2 case:

Table 2.1: text

No spin up	Deg	Energy	Magnetization
0	1	-8J	-4
1	4	0	-2
2	4	0	0
2	2	8J	0
3	4	0	2
4	1	-8J	4

Error Random number

The partition function:

$$\begin{aligned}
 Z &= \sum_i^M e^{-\beta E_i} = e^{-\beta 8J} + e^{-\beta 8J} + e^{\beta 8J} e^{\beta 8J} + 12 \\
 &= 2e^{-\beta 8J} + 2e^{\beta 8J} + 12 = 4 \left(\frac{e^{-\beta 8J} + e^{\beta 8J}}{2} \right) + 12 \\
 &= 4 \cosh(\beta 8J) + 12
 \end{aligned}$$

The energy:

$$\begin{aligned}
 \langle E \rangle &= k_B T^2 \left(\frac{\partial Z}{\partial T} \right)_{V,N} \\
 &= k_B T^2 \frac{\partial}{\partial T} \left[\ln \left(4 \cosh \left(\frac{8J}{k_B T} \right) + 12 \right) \right] \\
 \frac{\partial \ln Z}{\partial T} &= \frac{\partial Z}{\partial \beta} \frac{\partial \beta}{\partial T} = \frac{\partial \ln Z}{\partial \beta} \left(\frac{-1}{k_B T^2} \right) \\
 \langle E \rangle &= - \left(\frac{\partial Z}{\partial \beta} \right)_{V,N} = - \frac{\partial}{\partial \beta} \ln [4 \cosh(8J\beta) + 12] \\
 &= \frac{-1}{4 \cosh(8J\beta) + 12} 4 \sinh(8J\beta) 8J\beta \\
 &= \frac{-8J \sinh(8J\beta)}{3 \cosh(8J\beta) + 4}
 \end{aligned}$$

Following the same method, we found that:

$$\langle |M| \rangle = \frac{1}{Z} \sum_i^M M_i e^{\beta E_i} = \frac{(8J)^2 \cosh(8J\beta)}{\cosh(8J\beta) + 3}$$

$$\langle M \rangle = 0$$

$$\langle E^2 \rangle = \frac{8(e^{8J\beta} + 1)}{\cosh(8J\beta) + 3}$$

$$\langle M^2 \rangle = \frac{1}{Z} \left(\sum_i^M M_i^2 e^{\beta E_i} \right) = \frac{2(e^{8J\beta} + 2)}{\cosh(8J\beta) + 3}$$

We can use these to calculate the rest:

$$C_V = k\beta^2 (\langle E^2 \rangle - \langle E \rangle^2)$$

$$\chi = \beta (\langle M^2 \rangle - \langle M \rangle^2)$$

3 Method

Metropolis (T,A,...) Stokastisk matrise - konvergens (forhold egenverdier).

Hvilken random number engine

4 Result

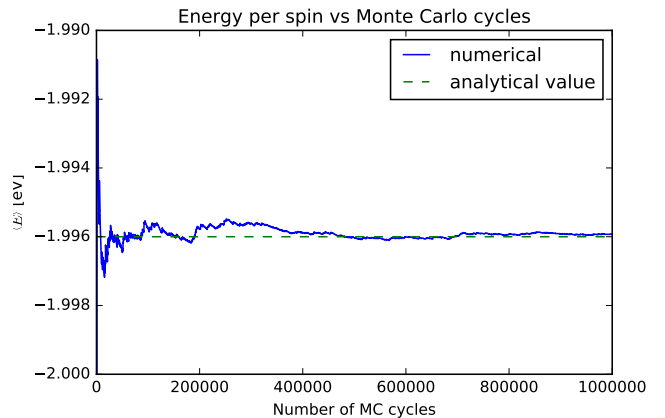


Figure 4.1: This is a plot of the expectation value of the energy per spin versus number of Monte Carlo cycles. The plot shows that at least $9 \cdot 10^6$ MC cycles are necessary for a good agreement.

5 Discussion

6 Conclusion

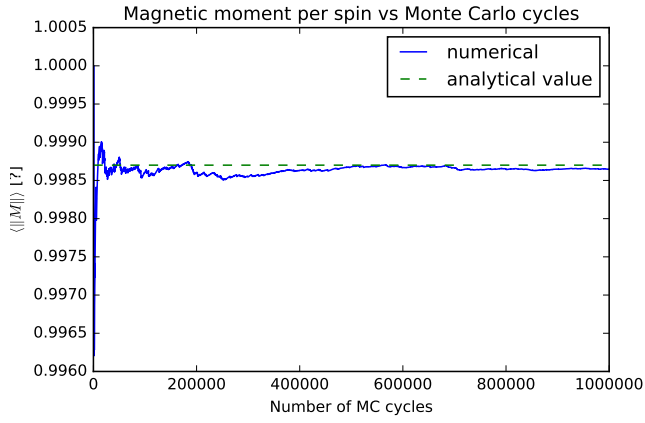


Figure 4.2: This is a plot of the expectation value of the mean absolute value of the magnetic moment per spin versus number of Monte Carlo cycles. The plot shows that at least $8 \cdot 10^6$ MC cycles are necessary for a good agreement, but all the way to 10^6 the value is a bit low.

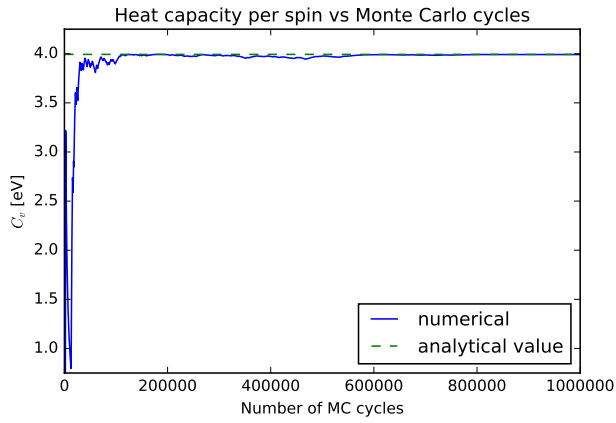


Figure 4.3: caption

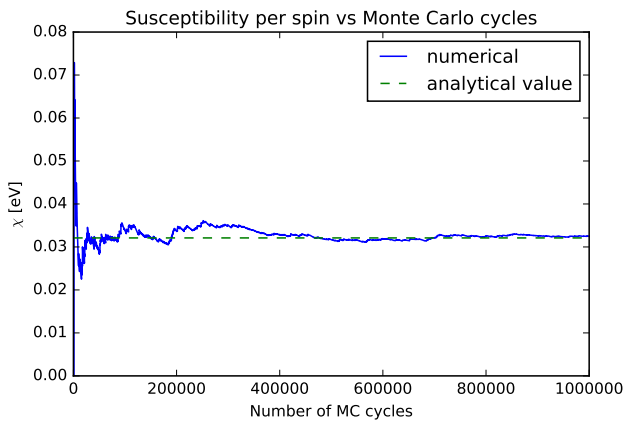


Figure 4.4: caption

References

Appendix

State	Spinn	Energi	Magnetization
0	↓↓↓↓	$-8J$	-4
1	↓↓↓↑	0	-2
2	↓↓↑↓	0	-2
3	↓↑↓↓	0	-2
4	↑↓↓↓	0	-2
5	↓↓↑↑	0	0
6	↓↑↓↑	0	0
7	↓↑↑↓	$8J$	0
8	↑↓↓↑	$8J$	0
9	↑↓↑↓	0	0
10	↑↑↓↓	0	0
11	↓↑↑↑	0	2
12	↑↓↑↑	0	2
13	↑↑↓↑	0	2
14	↑↑↑↓	0	2
15	↑↑↑↑	$-8J$	4