Project 4 FYS4150

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Abstract

Contents

1 Introduction

2 Theory

Boltzman Markhow chain - convergance

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:

$$Z = \sum_i^M e^{-\beta E_i} = e^{-\beta 8J} + e^{-\beta 8J} + e^{\beta 8J} e^{\beta 8J} + 12$$

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

$$= 4\cosh\left(\beta 8J\right) + 12$$

The energy:

$$\langle E \rangle = k_B T^2 \left(\frac{\partial Z}{\partial T}\right)_{V,N}$$

$$= k_B T^2 \frac{\partial}{\partial T}\left[\ln\left(4\cosh\left(\frac{8J}{k_B T}\right) + 12\right)\right]$$

$$\frac{\partial \ln Z}{\partial T} = \frac{\partial Z}{\partial \beta}\frac{\partial \beta}{\partial T} = \frac{\partial \ln Z}{\partial \beta}\left(\frac{-1}{k_B T^2}\right)$$

$$\langle E \rangle = -\left(\frac{\partial Z}{\partial \beta}\right)_{V,N} = -\frac{\partial}{\partial \beta}\ln\left[4\cosh\left(8J\beta\right) + 12\right]$$

$$= \frac{-1}{4\cosh(8J\beta) + 12} 4\sinh(8J\beta) 8J\beta$$

$$= \frac{-8J\sinh(8J\beta)}{3\cosh((J\beta) + 4}$$

Following the same method, we found that:

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

$$\langle M \rangle = 0$$

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

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

We can use these to calculate the rest:

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

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

3 Method

In this project we tried out many new concepts in our algorithm. We used Monte Carlo method.

3.1 Monte Carlo cycles

In Monte Carlo methods, the main properties are the mean value (Equation ??)

$$P(a \leq X \leq b) = \int_b^a p(x)\, dx \tag{1}$$

$$\langle h \rangle_X = \int h(x)\, p(x)\, dx \tag{2}$$

$$\langle x^n \rangle = \int x^n\, p(x)\, dx \tag{3}$$

$$\langle x \rangle = \int x\, p(x)\, dx \tag{4}$$

Table 4.1: This table compares the analytical values for L=2 with the numerical ones after 10^6 Monte Carlo cycles. The values are in units per spin.

	Numerical:	Analytical:
$\langle E \rangle$	-1.9958	-1.9960
$\langle E^2 \rangle$	15.9664	15.9679
$\langle M \rangle$	0.0451	0
$\langle M^2 \rangle$	3.9930	3.9933
$\langle \lvert M \rvert \rangle$	0.9986	0.9987
χ	3.9849	3.9933
C_V	0.0335	0.0321

3.2 Metropolis algorithm

3.3 Random number generator

3.4 Parallelizing

Metropolis (T,A,...) Stochastic matrix - convergences (forhold eigenvalue).

Hvilken random number engine

MPI:

- Develop codes locally, run with some few processes and test your codes. Do benchmarking, timing and so forth on local nodes, for example your laptop or PC. - When you are convinced that your codes run correctly, you can start your production runs on available supercomputers.

MPI functions:

4 Result

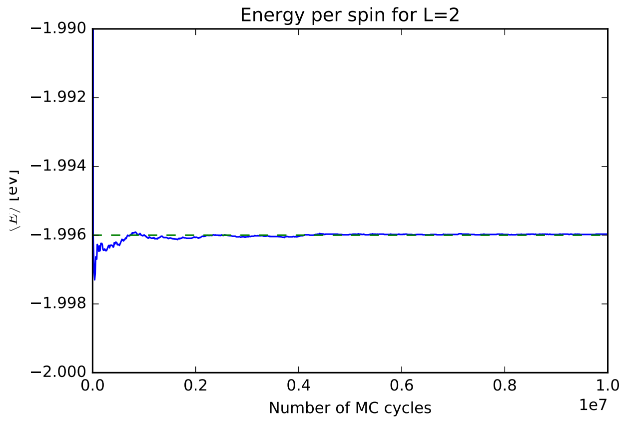

Figure 4.1: This is a plot of the expectation value of the energy per spin verus number of Monte Carlo cycles. The plot shows that at least $9 \cdot 10^5$ MC cycles are necessary for a good argeement.

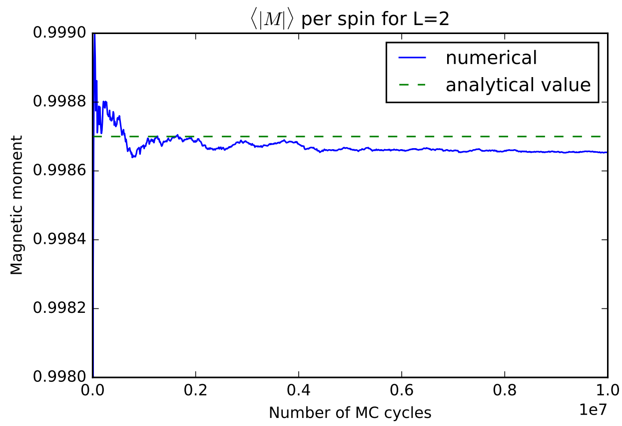

Figure 4.2: This is a plot of the expectation value of the mean absolute value of the magnetic moment per spin verus number of Monte Carlo cycles. The plot shows that at least $8 \cdot 10^5$ MC cycles are necessary for a good argeement, but all the way to 10^6 the value is a bit low.

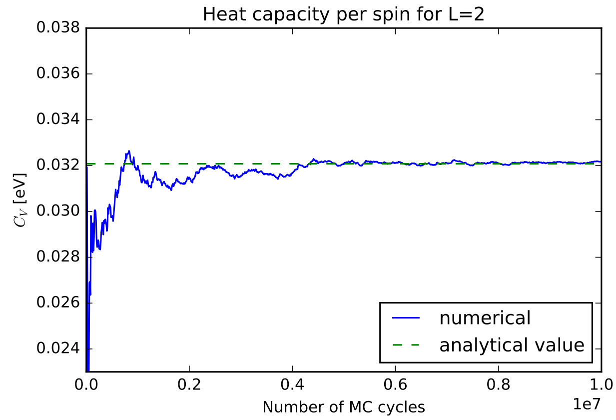

Figure 4.3: This is a plot of the heat capacity per spin verus number of Monte Carlo cycles. The plot shows that at least $6 \cdot 10^5$ MC cycles are necessary for a good argeement.

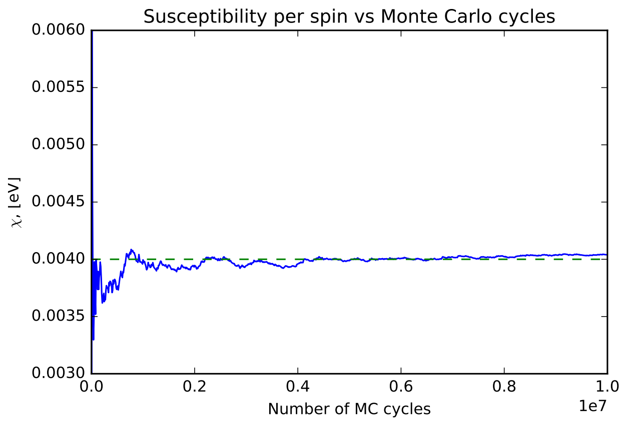

Figure 4.4: This is a plot of the susceptibility per spin verus number of Monte Carlo cycles. The plot shows that at least $6 \cdot 10^5$ MC cycles are necessary for a good argeement.

5 Discussion

6 Conclusion

References

Appendix

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