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

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

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:

MPI$_I nitMPI_I nit - initiatean MPI computation$

MPI$_F inalize MPI_F inalize - terminatethe MPI computati$

MPI$_C omm_s ize MPI_C omm_s ize - howmanyprocessespartic$

MPI$_C omm_r ank MPI_C omm_r ank - whichoneamI?(Anumb$
1.)

MPI$_S end MPI_S end - sendamessagetoaparticularprocess$

MPI$_R ecv MPI_R ecv - receiveamessagefromaparticularpr$

MPI$_r educe MPI_r educeor MPI_A llreduce MPI_A llreduce, se$

4 Result

M 1.0000 1.0000 1.0000 1.0000 -8 <E>, <E^2 >, $< M >, < M^2 >, < |M| >, Cv, XExpect : -1.995815$ $-1.996015.967903.99330.99873.99330.0321$

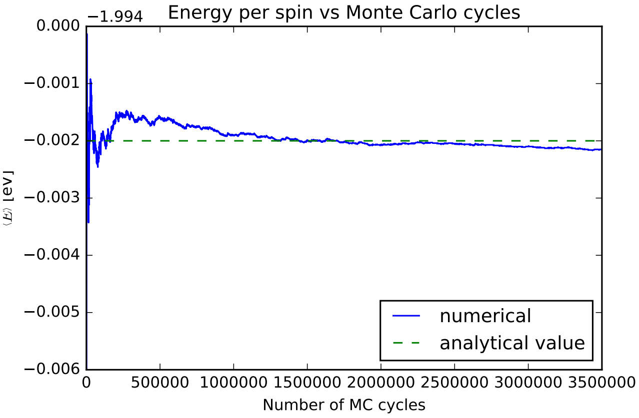

Figure 4.1: This is a plot of the expectation value of the energy per spin verus number of Monte Carlo cycles. The plot shows that at least $9 \cdot 10^5$ MC cycles are necessary for a good argeement.

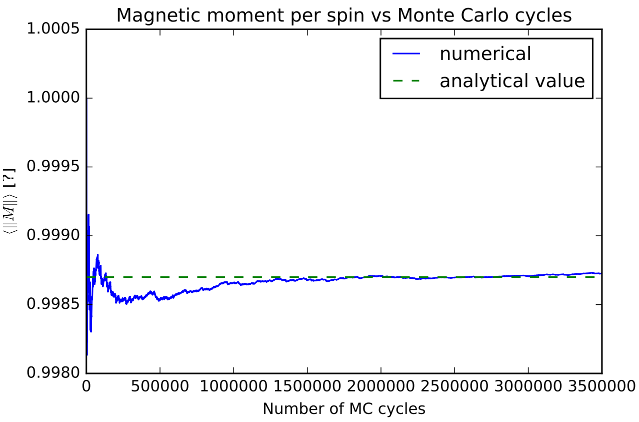

Figure 4.2: This is a plot of the expectation value of the mean absolute value of the magnetic moment per spin verus number of Monte Carlo cycles. The plot shows that at least $8 \cdot 10^5$ MC cycles are necessary for a good argeement, but all the way to 10^6 the value is a bit low.

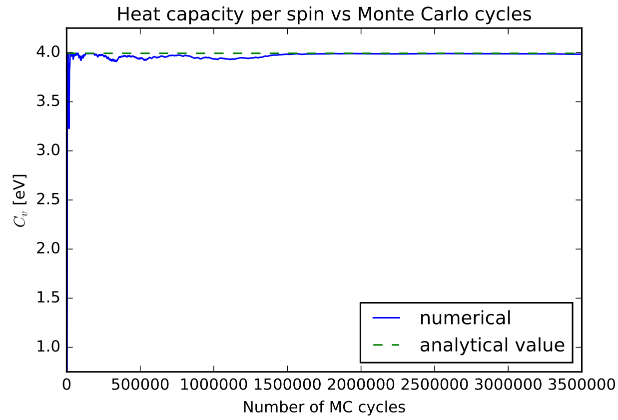

Figure 4.3: This is a plot of the heat capacity per spin verus number of Monte Carlo cycles. The plot shows that at least $6 \cdot 10^5$ MC cycles are necessary for a good argeement.

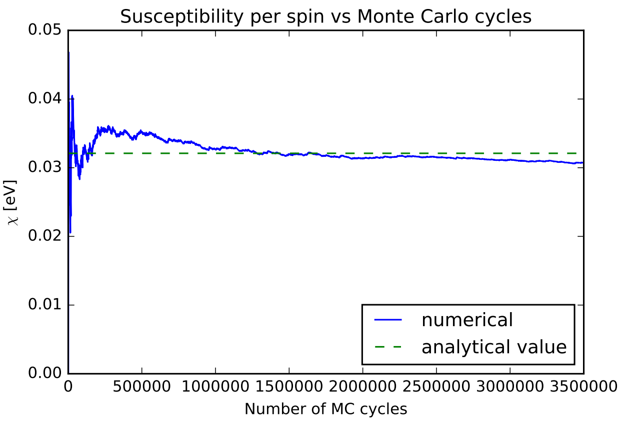

Figure 4.4: This is a plot of the susceptibility per spin verus number of Monte Carlo cycles. The plot shows that at least $6 \cdot 10^5$ MC cycles are necessary for a good argeement.

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