Project 4 FYS4150

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Abstract

Contents

1 Introduction

2 Theory

Bolzman 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

2.1 Introduction to statistics

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

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

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

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

2.2 Magnet - properties

Energy, magnetic moment, susceptibility, heat capacity.

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu} \tag{5}$$

Boltzman Markhow chain - convergance

L=2 case:

Table 2.2: 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

OBS: Bruker forventing av abs(M) i susceptbilitet.

VILDE:

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 goal is to

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

4.1 The L=2 case

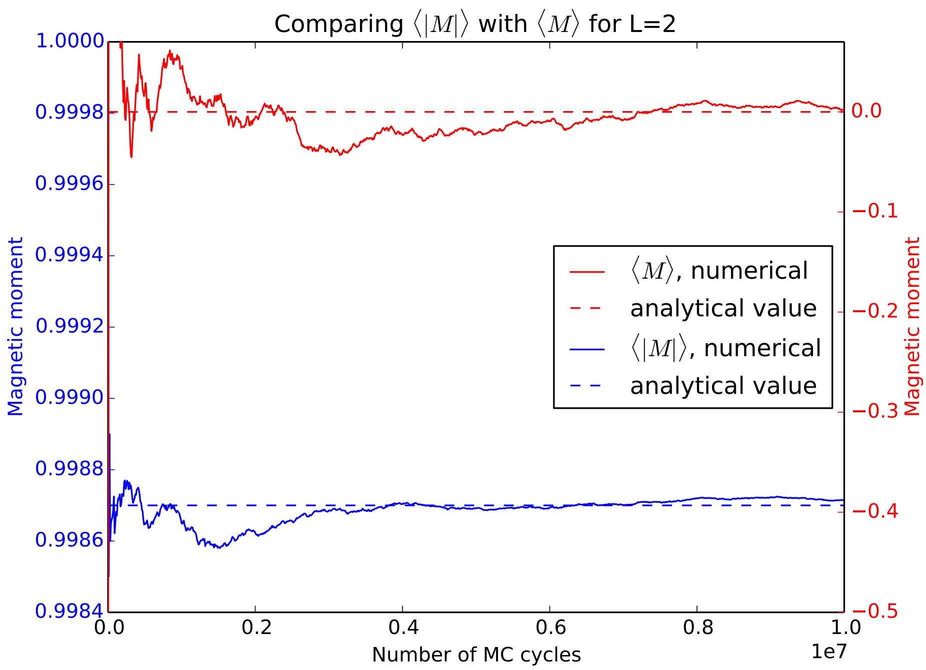
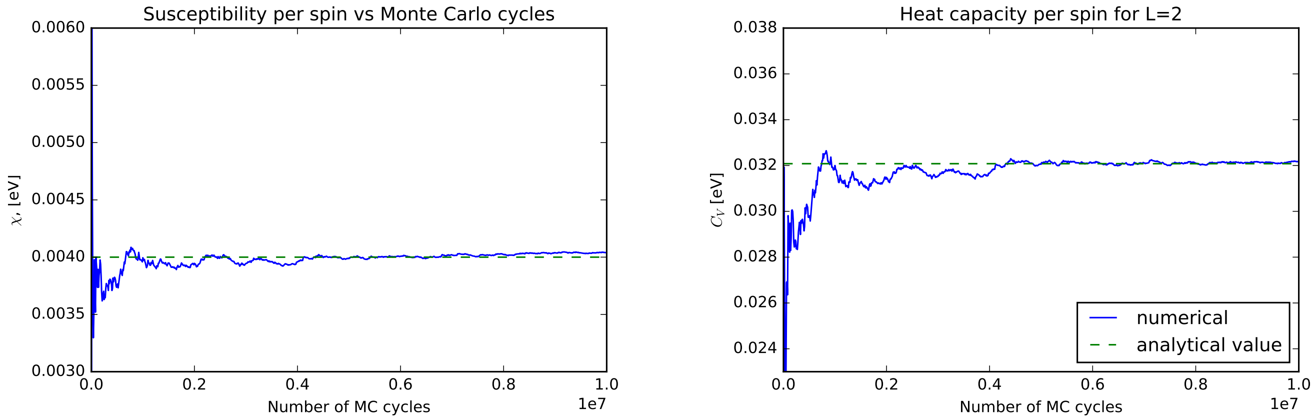


Figure 4.1



(a) (b)

Figure 4.2: $\theta/2\theta$ scan around the (0002) peak and (0004) peak of ZnO and GaN.

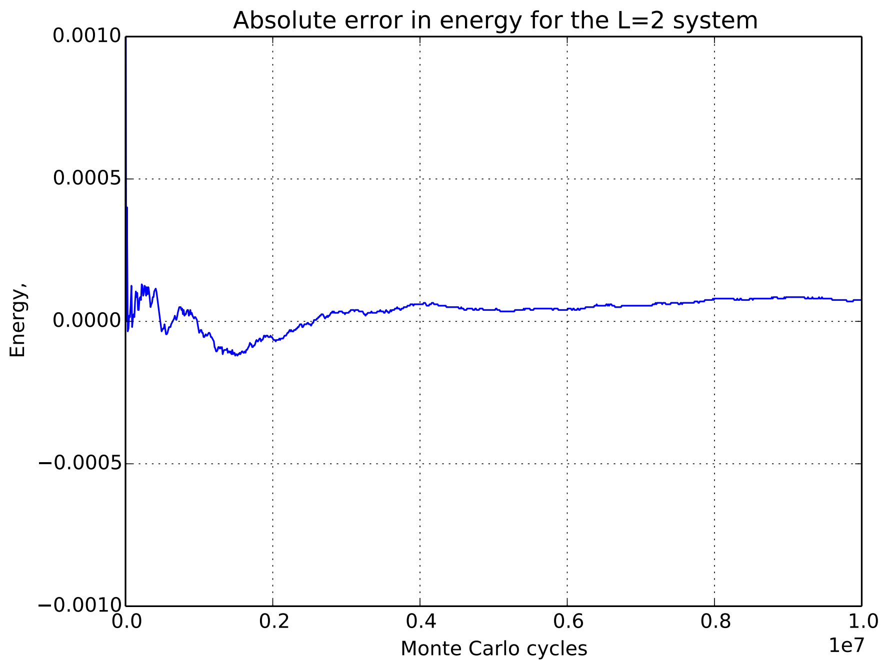


Figure 4.3

4.2 The L=20 system

4.2.1 Initial ordering of the system

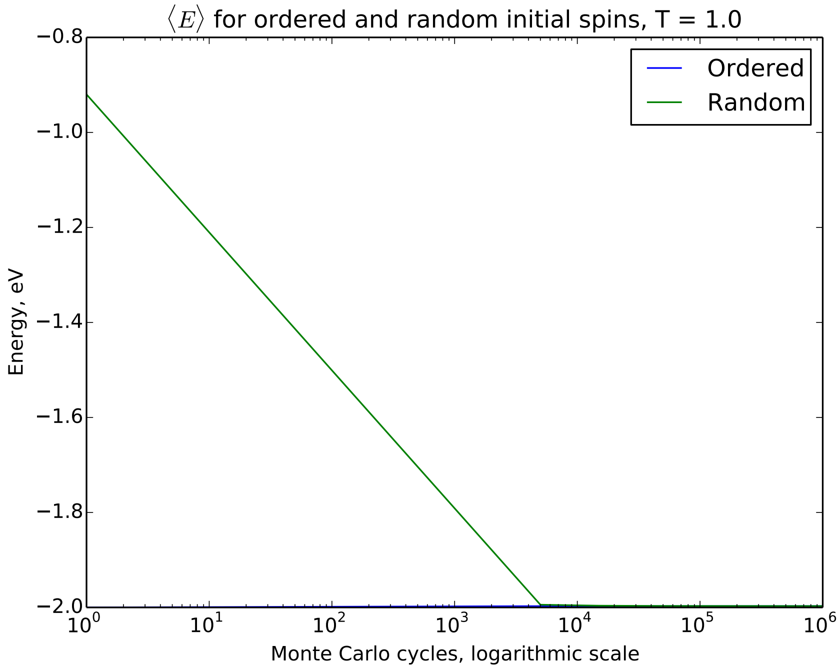


Figure 4.4

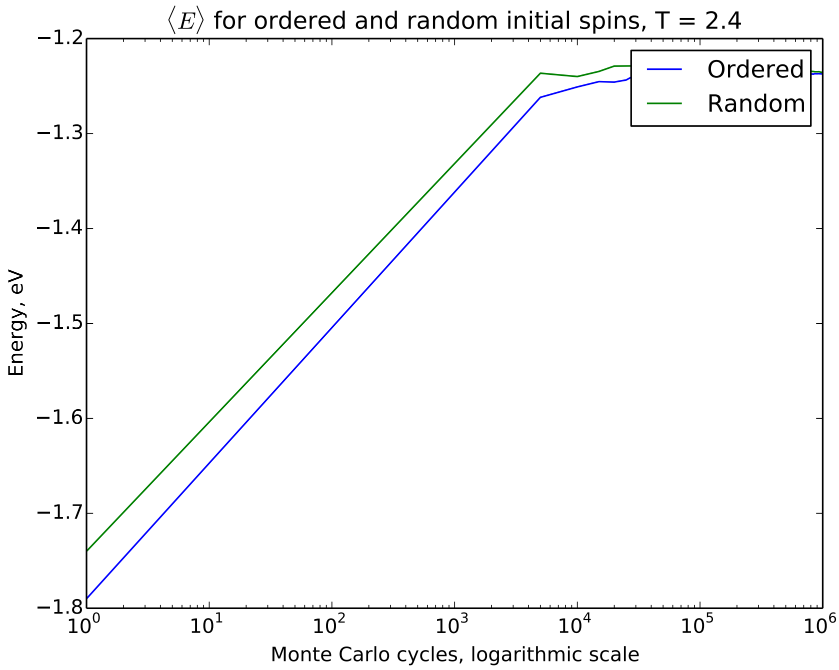


Figure 4.5

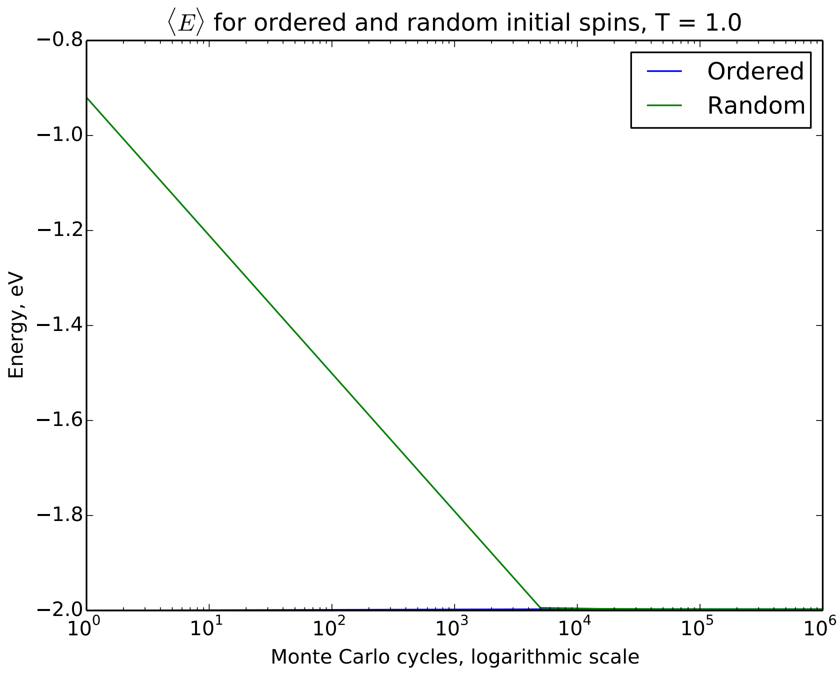


Figure 4.6

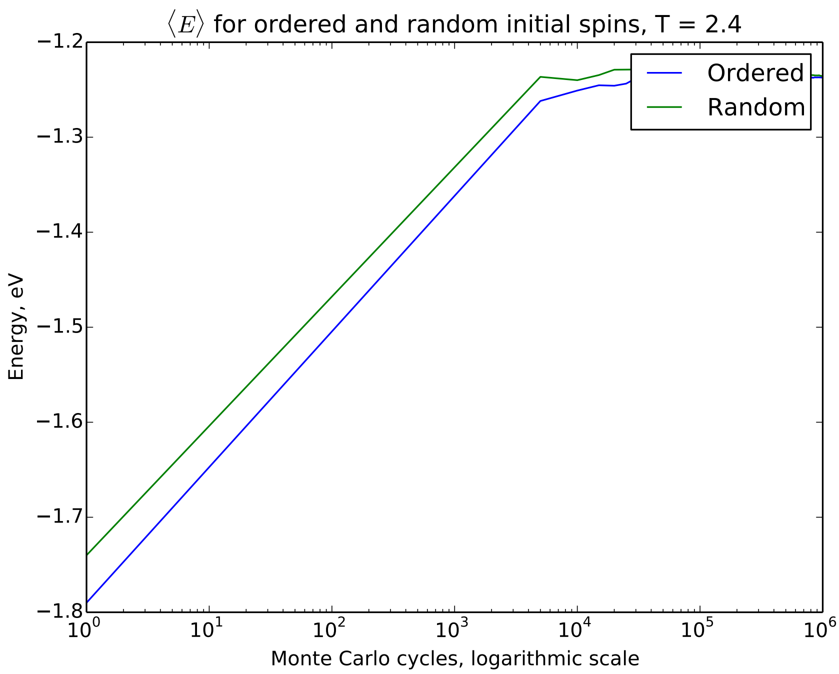
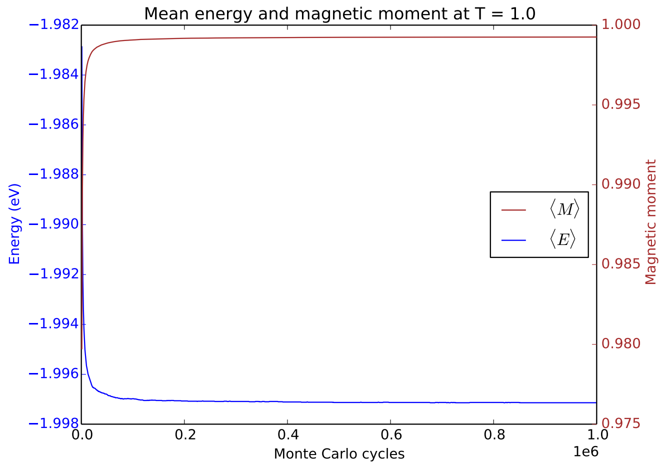
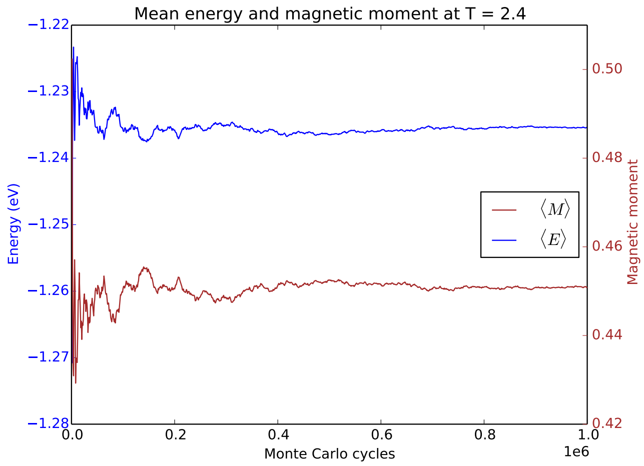


Figure 4.7

4.2.2 Equilibrium time for the random L=20 system

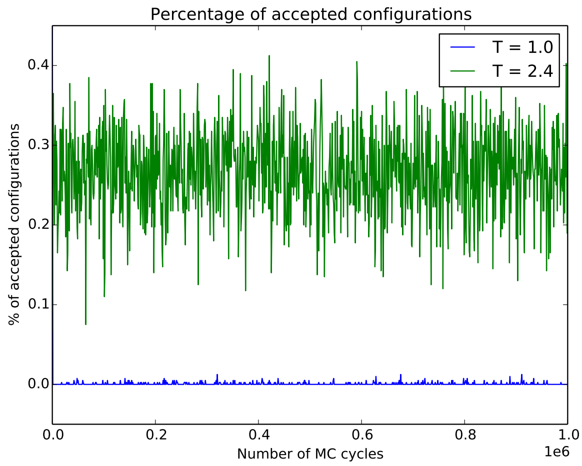


(a)

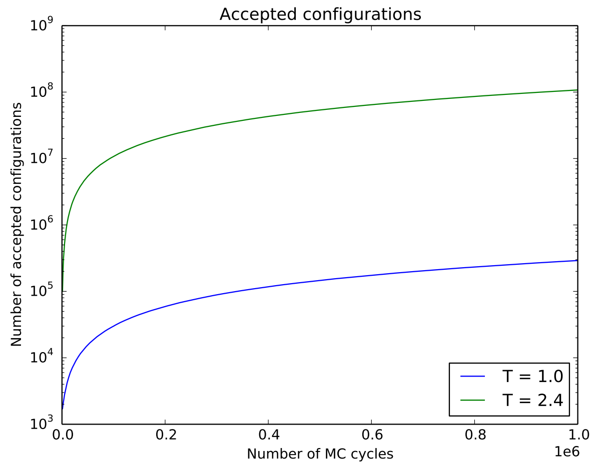


(b)

Figure 4.8



(a)



(b)

Figure 4.9

4.2.3 Probability distrubition for the L=20 system

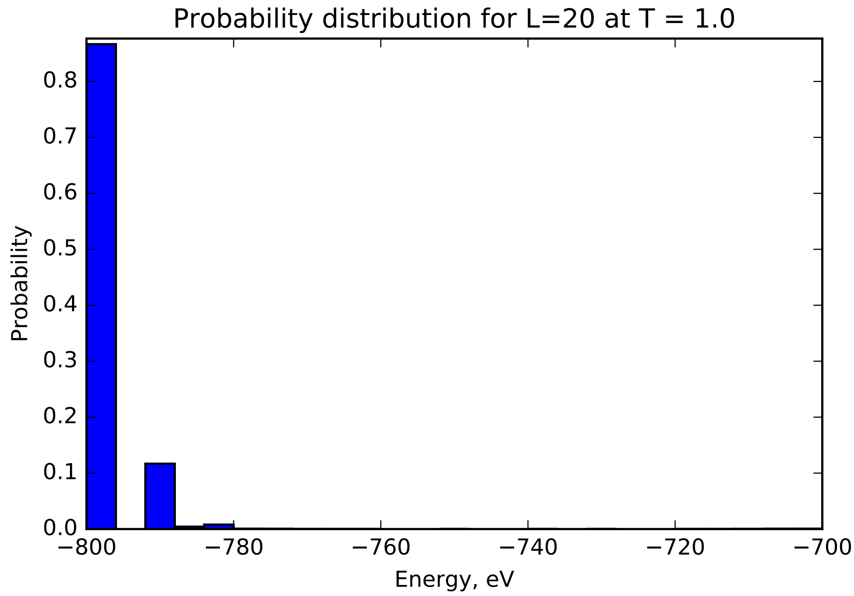


Figure 4.10

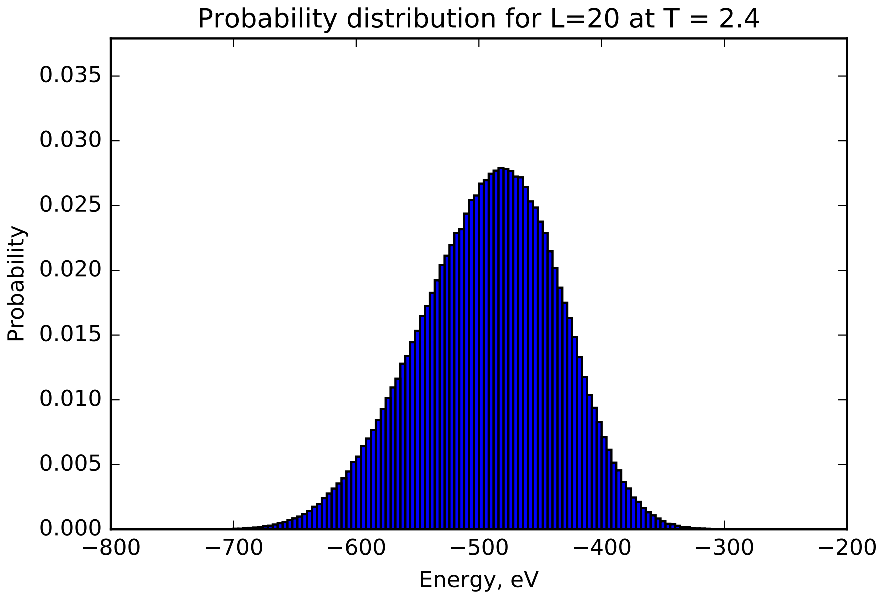


Figure 4.11

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

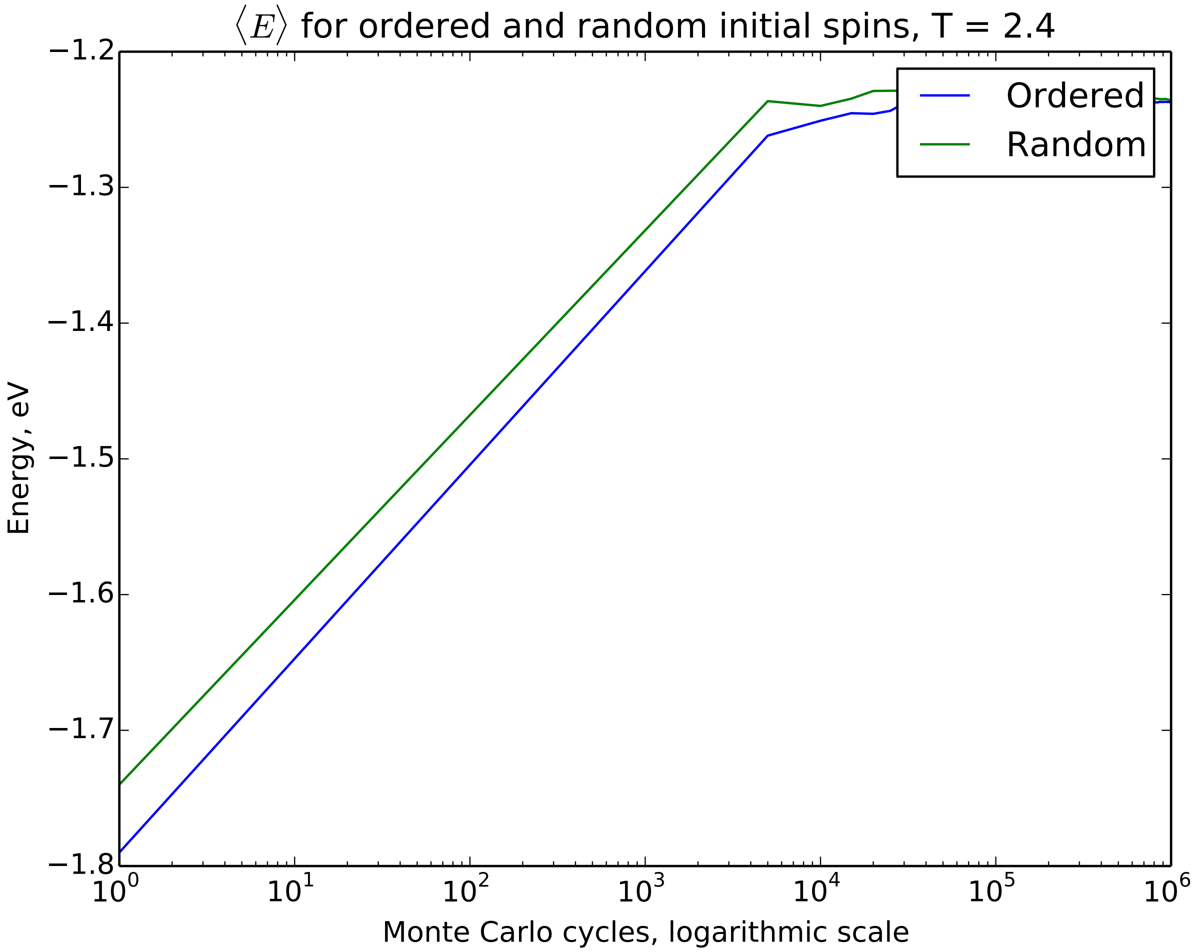


Figure 6.1