Project 4 FYS4150

Kjetil Karlsen

November 16, 2017

Abstract

To do:
Enhet akse ($T' = \frac{k_b}{J}T$), $E' = x$, $E = xJ$
Error estimation
Problem: Ulike T_C for varmekapasitet og X !!!!!
Korrelasjonslengde? Vits plotte? Autokorrelation: NEI
Tidsberegning Parallell

Contents

1 Introduction

2 Theory

Ising model

Markhow chain - convergance Error Random number ?????

2.1 The Ising model

The Ising model is a model used to simulate magnetic phase transitions of solids. In this project a somewhat simplified version of the model will be used, assuming no external magnetic field and a finite, 2 dimentional system. It is also assumed that the each spin can only take the values $s = \pm 1$. In this model only the nearest neighbours affect each other, excluding long range effects. The energy in a system of a total of N spins is then defined as

$$E = -J \sum_{\langle jk \rangle}^{N} s_k s_l \tag{1}$$

with J being a coupling constant and $\langle jk \rangle$ indicating that the sum is over the nearest neighbours only. The useful quantity Energy per spin is defined as $E_{spin} = \frac{E}{N}$.

2.1.1 Statistical physics in the Ising model

The spins in the Ising model follows Boltzmann statistics, meaning that the probability of a state $|i\rangle$ is defined as

$$P(E_i) = \frac{e^{-E_i \beta}}{Z_\beta} \tag{2}$$

with the partition function $Z_\beta = \int dE\ e^{-E\beta}$ normalizes the expression and $\beta = (k_B T)^{-1}$. The partition function used in the project is discrete,$Z_\beta = \sum_i^N e^{-E_i \beta}$. As the temperature T increases, the probability of each state decreases, giving a broader distribution of probable states.

In order to characterize the system, the mean energy, mean magnetization and mean absolute magnetization are important. The macroscopic property of mean energy $\langle E \rangle$ is needed to define the heat capacity C_V of the system, while the microscopic effect of mean magnetization and the magnetic moment leads to the susceptibility χ. These are defined below:

$$\langle E \rangle = \frac{1}{Z_\beta} \sum_i^N E_i P_\beta(E_i) \tag{3}$$

$$\langle M \rangle = \frac{1}{Z_\beta} \sum_i^N M_i P_\beta(E_i) \tag{4}$$

$$\langle |M| \rangle = \frac{1}{Z_\beta} \sum_i^N |M|_i P_\beta(E_i) \tag{5}$$

$$C_V = \frac{1}{k_B T^2} \left(\langle E^2 \rangle - \langle E \rangle^2 \right) \tag{6}$$

$$\chi = \frac{1}{k_B T} \left(\langle M^2 \rangle - \langle M \rangle^2 \right) \tag{7}$$

2.1.2 Periodic boundary conditions

At the boundaries of a finite spin matrix it is fewer nearest neighbours than in the bulk of the matrix. This is analogous to a surface of a material. By assuming periodic boundary conditions, the effects of the surface is neglected and easy to handle. For a 1 dimensional case with N spins, the neighbours of spin S_N is S_{N-1} and S_1.

2.2 Phase transitions

Regardless of the matrix size of the 2 dimensional system, there are only 16

Energy, magnetic moment, susceptibility, heat capacity, critical temperature:

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu} \tag{8}$$

Analytical solution

If one has experimental data from two systems with different matrix sizes, L and L', and doing some simple algebra, the following expression emerges for $T_C(\infty)$:

$$T_C(\infty) = T_C(L) - aL^{-1/\nu} = T_C(L) - \frac{T_C(L') - T_C(L)}{\frac{1}{L'} - \frac{1}{L}} L^{-1/\nu} \tag{9}$$

2.3 Simple example of the Ising model

L=2 case:

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

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

Energy:

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

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

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

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

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

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

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:

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

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

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

3 Method

Metropolis (T,A,...) Stokastisk matrise - konvergens - Markhov chain. Equilibrium- hva skjer med Z?

Hvilken random number engine ???

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

VILDE:

3.1 Monte Carlo cycles

In Monte Carlo methods, the goal is to

3.2 Metropolis algorithm

3.3 Random numbers

Ikke uavhengig Periode Hvilken generator

3.4 Parallelizing

Speedup

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

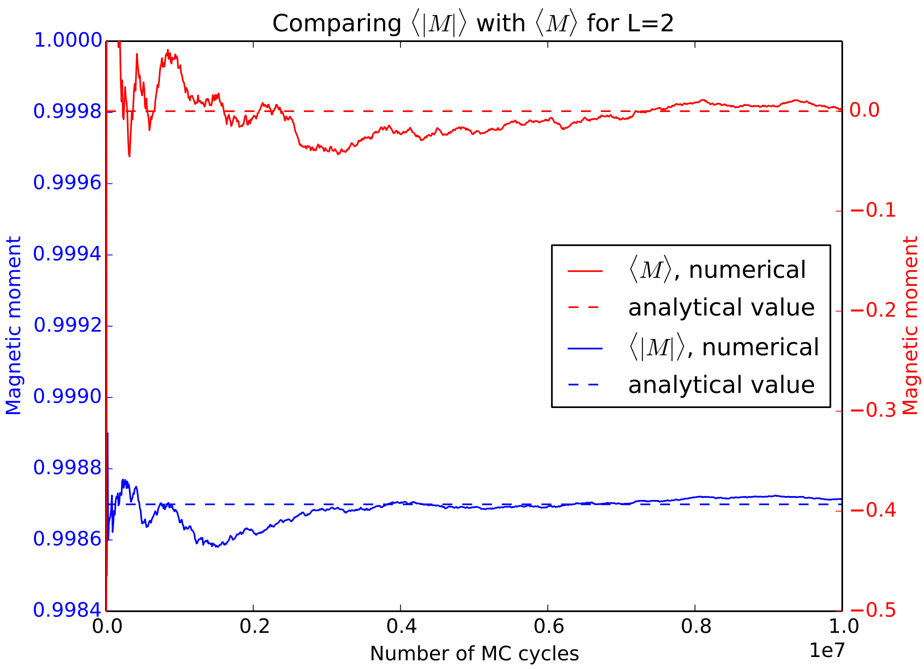
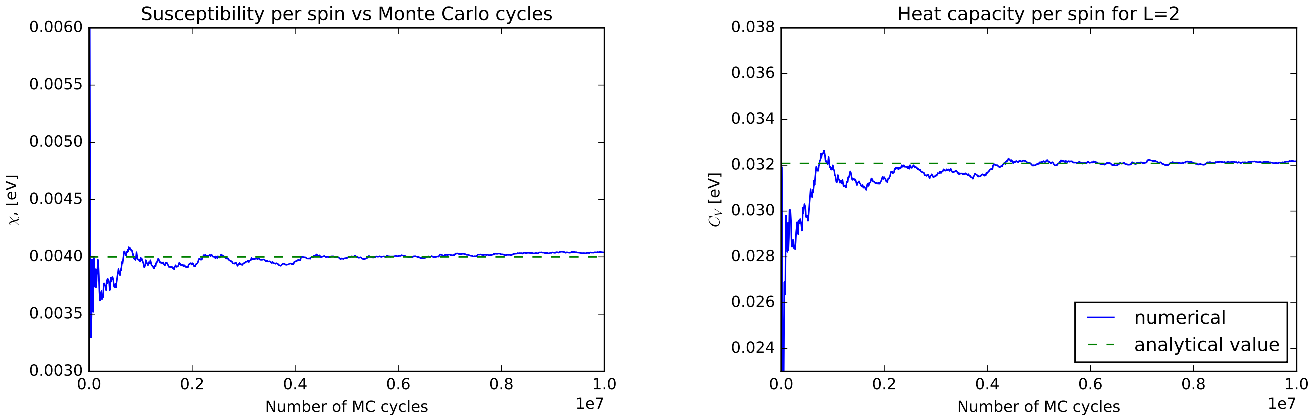


Figure 4.1

Se forelesningsnotat for kommentar + diskusjon!



(a) (b)

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

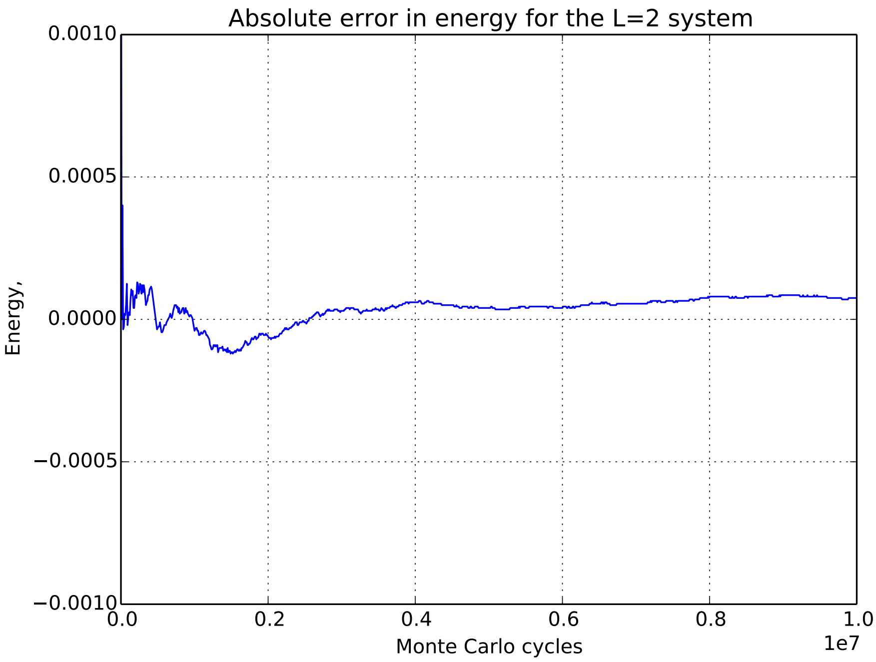


Figure 4.3

OBS! Need an number of MC cycles necessary!

All calculations in this subsection are at T = 1.0 K.

4.2 The L=20 system

HMM: Should define an area that is enough for equilibrium!

OBS: Need the number of MC cycles to reach equilibrium!

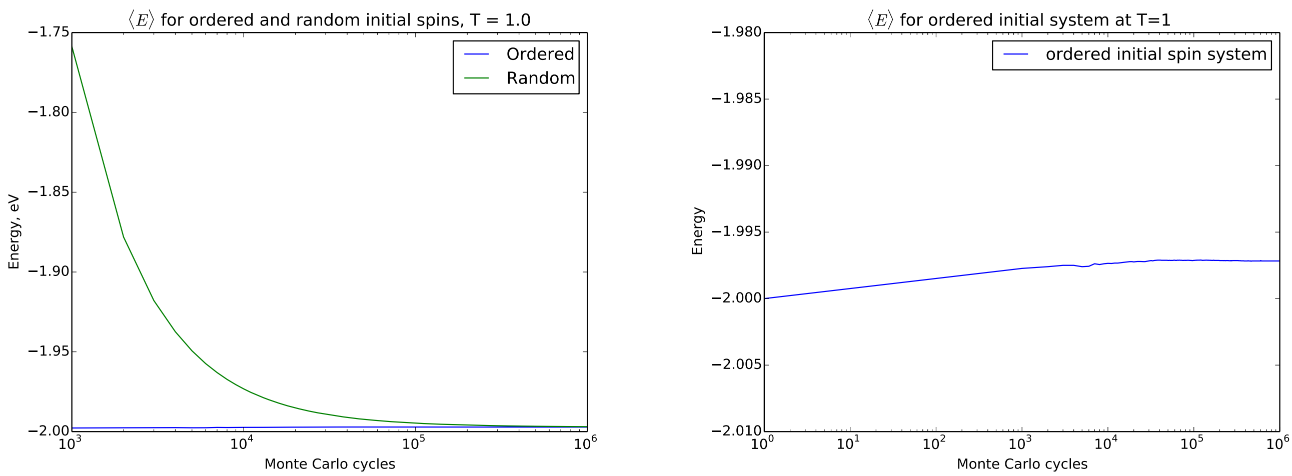
OBS: Need equilibration time! (5 1e5?)

OBS: Comment accepted configs T dependency

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

4.2.1 Initial ordering of the system



(a) (b)

Figure 4.4

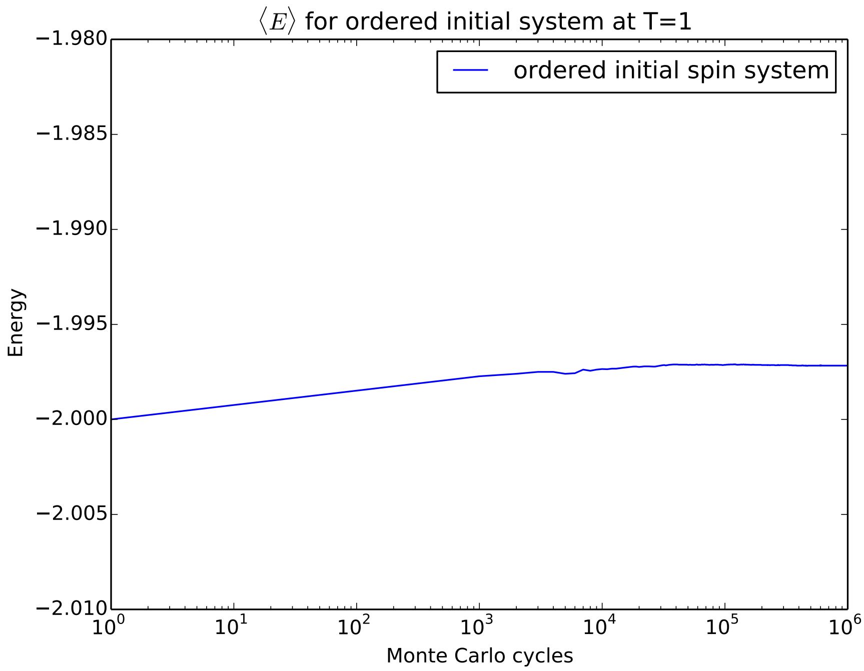


Figure 4.5: Plot of the

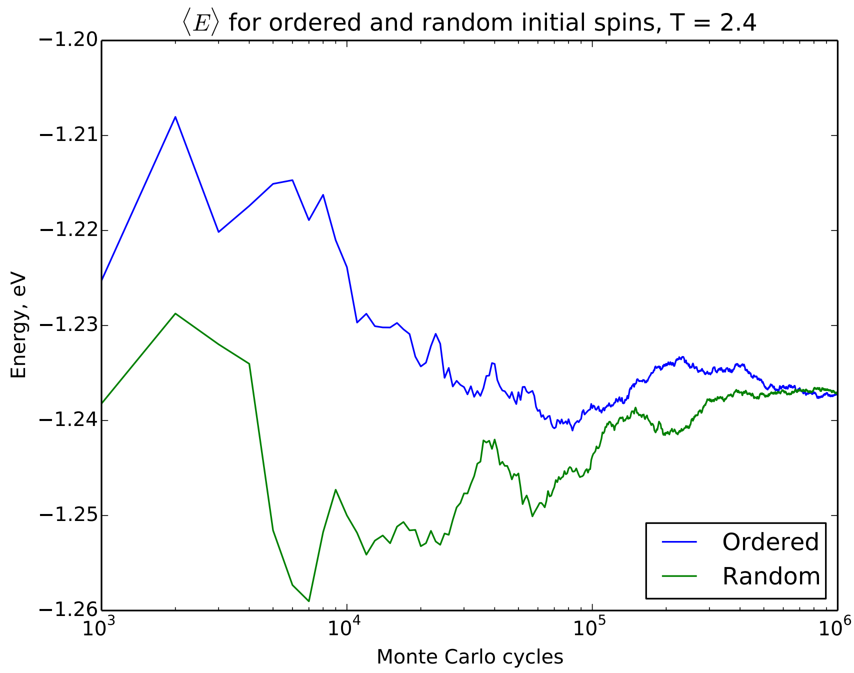
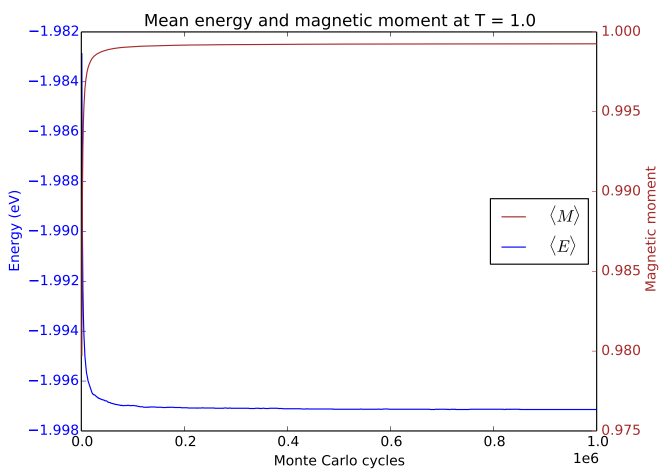
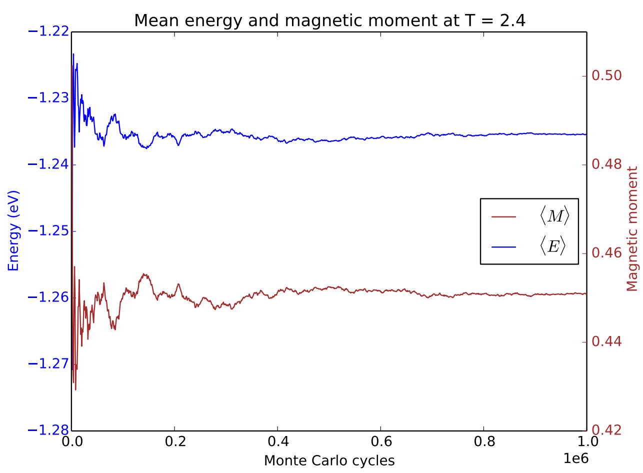


Figure 4.6

4.2.2 Equilibrium time for the random L=20 system

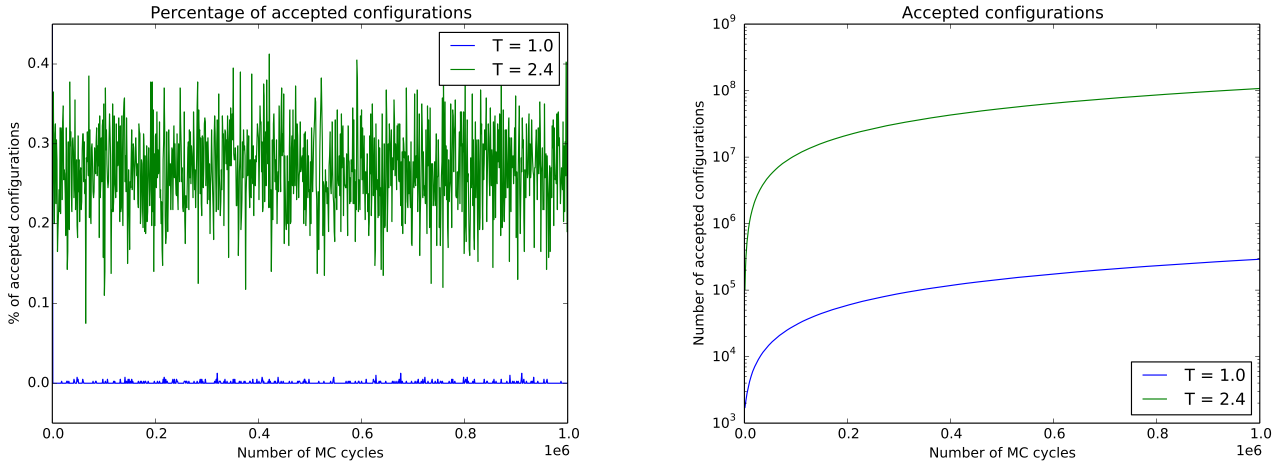


(a)



(b)

Figure 4.7



(a) (b)

Figure 4.8

4.2.3 Probability distrubition for the L=20 system

OBS: Compare result with computed variance!

OBS: Discuss behavior (In Discussion - maybe just merge result and discussion?)

Computed variance (from same dataset?):

$$\sigma_E^2 = \left\langle E^2 \right\rangle - \left\langle E \right\rangle^2$$

T = 1.0 K:

$$\sigma_E^2 = 1595.45 - (-1.997)^2 = 1591.46$$

T = 2.4 K:

$$\sigma_E^2 = 620.734 - (-1.23759)^2 = 619.20$$

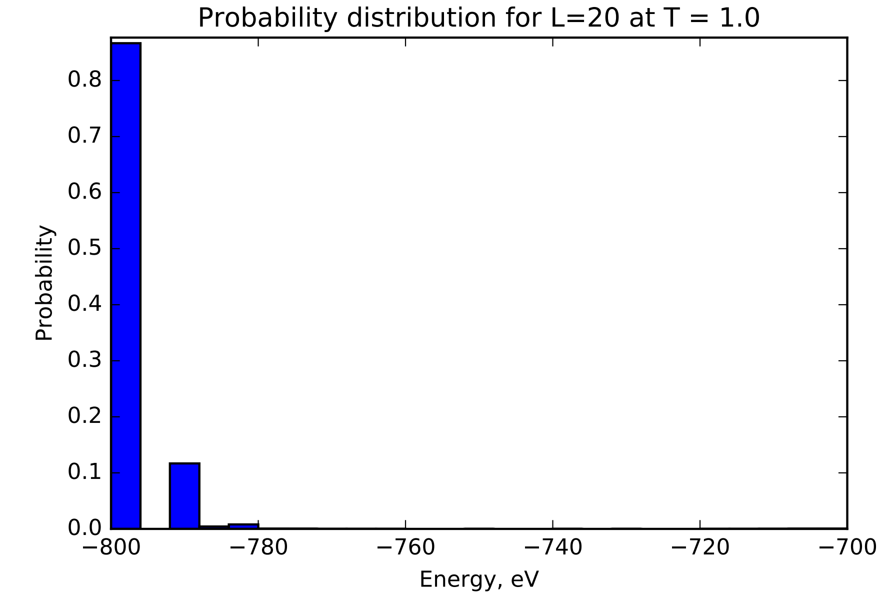


Figure 4.9

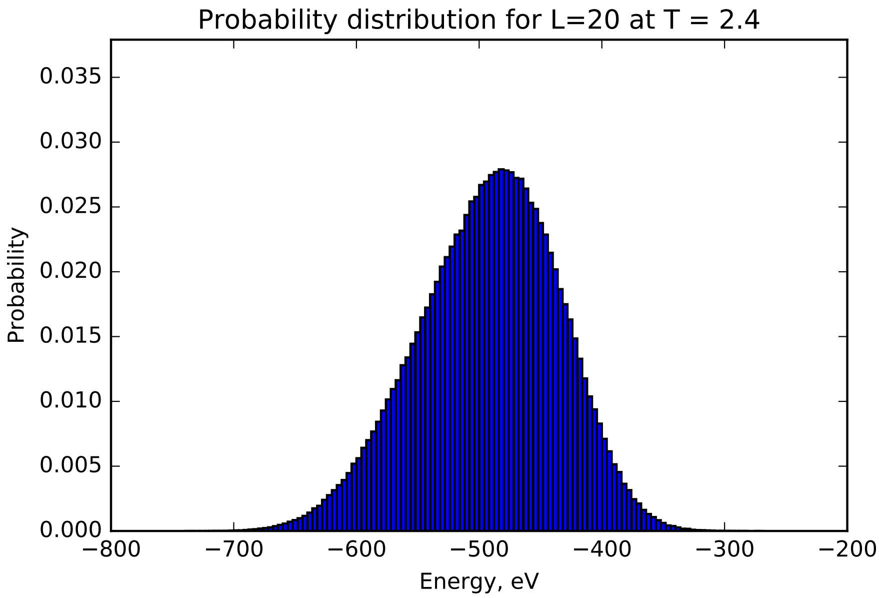


Figure 4.10

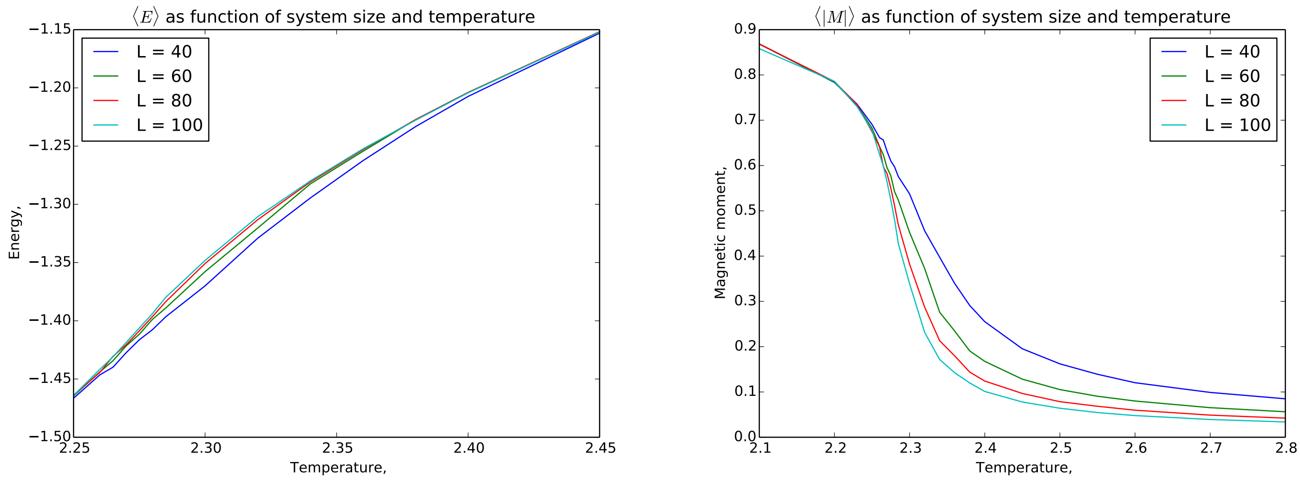
4.3 Phase transition and Critical temperature

OBS: Plot of E, M, Cv, X as functions of T (put L as legend and plot together)

OBS: Indication of phase transition? (Peak - at least for Cv and X)

OBS: Use Equation 11 to extract T_C.

Timing parallellisering



(a) (b)

Figure 4.11

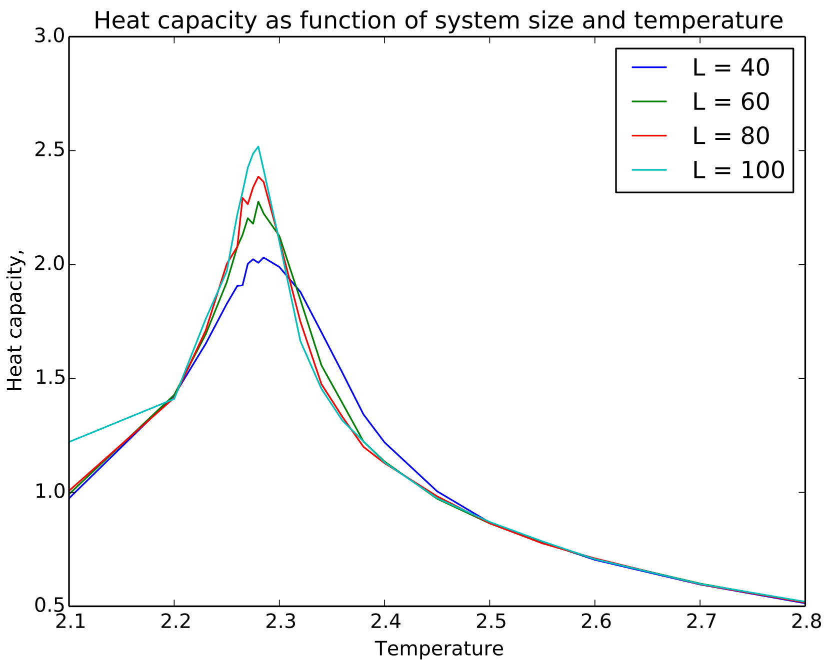


Figure 4.12

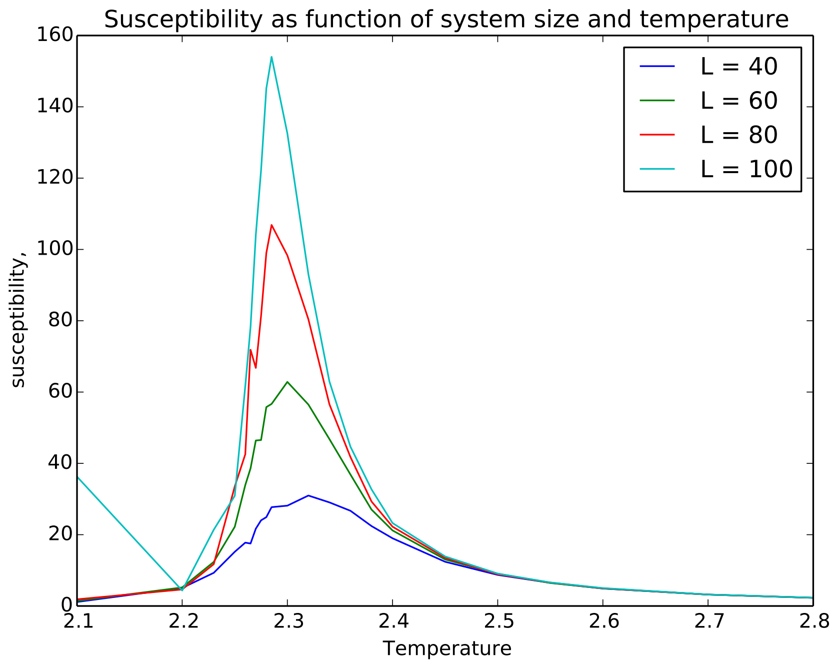


Figure 4.13

Table 4.2: text

L	T_C
40	2.29
60	2.28
80	2.28
100	2.28

5 Discussion

6 Conclusion

References

Appendix

Table 6.1: Table of all the possible microstates for the L=2 system

State	Spinn	Energi	Magnetization
1	↓ ↓ ↓ ↓	−8J	−4
2	↓ ↓ ↓ ↑	0	−2
3	↓ ↓ ↑ ↓	0	−2
4	↓ ↑ ↓ ↓	0	−2
5	↑ ↓ ↓ ↓	0	−2
6	↓ ↓ ↑ ↑	0	0
7	↓ ↑ ↓ ↑	0	0
8	↓ ↑ ↑ ↓	8J	0
9	↑ ↓ ↓ ↑	8J	0
10	↑ ↓ ↑ ↓	0	0
11	↑ ↑ ↓ ↓	0	0
12	↓ ↑ ↑ ↑	0	2
13	↑ ↓ ↑ ↑	0	2
14	↑ ↑ ↓ ↑	0	2
15	↑ ↑ ↑ ↓	0	2
16	↑ ↑ ↑ ↑	−8J	4