Project 4 FYS4150

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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
Diskutere bredde Tc peak? Teoridel - se side 431 i kompedium

Contents

1 Introduction

2 Theory

The theory and method sections are based on chapter 12 and 13 in Jensen, [1].

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

A phase transition happens when a thermodynamically stable state of a system changes abruptly as one or more thermodynamical variables describing the structure reaches a critical value. In addition to changing state, macroscopic properties of the system must change. Melting of a solid is a example of an everyday phase transition, depending on a critical pressure and a critical temperature. At a critical temperature (T_C) the Ising model undergoes a second order phase transition, affecting both the mean energy and magnetization.

A first order phase transition is a gradual change from a phase to another and have two phases that coexist at the critical point, for example the melting of ice. The long range ordering exist in each phase, which gives a relatively large correlation length. For a second order phase transition, in the Ising model caused by Boltzmann statistics , the correlation length spans the entire system at the critical point. This means that the two phases on either side of the critical point is the same.

For a finite lattice the correlation length, mean magnetization, susceptibility and heat capacity is described by the following equations near the critical temperature.

$$\chi(T) \simeq (T_C - T)^{-\alpha} \tag{8}$$
$$\xi(T) \simeq |T_C - T|^{-\nu} \tag{9}$$
$$C_V(T) \simeq |T_C - T|^{-\gamma} \tag{10}$$
$$\langle M \rangle \simeq |T - T_C|^{\beta} \tag{11}$$
$$\tag{12}$$

The critical exponents α, β, ν and γ are all positive. From equation 8-10 it is clear that χ, $\xi(T)$ and C_V diverges to infinity at $T = T_C$. As the correlation length spans the whole system, it is limited by the lattice size, L. The critical temperature is related to the finite scaling by equation 13

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu} \tag{13}$$

2.3 Simple example of the Ising model

It is possible to model the 2×2 Ising model with periodic boundary conditions analytically. This specific system has $N = 2^{L^2} = 2^4 = 16$ different micro states.

Table 2.1: Overview of the degeneracy of the $L = 2$ system. See table 6.1 for all the different microstates

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

From table 2.1 it is possible to calculate the partition function of the system:

$$Z = \sum_i^M e^{-\beta E_i} = 2e^{-\beta 8J} + 2e^{\beta 8J} + 12 = 4\cosh(\beta 8J) + 12$$

The mean energy is given as a derivation by parts of $\ln Z$ with regards to β:

$$\langle E \rangle = -\left(\frac{\partial \ln Z}{\partial \beta}\right)_{V,N} = -\frac{\partial}{\partial \beta}\ln\left[4\cosh(8J\beta) + 12\right] = \frac{-8J\sinh(8J\beta)}{3\cosh(J\beta) + 4}$$

By investigating table 2.1, the mean magnetization $\langle M \rangle$ must be 0. However, that is not true for the mean absolute magnetization:

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

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

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

We can use these to calculate the rest:

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

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

Describes all the nearest neighbour interactions possible in all systems

To do: beskrive alle data: tabell, Eavg Mavg, Z, Cv, X,

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 0.5e6 v 1e6 - mulige feil (likevekt tidlig - liten effekt)

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

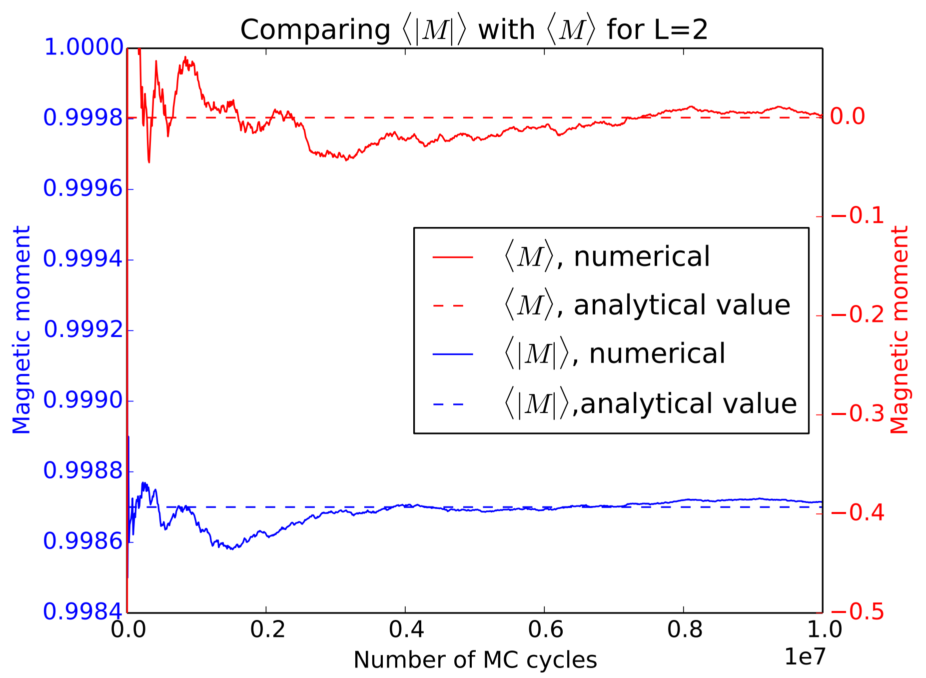
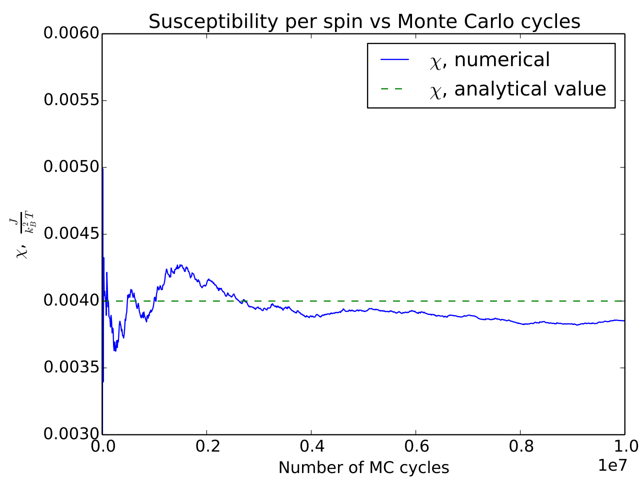
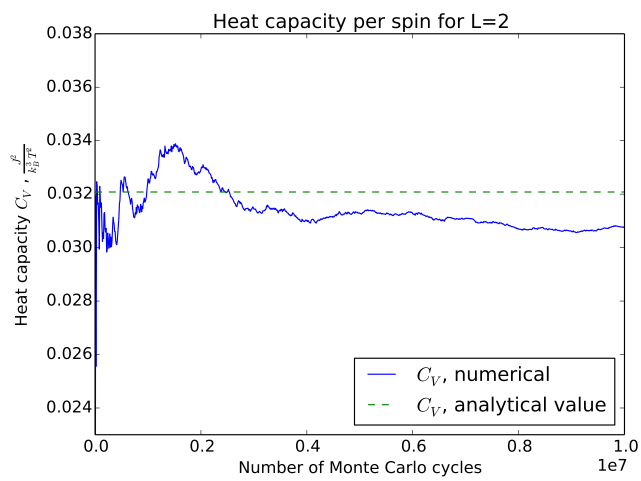


Figure 4.1

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.

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

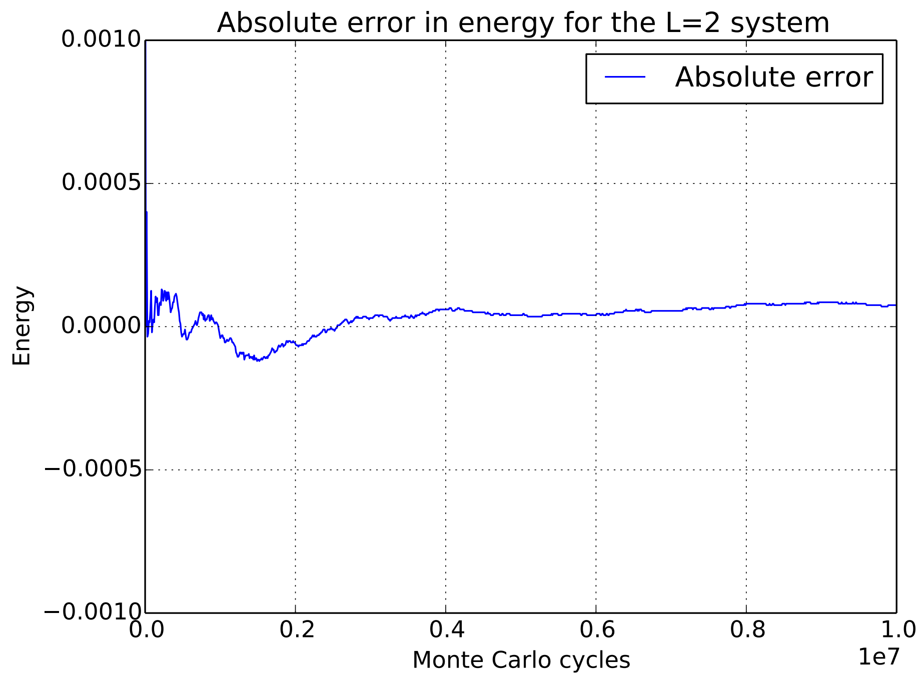


Figure 4.3

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

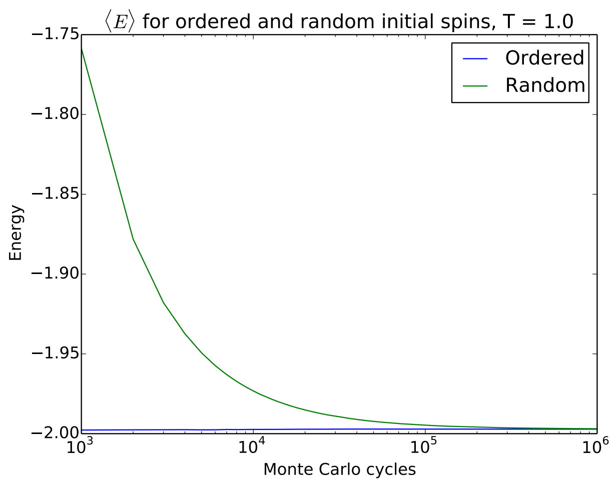
HMM: Should define an area that is enough for equilibrium!

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

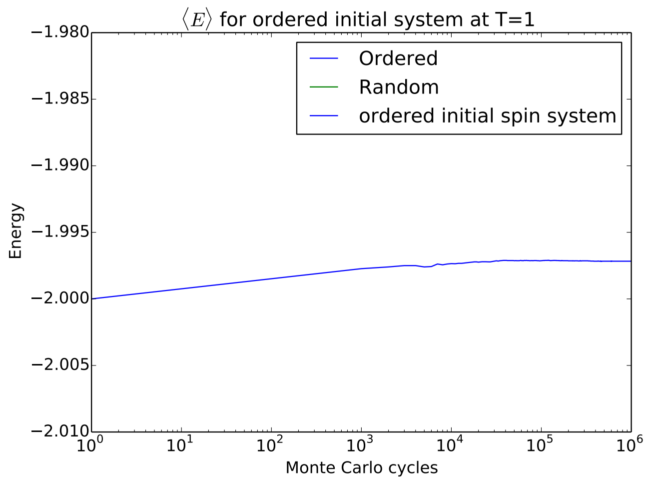
OBS: Need equilibration time! (5 1e5?)

OBS: Comment accepted configs T dependency

4.2.1 Initial ordering of the system



(a)



(b)

Figure 4.4

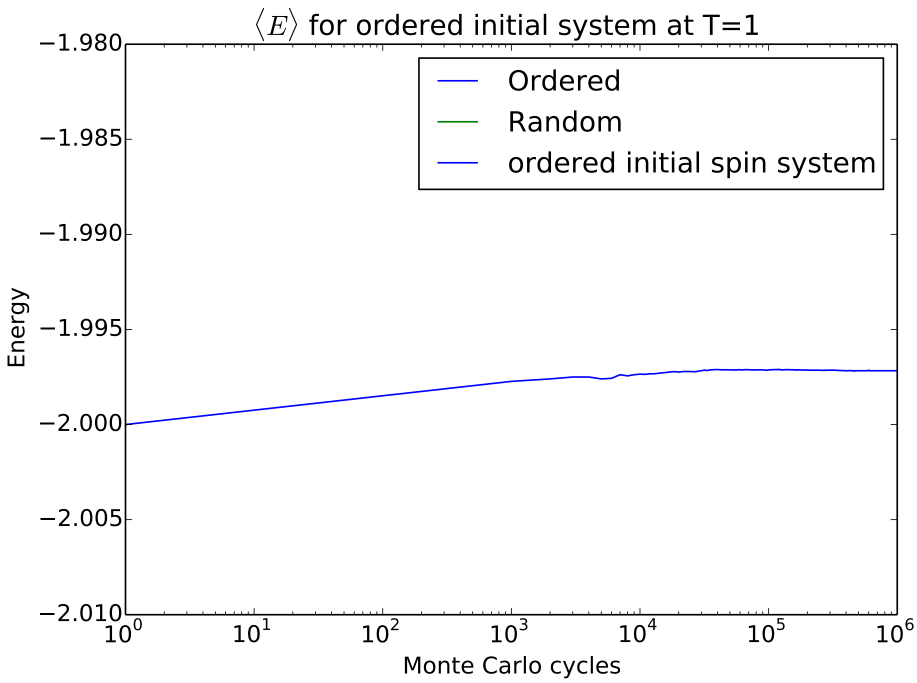


Figure 4.5: Plot of the

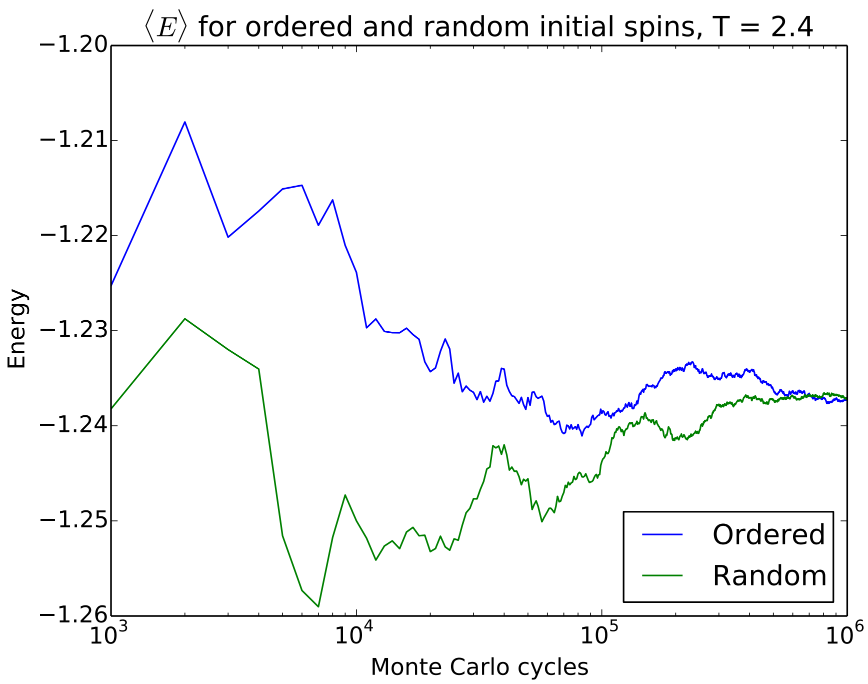
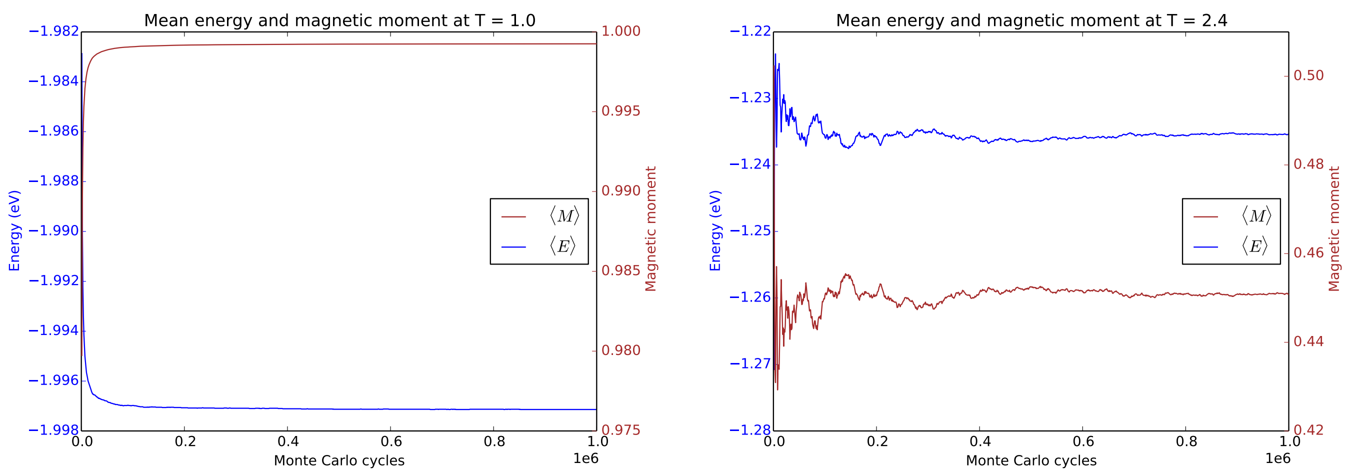


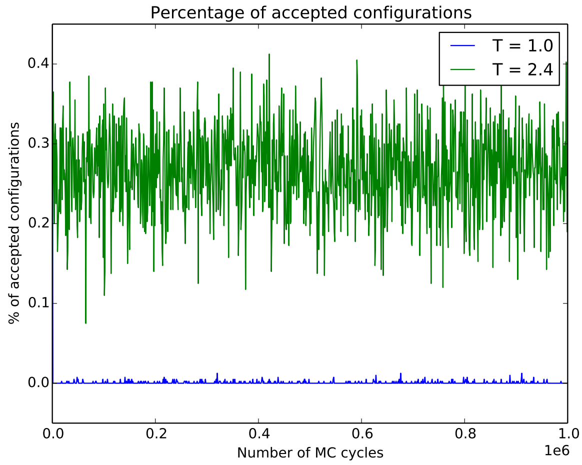
Figure 4.6

4.2.2 Equilibrium time for the random L=20 system

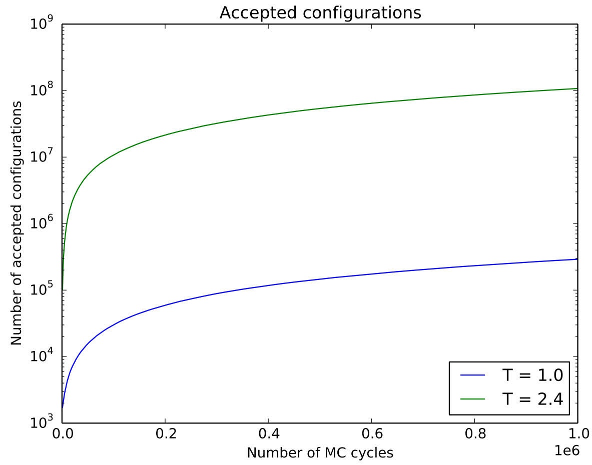


(a) (b)

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:

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

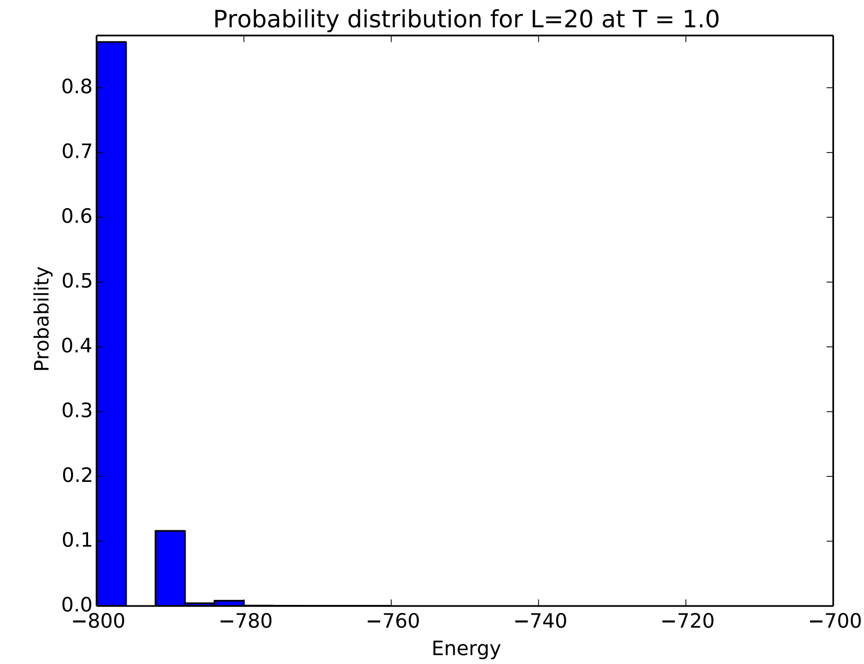


Figure 4.9

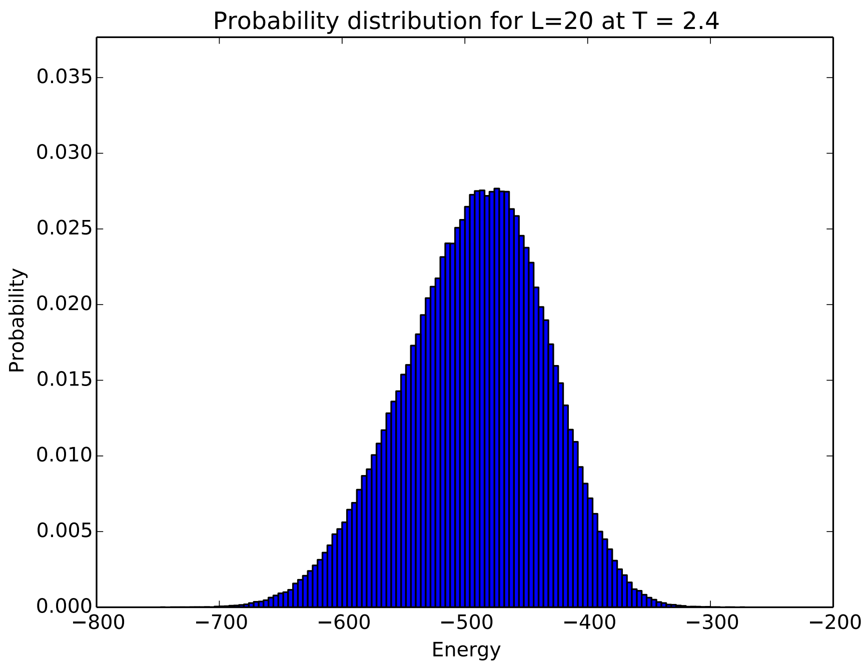


Figure 4.10

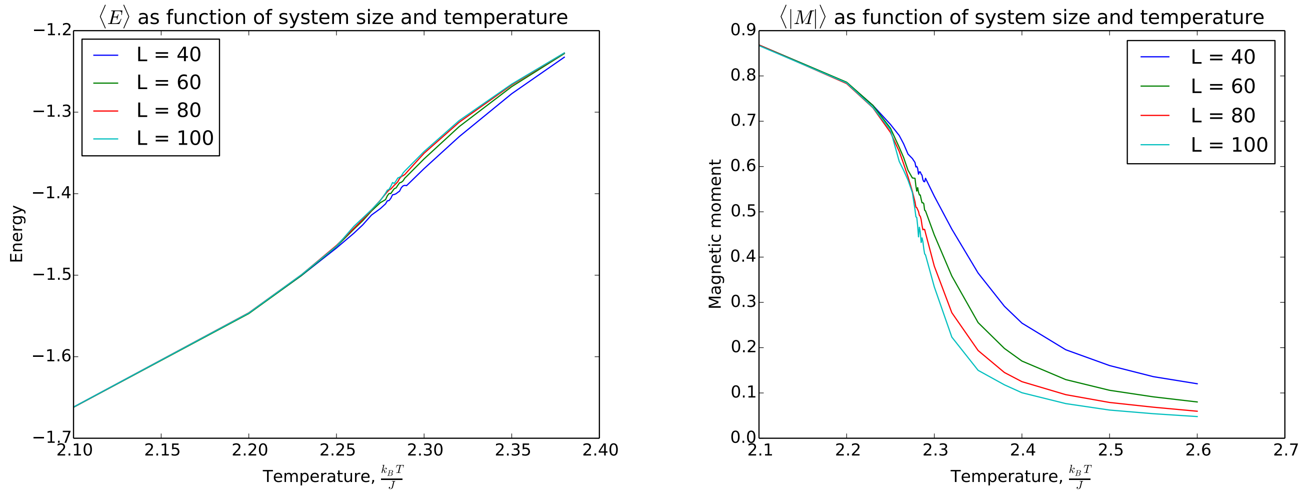
4.3 Phase transition and Critical temperature

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 13 to extract T_C.

Timing parallellisering



(a) (b)

Figure 4.11

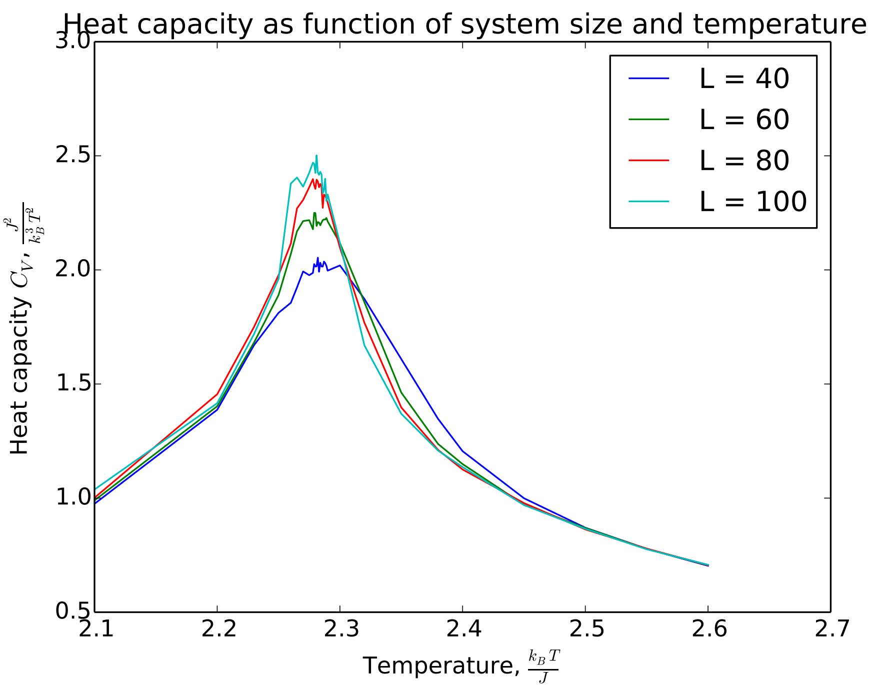


Figure 4.12

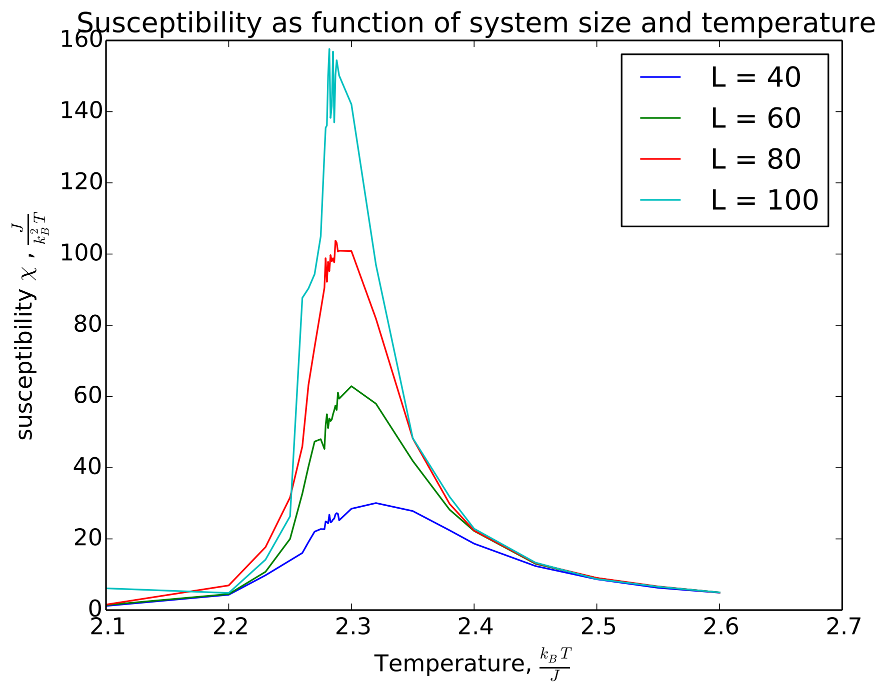


Figure 4.13

Table 4.2: text

L	T_C
40	2.28
60	2.28
80	2.28
100	2.28

5 Discussion

Phase transition As the temperature is increased, the Boltzmann distribution predicts that more states will become stable, lowering the energy necessary to change state of each spin. This can be seen in figure 4.11b from the fact that $\langle M \rangle$ approaches 0 after T_C

6 Conclusion

References

[1] Morten Hjorth-Jensen. Computational physics: Lecture notes fall 2015. Department of Physics, University of Oslo, 8 2015. Chapter 12 and 13.

Appendix

Table 6.1: Alle the microstates of the 2×2 Ising model

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