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:

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

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

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

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

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

By using the same methods as above, the expressions for $\langle E^2 \rangle$ and $\langle M^2 \rangle$ is found to be:

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

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

Combining these gives the expressions for the heat capacity and susceptibility from equations 6 and 7.

$$C_V = k\beta^2\left(\left\langle E^2 \right\rangle - \langle E \rangle^2\right) = \frac{\beta(8J)^2}{T}\left(\frac{\cosh^2 x - \sinh^2 x + 3\cosh x}{(\cosh x + 3)^2}\right) = \frac{(8J)^2}{k_B T^2}\frac{3\cosh x}{(\cosh x + 3)^2}$$

with $x = 8J\beta$. Similary, χ is found to be

$$\chi = \beta\left(\left\langle M^2 \right\rangle - \langle M \rangle^2\right) = \frac{8\beta\left(e^x + 1\right)}{\cosh x + 3}$$

The real usefulness of the $L = 2$ periodic system is that it describes all the nearest neighbour interactions, for any lattice size.

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

3 Method

We want to study the Ising model at equilibrium. However, the system has to start from a initial condition. Markov chains are useful for this.

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

3.1 Markov chains

The idea behind the markov chains is to make a random movement with a given probability of actually making the move, describing the microscopic principle of Brownian motion. This is often done by an eigenvalue problem, using a stochastic matrix W with the probabilities of making a move. As the eigenvalue of a $L \times L$ stochastic matrix has L eigenvalues with $\lambda_1 = 1,\ \lambda_i < 1$, it will eventually converge towards a equilibrium eigenvector through the relation $w_N = W^n w_0$. The steady state is reached when $w_{i+1} = W w_i$. In real life, this corresponds for instance to a particle diffusing through a solid. This particle has at every given moment a specific energy and in order to diffuse it has to overcome an energy barrier. However, a markov chain needs to obey the principles of ergodicity and detailed balance.

3.2 Metropolis algorithm

The matrix W is often unknown and in the metropolis algorithm it is instead described by $W = AT$. The acceptance probability of the problem is handled by matrix A, while the physics of the problem is handled by matrix T, describing the likelihood of making a transition. The detailed balance guaranties that the most likely state is reached, ie. that the probability of state w_i to transit to state w_j is the same as back from w_j to w_i: $w_j T(j \to i) A(j \to i) = w_i T(i \to j) A(i \to j)$.

In this project, the probability of a certain state is $w_i = \frac{1}{Z_\beta} e^{-\beta E_i}$ and the physics of moving between w_i and w_j is the same, one gets the following relation:

$$w_j = \frac{A(i \to j)}{A(j \to i)} w_i = e^{-\beta \Delta E} w_i \tag{14}$$

A system developing like this, with $\Delta E = E_j - E_i$ will reach the most likely state eventually. However, a real system fluctuates around the equilibrium. In order to ensure this, it must be probable to reach a state with higher energy than the previous. For the algorithm used in this project, all situations where the energy got lower by making a random transition, $E_{i+1} < E_i \Rightarrow \frac{w_{i+1}}{w_i} \geq 1$ was accepted. But also some states with $\frac{w_{i+1}}{w_i} > 1$ was accepted by random acceptance. Another important feature of equation 14 is that there is no need to calculate the partition function, which for large systems would lead to numerical errors.

For each Monte Carlo cycle our algorithm tried L^2 transitions, accepting only those transitions that fulfilled the requirements set in the previous section. This was done in order to directly compare how different matrix sizes converged to an equilibrium as a function of Monte Carlo cycles.

3.3 Random numbers

An ideal random number generator is not deterministic and produces an infinite number of different random numbers. However, this is not the case for a real generator. Every computer generated pseudo random generator will reproduce the same set of random numbers after a given period, which should be as large as possible. This means that a deterministic computer cannot produce a true random number, but a good pseudo random number generator has a negligible correlation between the different numbers. In this project the Mersene Twister 19937 generator (64 bit) was used, which has a period of 2^{19937}.

3.4 Parallelizing and speed up

Parallel computing represents a big increase in speed of these simple Monte Carlo calculations. When computing in parallel, the same program runs on a multitude of threads, effectively doing several experiments at the same time. A computer with two CPU's will be able to run the two programs parallel, collecting the data in the end. For this project parallel computing was utilized to split up the number of Monte Carlo cycles by the number of available CPU's. Assuming that the number of Monte Carlo cycles the system need to reach equilibrium is negligible compared to the total Monte Carlo cycles in the experiment, this approach is reasonable. By running on computer with p CPU's, this should give a speedup, defined by $Speedup(code, sys, p) = T_1/T_p$ of approximately 0.5.

Another way to increase the speed of the algorithm is to precalculate the energy. As there are only 16 changes in energy by changing a single spin, discussed in section 2.3, it is possible to pre-calculate $e^{-\beta\Delta E}$ Prekalkulere energi

3.5 Unit tests

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

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

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

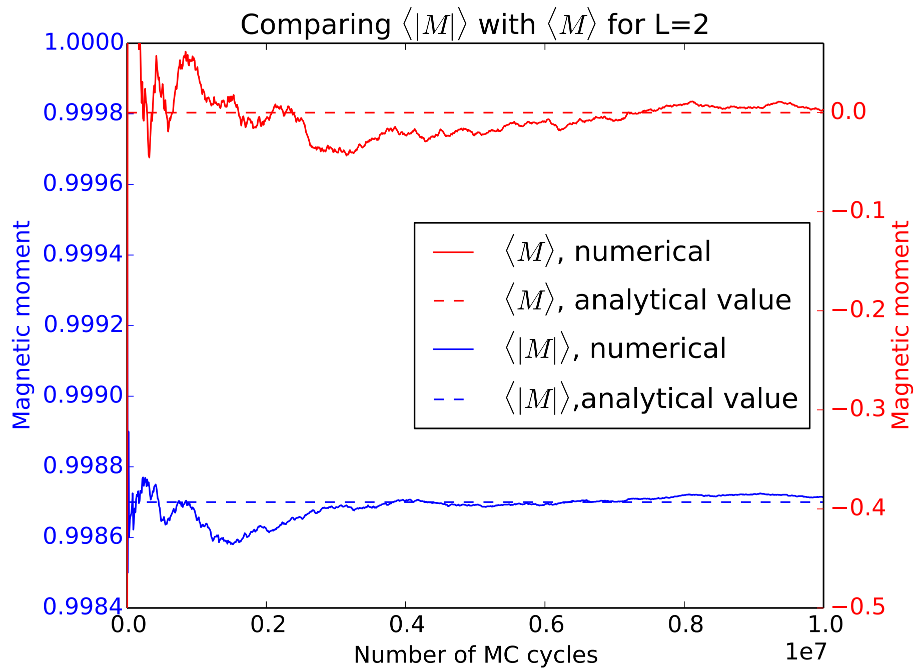
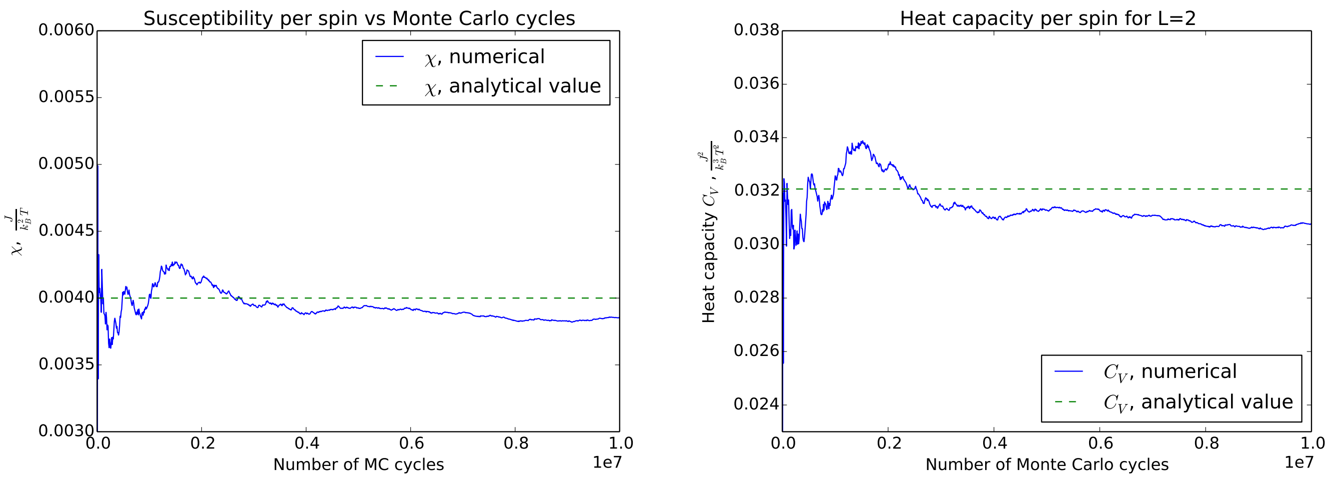


Figure 4.1

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

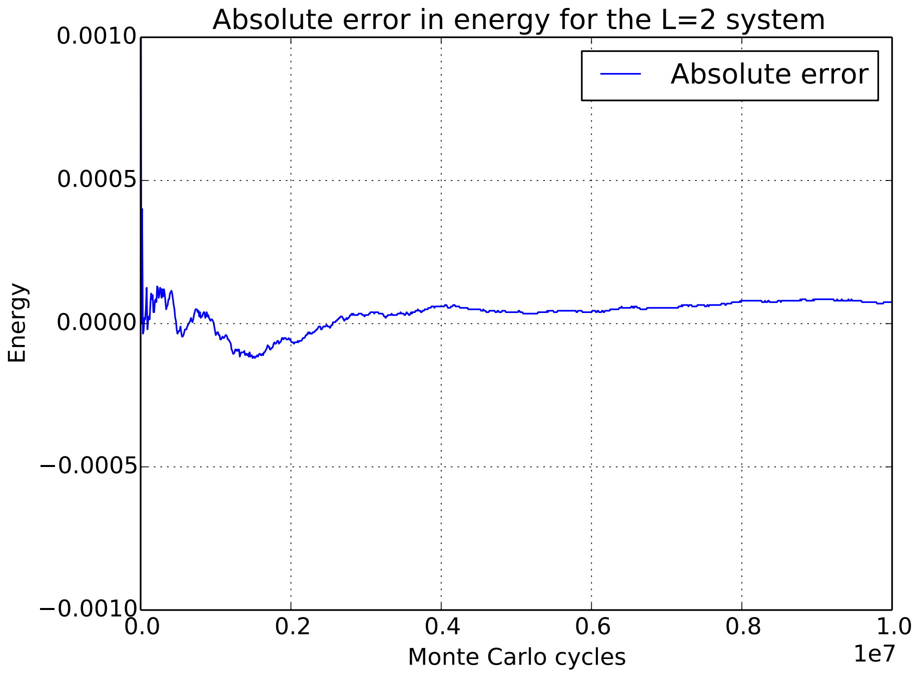


Figure 4.3

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

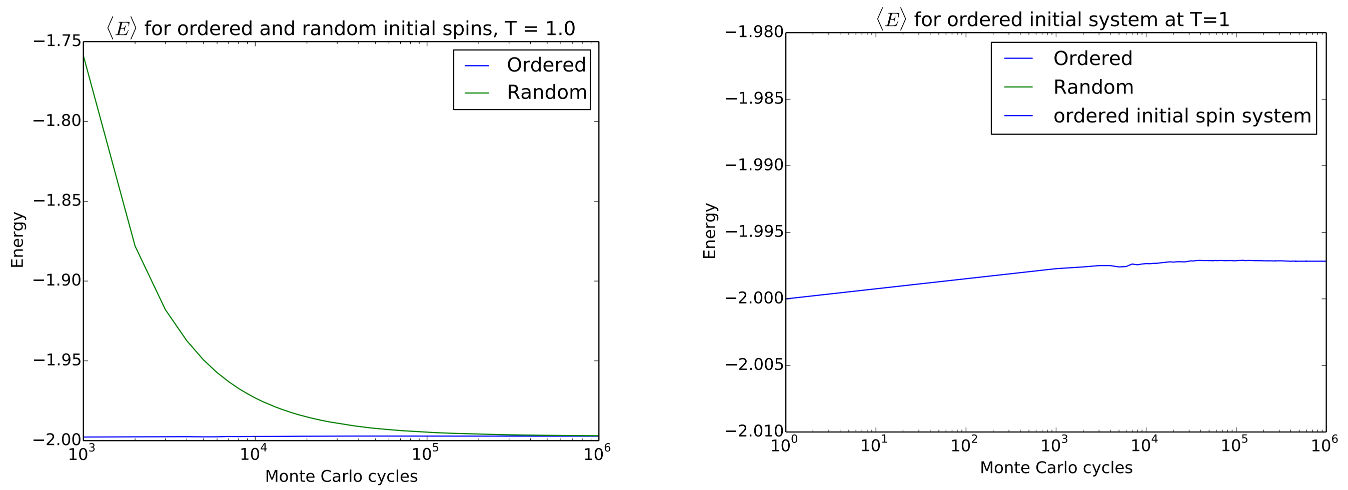
HMM: Should define an area that is enough for equilibrium!

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

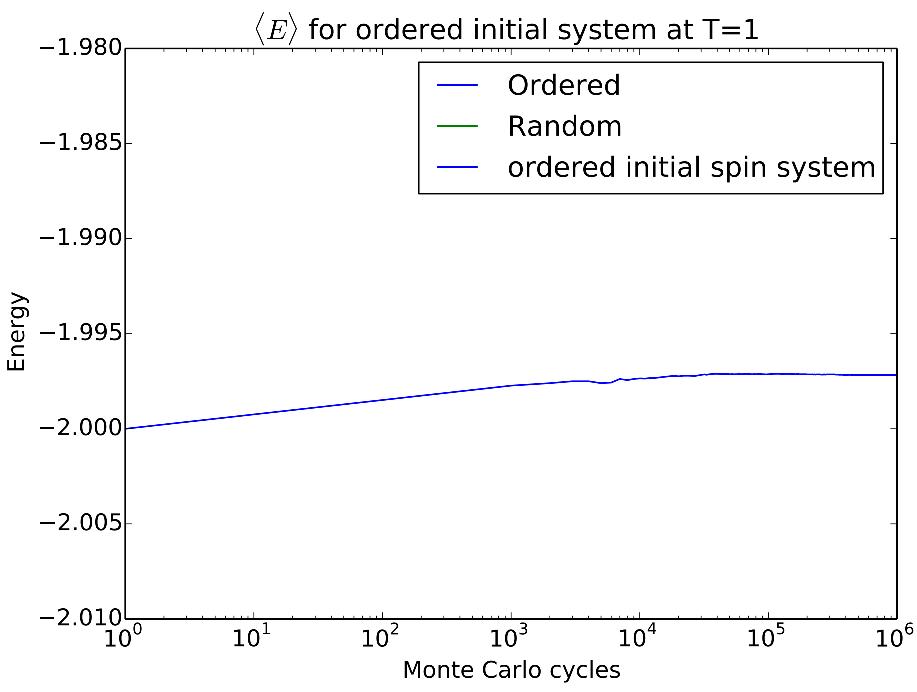


Figure 4.5: Plot of the

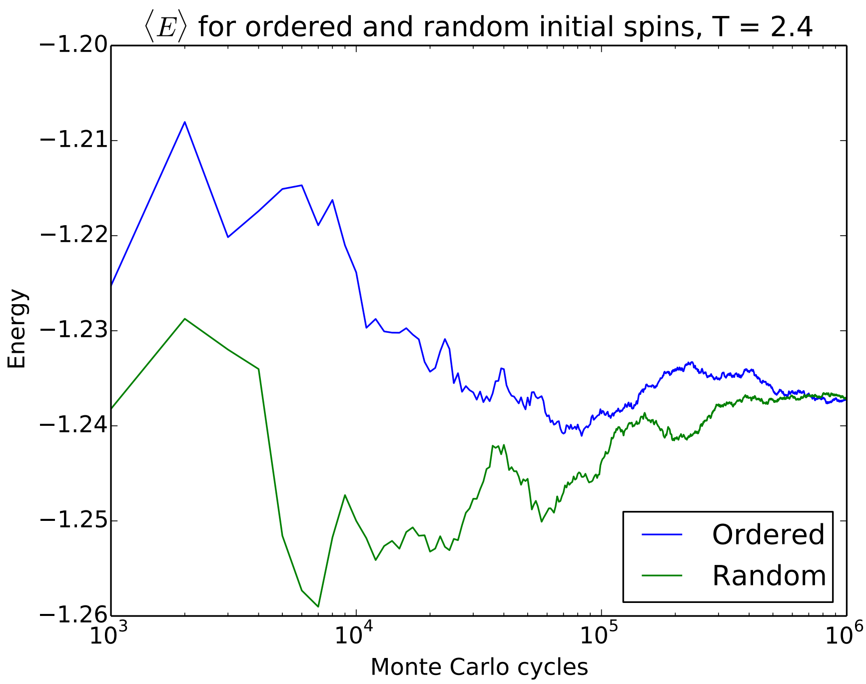
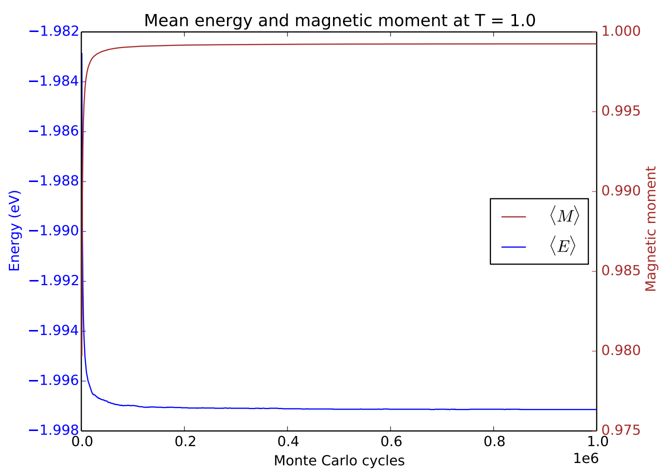
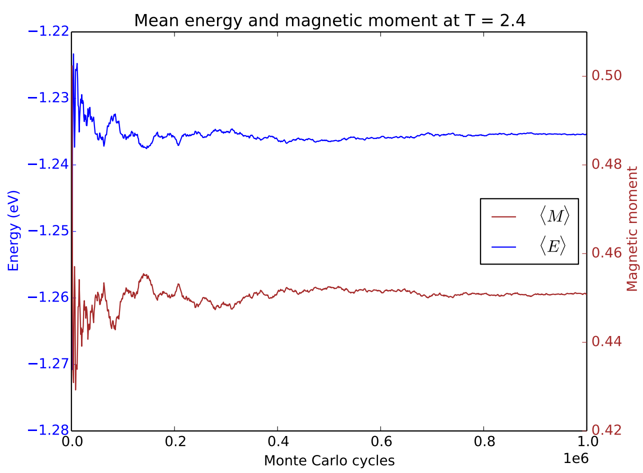


Figure 4.6

4.2.2 Equilibrium time for the random L=20 system

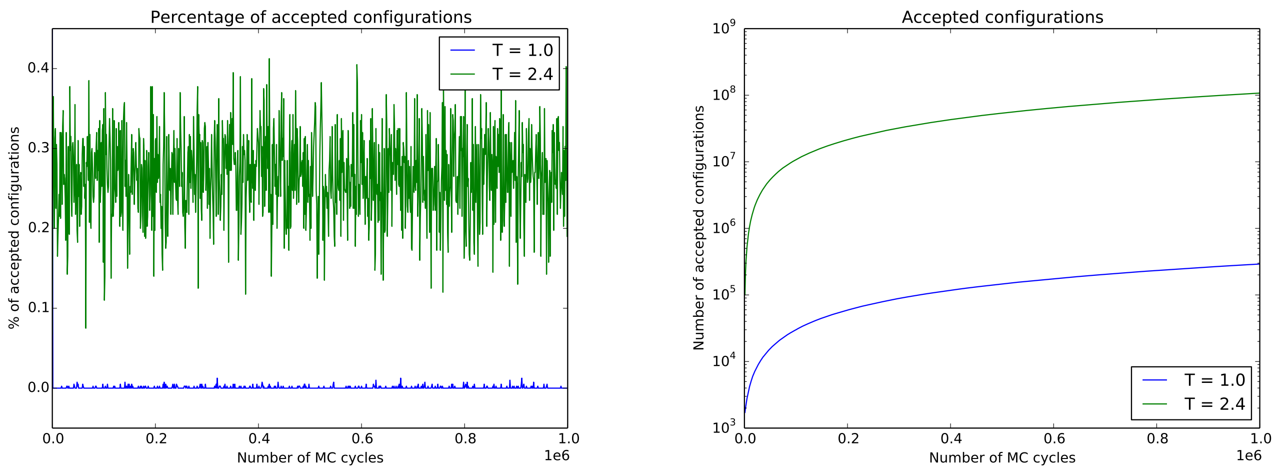


(a)



(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:

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

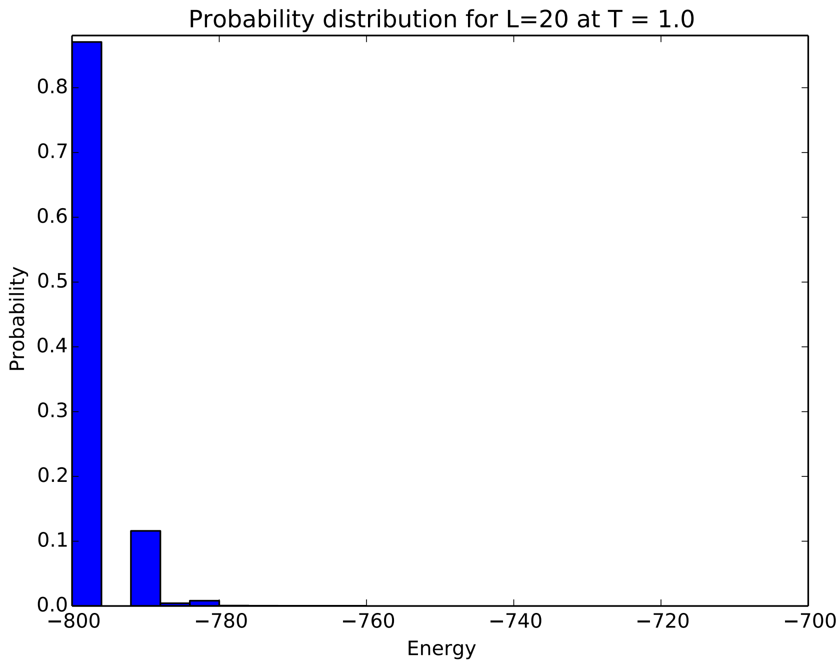


Figure 4.9

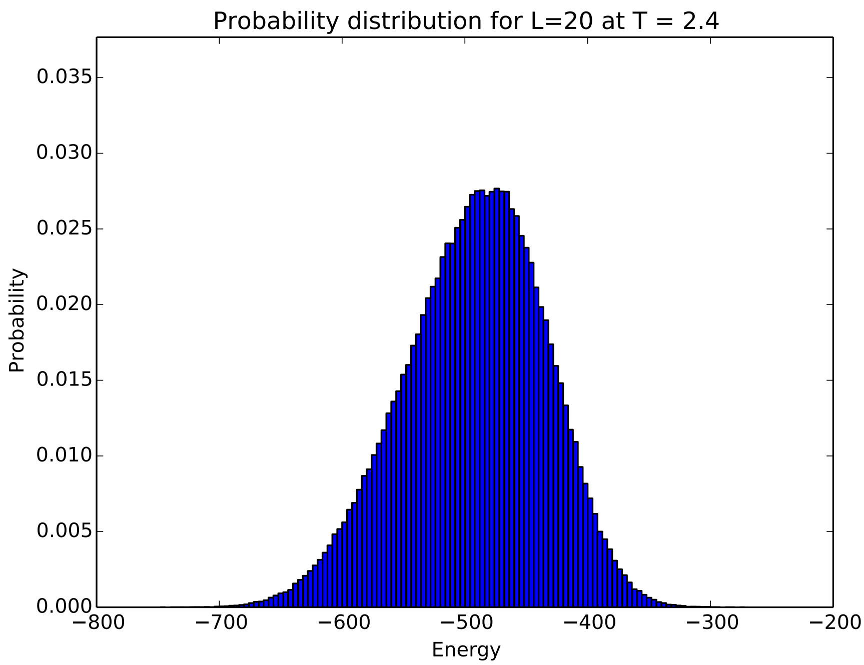


Figure 4.10

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

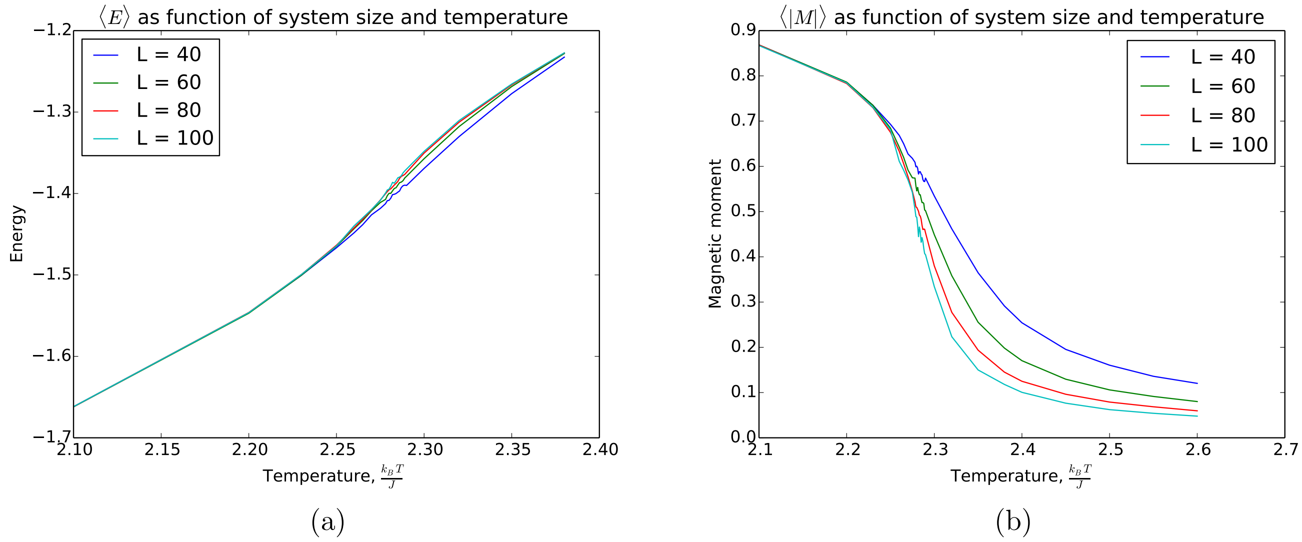


Figure 4.11

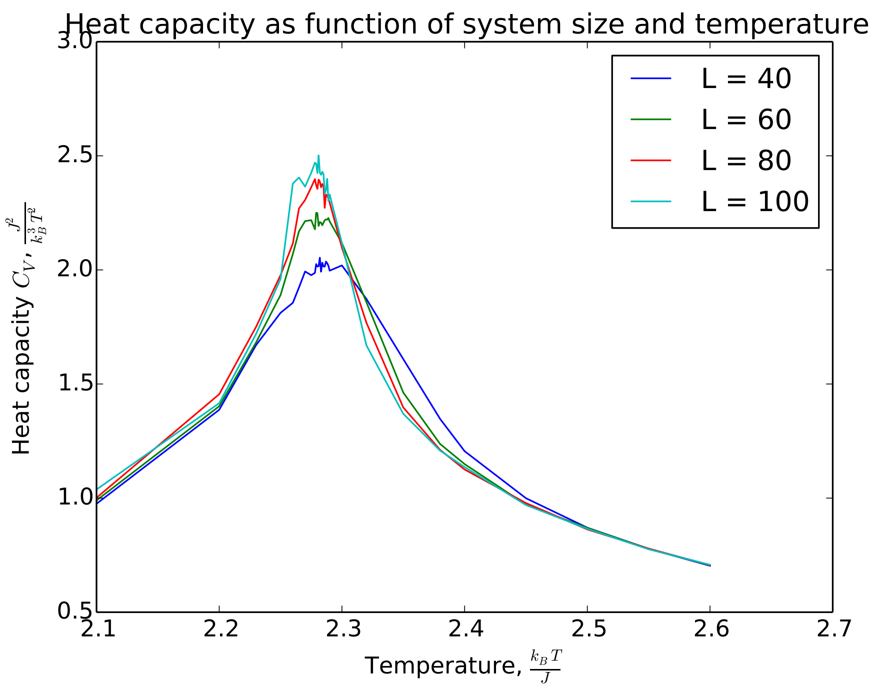


Figure 4.12

Table 4.3: L=80 and MC cycles is 1e6.

Number of processors:	CPU time [s]:
1	513.069
2	306.975

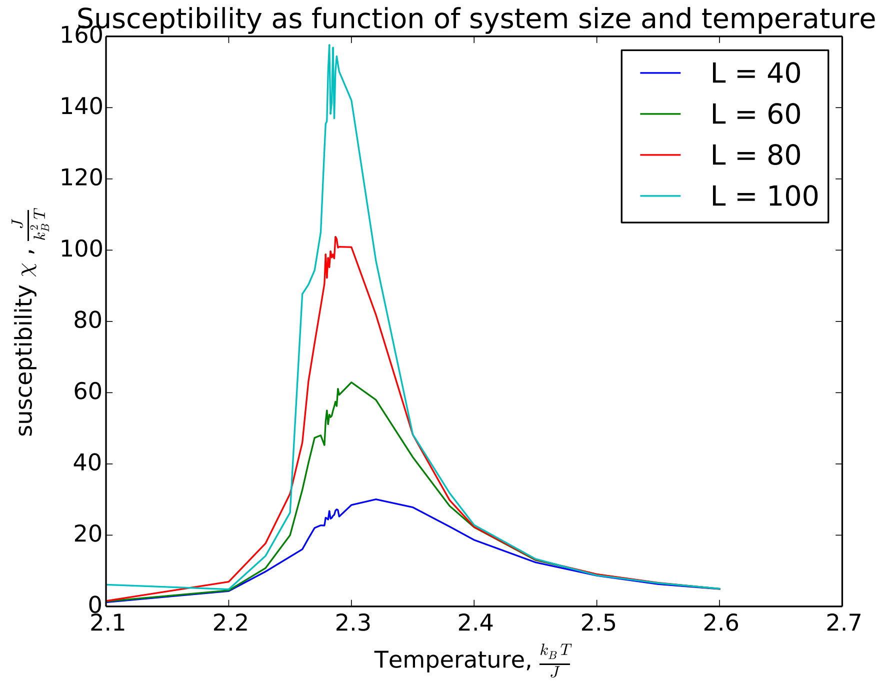


Figure 4.13

Table 4.2: text

L	T_C
40	2.28
60	2.28
80	2.28
100	2.28

Exact $T_C = kTC/J = 2/\ln\left(1+\sqrt{2}\right) \approx 2.269$ [2]

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.

[2] Lars Onsager. Crystal statistics. i. a two-dimensional model with an order-disorder transition. *Phys. Rev.*, 65:117–149, Feb 1944.

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