Project 4 FYS4150

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Abstract

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1 Introduction

2 Theory

2.1 Ising model

The two dimensional Ising model is a statistical model that allows us to investigate the temperature dependence of different properties of a magnet. The model consists of a two dimensional lattice of spins that can be in two different states, spin up, $\uparrow$, or spin down, $\downarrow$ [1]. In our system we do not have an applied field, $B_a = 0$.

The energy of our system is then:

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

where in our system $J > 0$, giving a ferromagnetic ordering, and s_k, $s_l = \pm 1$.

2.2 Introduction to statistics

The methods in this project require some statistics. Equation 2 shows the probability density and in the Ising model, the probability distribution is Boltzmann distribution (Equation 3) where Z is the partition function that normalizes the probability (Equation 4).

$$P(a \leq X \leq b) = \int_b^a p(x)\,dx \tag{2}$$

$$P_i(\beta) = \frac{e^{-\beta E_i}}{Z} \tag{3}$$

$$Z = \sum_{i=1}^{M} e^{-\beta E_i} \tag{4}$$

In this project we are looking at different properties of a magnet. That is energy, magnetic moment, heat capacity and susceptibility. To get out this data form our Ising model, we need some statistical terms. We will use Monte Carlo cycles and the Metropolis algorithm to calculate the first order moment (Equation 5), the mean value (Equation 6) of the energy and the magnetic moment.

$$\langle x^n \rangle = \int x^n\, p(x)\,dx \tag{5}$$

$$\langle x \rangle = \int x\, p(x)\,dx \tag{6}$$

The mean value of the energy is then:

$$\langle E \rangle = \int E\,p(E)\,dE = \int E \int_b^a \frac{e^{-\beta E_i}}{\sum_{i=1}^{M} e^{-\beta E_i}}\,dE_i\,dE$$

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

Boltzman

2.3 Magnetic properties

The energy of this system is found by Helmholtz free energy:

$$F = \langle E \rangle - TS = -kT \ln Z$$

$$\ln Z = -F/kT = -F\beta$$

$$\langle E\ \rangle = -\frac{\partial \ln Z}{\partial \beta}$$

Energy, magnetic moment, susceptibility, heat capacity.

derivative of F (with respect to T/external magnetic field): E, M

second derivative of F (_,,_): X, Cv

Second order phase transition. Correlation length diverges (spin correlation - they all "feel" each other? - they all change?) The spin gets more and more correlated as $T \to T_C$. Correlation length increases - second order - span the whole system.

The Ising model exhibits a second-order phase transition since the heat capacity diverges.

T< Tc : Spontanious magnetization - ferromagnetic

T > Tc : Net magnetication = zero - paramagnetic

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu} \tag{7}$$

Markhow chain - convergance

2.4 Our problem

Monte Carlo sampling function:

The probability of finding the state in state i:

$$P(E_i) = \frac{e^{-\beta E_i}}{Z}$$

To calculate Z we need to know the energy of all states:

$$Z = \sum_i^M e^{-\beta E_i}$$

We can do this for the small lattice where L=2.

2.5 Analytical solutions for L=2

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:

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

$$\langle M \rangle = 0$$

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

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

We can use these to calculate the rest:

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

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

3 Method

In this project we tried out many new concepts in our algorithm.

```
for(i =0; i<temperature.size();i++){
   T = temperature[i];
   for(MC = 1; MC < MCcycles.size(); MC++){
       for(i=0; i< L*L; i++){
           ix, iy = random(i);
           // with random spin generator
           Matrix(ix, iy) *= -1;
           dE = dEs[i];
           // dEs = vec({})
           MetropolisAlgorithm();
           // decide if the flip is accepted
           if(flip is accepted){
               Energy += dE;
               Magnetic += dM;
           }
      }
      //Add the new values to the sum of the
     values:
      mean_E += Energy;
      mean_E2 += Energy*Energy;
      mean_M += Magnetic;
      sum M\^2 += M\^2;
      sum |M| += |M|;
   }
//Before print, the values are divided by
    the number of Monte Carlo cycles to find
     the mean values.
}
```

3.1 Monte Carlo cycles

In Monte Carlo methods, the goal is to compute as many possible outcomes of the systems properties and find the mean value of them. By computing enough times, a steady state will be reached.

3.2 Metropolis algorithm

The metropolis algorithm is an algorithm that takes the system to the steady state. We want to find out what the real state of the system is when the outer parameters are what they are, for example temperature.

- Calculate total energy of initial lattice, E_{tot}

- Pick a random spin in the lattice

- Flip the spin

- Calculate the change in energy, ΔE (only five possibilities)

- If $\Delta E \leq 0$ - accept because we want to move to a state with the lowest energy

- If $\Delta E > 0$ - calculate $\omega = e^{-\beta \Delta E}$

- Compare ω with a random number r, if $r \leq \omega$ - accept new configuration

- Update mean values

- Repeat

Should show how to find the five ΔEs.

3.3 Random number generator

3.4 Parallelizing

3.5 Unit tests

Check the L=2 result with the analytical one - We did it visually

Make a small matrix (ordered initial), calculate energy - flip one spin, calculate energy - is the change in energy what we expect?

- Should have had it underveis - Kan neste gang lage tester som gjør at når vi implementerer nye ting som for eksempel classes eller paralelleisering, vet at det ikke har skjedd noe galt.

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:

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 Result

4.1 Matrix dimension L=2

OBS! Need an number of MC cycles necessary!

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

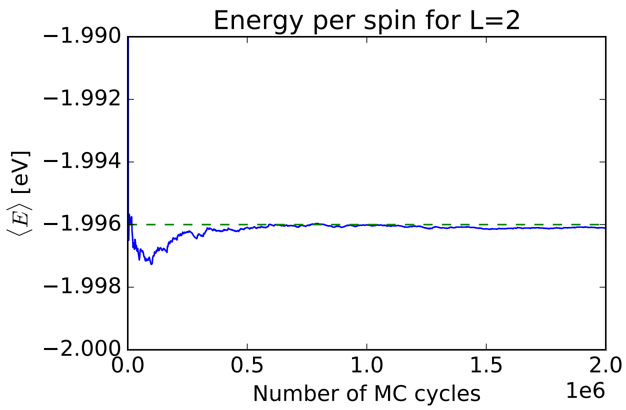

Figure 4.1: This is a plot of the expectation value of the energy per spin verus number of Monte Carlo cycles. The plot shows that we have a good agreement after $5 \cdot 10^5$ MC cycles.

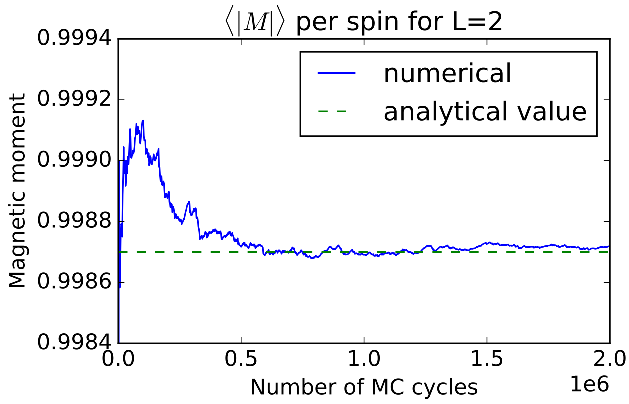

Figure 4.2: This is a plot of the expectation value of the mean absolute value of the magnetic moment per spin verus number of Monte Carlo cycles. The plot shows that we have a good agreement after $5 \cdot 10^5$ MC cycles.

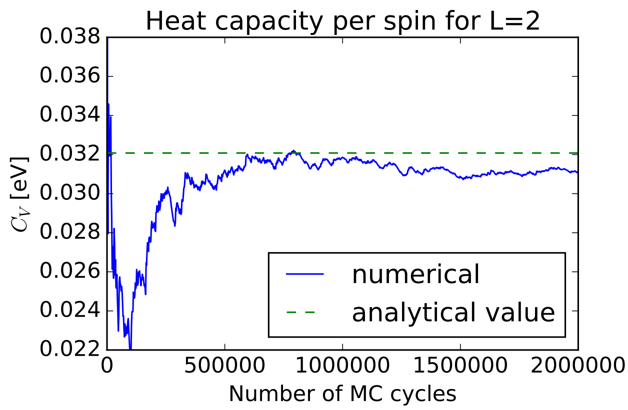

Figure 4.3: This is a plot of the heat capacity per spin verus number of Monte Carlo cycles. The plot shows that we have a good agreement after $5 \cdot 10^5$ MC cycles.

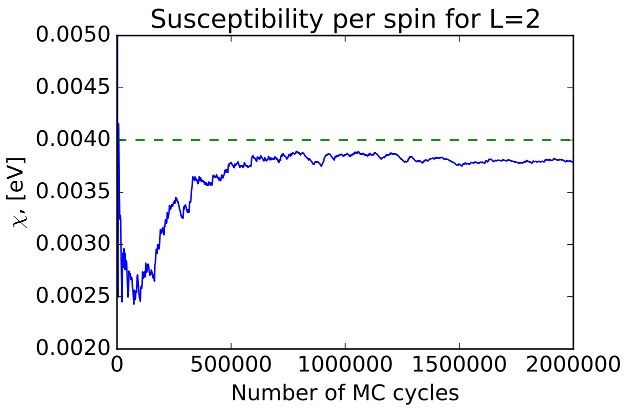

Figure 4.4: This is a plot of the susceptibility per spin verus number of Monte Carlo cycles. The plot shows that we have a good agreement after $5 \cdot 10^5$ MC cycles.

4.2 Matrix dimension L = 20

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 Different temperatures

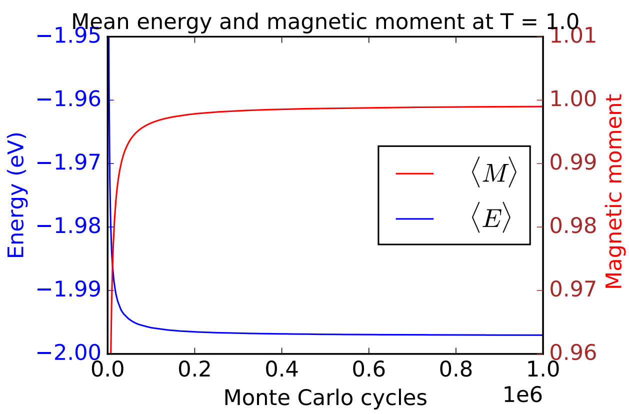

Figure 4.5: This is a plot of both the expectation value of the energy and absolute magnetic moment per spin verus number of Monte Carlo cycles at T = 1.0 K. The plot shows that an equilibrium is reached already at $2 \cdot 10^5$ MC cycles.

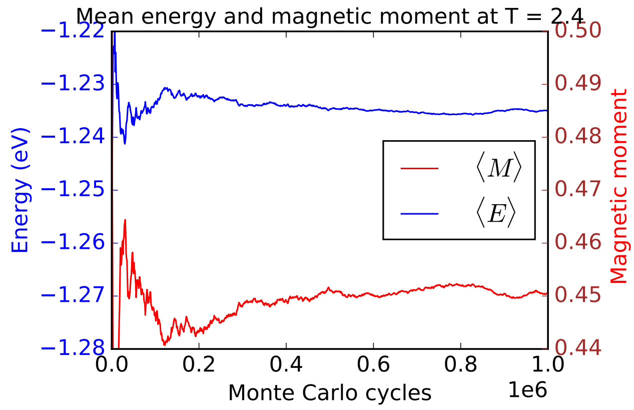

Figure 4.6: This is a plot of both the expectation value of the energy and absolute magnetic moment per spin verus number of Monte Carlo cycles at T = 2.4 K. The plot shows that an equilibrium is reached at around $5 \cdot 10^5$ MC cycles.

4.2.2 Initial state

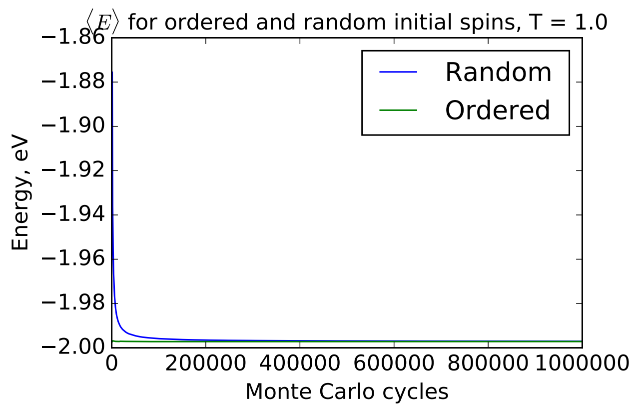

Figure 4.7: This is a plot of both the expectation value of the energy and absolute magnetic moment per spin verus number of Monte Carlo cycles at T = 1.0 K. The plot shows the difference in the behaviour of the ordered initial state and a random initial state.

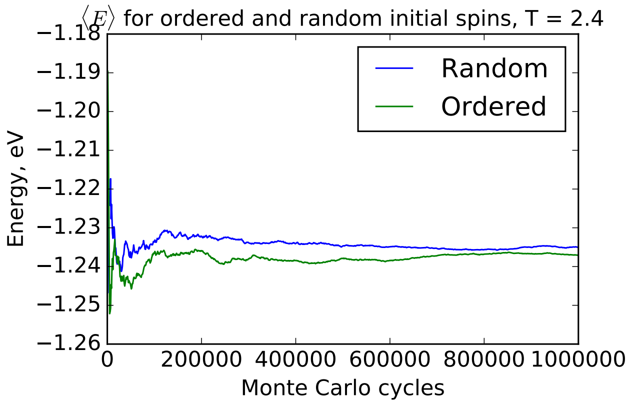

Figure 4.8: This is a plot of both the expectation value of the energy and absolute magnetic moment per spin verus number of Monte Carlo cycles at T = 2.4 K. The plot shows the difference in the behaviour of the ordered initial state and a random initial state.

4.2.3 Accepted configurations

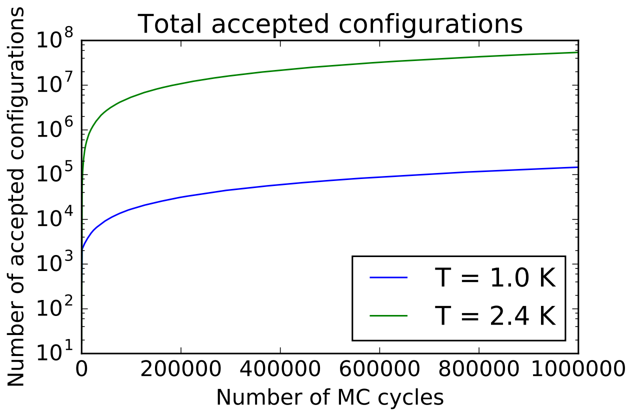

Figure 4.9: This is a plot of the total number of accepted configurations versus number of Monte Carlo cycles with random initial state.

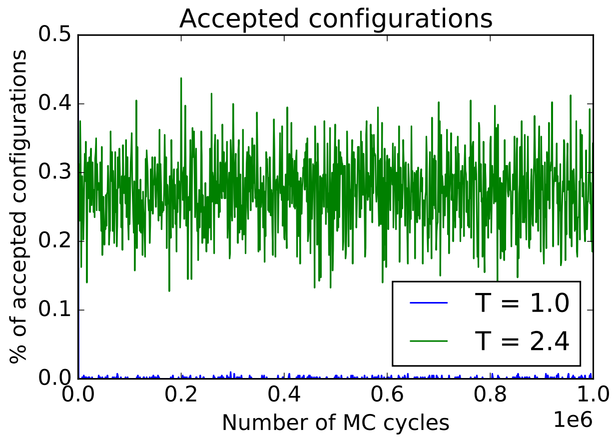

Figure 4.10: This is a plot of the percentage accepted of attempted configurations versus Monte Carlo cycles with random initial state.

4.3 Energy probability

OBS: Compare result with computed variance!

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

Computed variance (from same dataset?):

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

$$\text{FWHM} = 2\sqrt{2ln2}\sigma \approx 2.355\sigma$$

T = 1.0 K:

$$\sigma_E^2 = 638181 - (-798.855)^2 = 11.69$$

$$\sigma = 3.42$$

$$\text{FWHM} \approx 2.355 \cdot 3.24 = 7.63$$

T = 2.4 K:

$$\sigma_E^2 = 247886 - (-494.628)^2 = 3229.14$$

$$\sigma = 56.8$$

$$\text{FWHM} \approx 2.355 \cdot 56.8 = 133.76$$

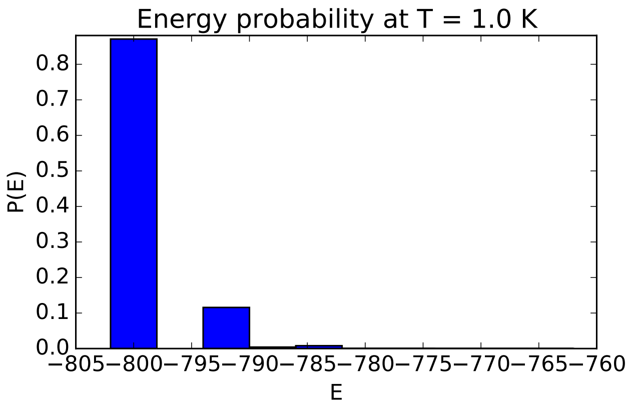

Figure 4.11: This is a plot of the energy probability when T = 1.0 K. The energy is the total energy of the 2D lattice with 20 × 20 spins.

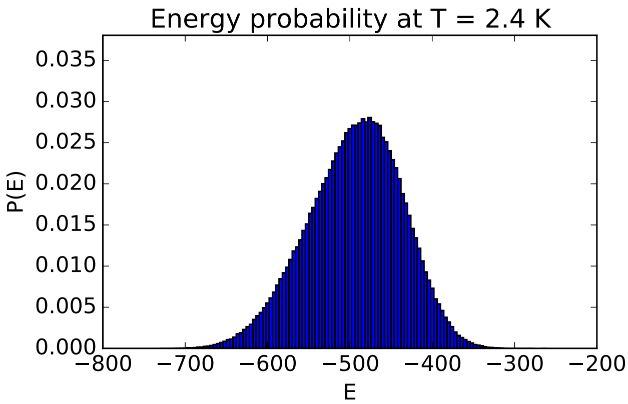

Figure 4.12: This is a plot of the energy probability when T = 2.4 K.The energy is the total energy of the 2D lattice with 20 × 20 spins.

4.4 Increasing dimensionality/ Critical temperature

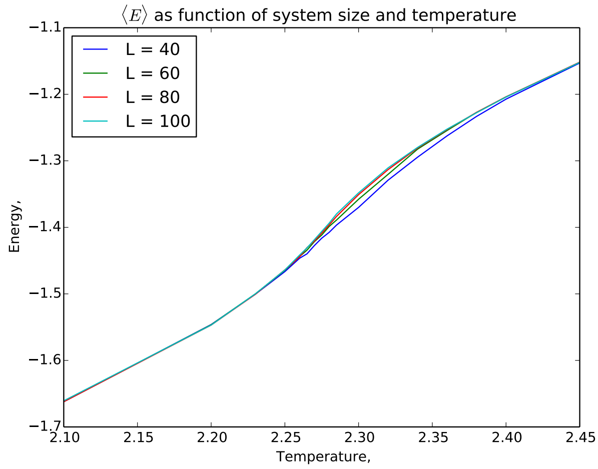

Figure 4.13: This is a plot if the energy versus temperature around the critical temperature for the different lattice sizes with L = 40, L = 60, L = 80 and L = 100.

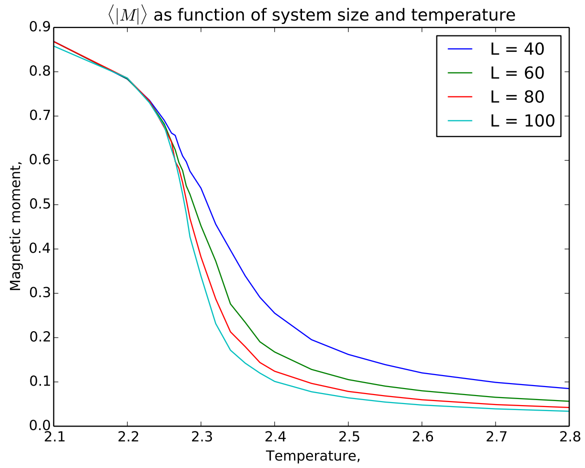

Figure 4.14: This is a plot if the absolute magnetic moment versus temperature around the critical temperature for the different lattice sizes with L = 40, L = 60, L = 80 and L = 100.

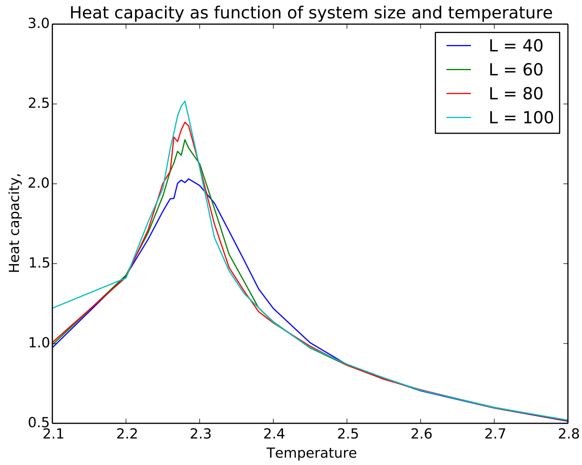

Figure 4.15: This is a plot if the heat capacity versus temperature around the critical temperature for the different lattice sizes with L = 40, L = 60, L = 80 and L = 100.

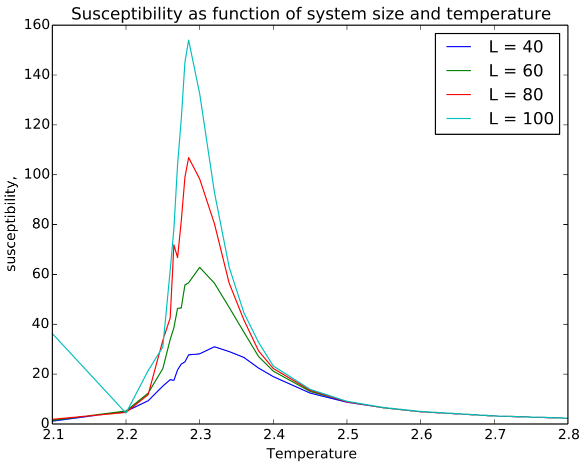

Figure 4.16: This is a plot if the susceptibility versus temperature around the critical temperature for the different lattice sizes with L = 40, L = 60, L = 80 and L = 100. The exact value is $T_C = kTC/J = 2/\ln(1+\sqrt{2}) \approx 2.269\,\mathrm{k_B\,K}$ [2].

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

OBS: Compare behaviour with equations?

OBS: Use Equation 7 to extract T_C.

Getting these equations from 7 where $\nu = 1$:

$$T_C(40) - T_C(\infty) = a \cdot 40^{-1}$$
$$T_C(60) - T_C(\infty) = a \cdot 60^{-1}$$
$$T_C(80) - T_C(\infty) = a \cdot 80^{-1}$$
$$T_C(100) - T_C(\infty) = a \cdot 100^{-1}$$

Table 4.2: L=60 and MC cycles is 1e6.

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

(Sett inn tall!)

$$T_C(\infty) = -a \cdot 40^{-1} + 2.28 \tag{8}$$
$$T_C(\infty) = -a \cdot 60^{-1} + 2.27 \tag{9}$$
$$T_C(\infty) = -a \cdot 80^{-1} + 2.28 \tag{10}$$
$$T_C(\infty) = -a \cdot 100^{-1} + 2.27 \tag{11}$$

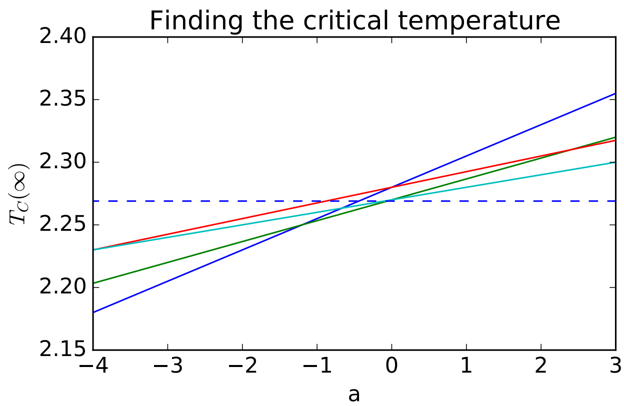

Figure 4.17: This is a plot of Equation 7 with different values of L (See Equations 8 - 11). The interssections represent the solution. They should have all had a cross section in the same place, and the y-value of the intersection would have been the critical temperature when $L \to \infty$.

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

5 Discussion

6 Conclusion

References

[1] Ising model. https://en.wikipedia.org/wiki/Ising_model. Accessed: 2017-11-17.

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

Appendix

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