UiO : Department of Physics
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# Studies of phase transitions in magnetic systems

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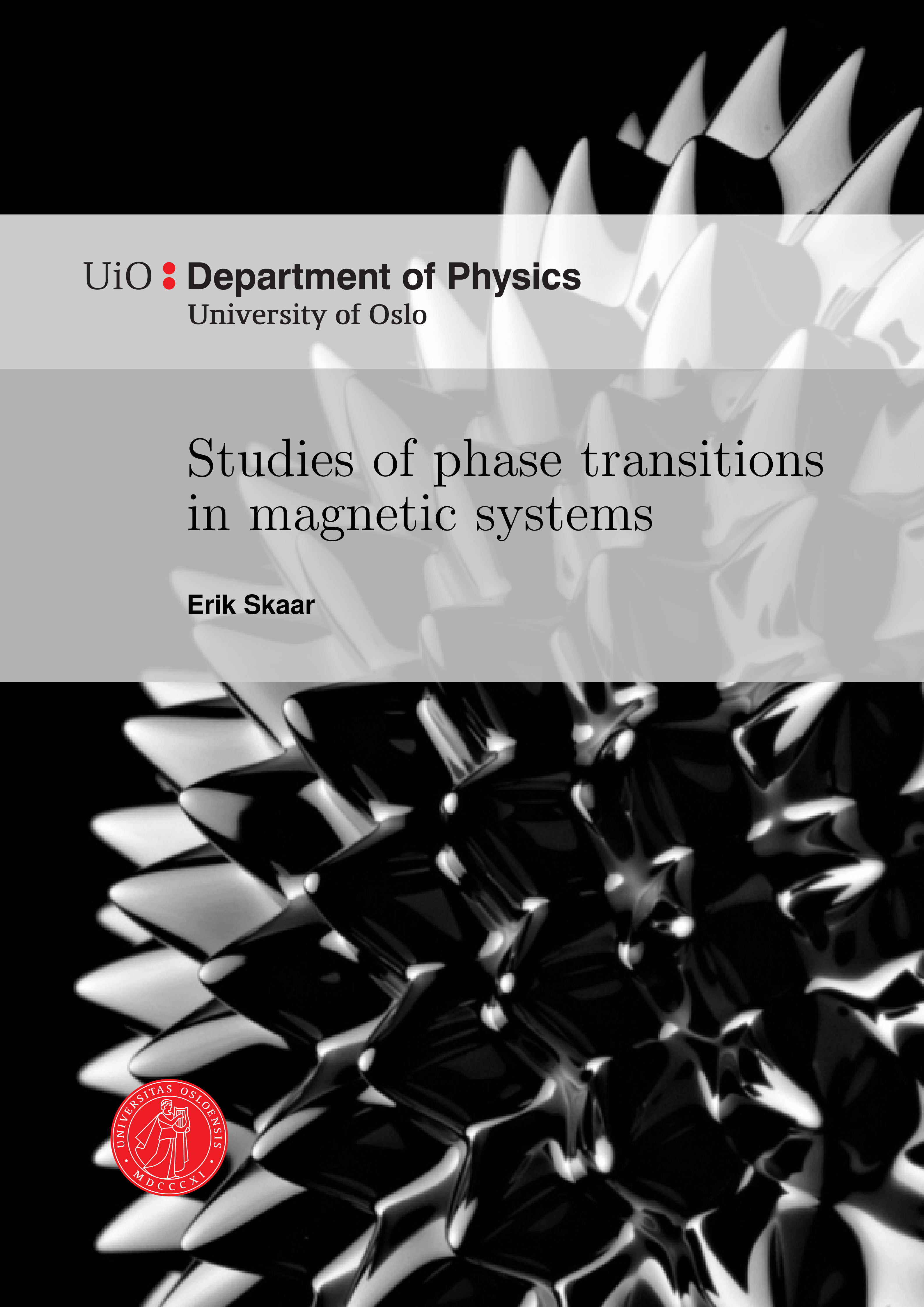


# Contents

## Abstract

# 1 Introduction

These laws are not enough to solve the motion of the planets. From the laws one can derive differential equations for the motion, which are not trivial or even possible to solve analytically. This is where computational methods are useful. With the tools developed in computtational physics we can make a prediction to the motion of the planets in our solar system.[1] And because of our assignment we kind of have to do this to pass the course.[2]

[1] Semester page for FYS3150 - Autumn 2017.

# 2 Theory

## 2.1 the Ising model

The Ising model describes a coupled system. Where only the nearest neighbor affect each other. In this report the Ising model will be applied to a two dimensional magnetic system. This will be a grid of spins, where each spin $s_i$ can either have 1 or 0 as value. The total energy is expressed as:

$$E = -\sum_{<i,j>} J_{i,j} s_i s_j$$

Where the symbol $<$ kl $>$ indicates that we sum over nearest neighbors only. If we assume that each coupling has the same magnitude J, then the energy is expressed as:

$$E = -J \sum_{<i,j>} s_i s_j \tag{1}$$

### 2.1.1 Periodic boundary conditions

When working with a finite matrix we run into a problem with the boundaries. They are missing neighbours. We solve this by introducing periodic boundary conditions. This means that the right neighbour for $S_n$ is assumed to take the value of $S_1$.

## 2.2 Statistical physics

### 2.2.1 the partition function

Boltzmann distribution is used as the probability distribution. Boltzmann distribution states the probability for $E_i$ is proportional to $e^{-\beta E_i}$ , where $\beta$ is $\frac{1}{k_B T}$. k is the Boltzmann constant. For this to be a probability distribution, it needs to be normalized. To normalize the distribution divide the sum of probabilities by a constant Z:

$$1 = \frac{\sum_i e^{-\beta E_i}}{Z}$$
$$Z = \sum_i e^{-\beta E_i}$$

Z is called the partition function.

### 2.2.2 Calculation of values

The partition function is very useful. In combination with the Boltzmann distribution we get a expression for the probability.

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

For finding a mean value, one can simply make a sum over $P(E_i)$ multiplied by the value of interest. For instance the mean energy is given by:

$$\langle E \rangle = \sum_i E_i P(E_i)$$

Expressions for important expectation values can be derived such for the energy E, magnetic moment |M|, specific heat capacity $C_v$ and the susceptibility $\chi$. The expressions used in this report are listed below[1]:[2]

$$\langle E \rangle = \sum_i E_i P(E_i) \tag{2}$$

$$\langle |M| \rangle = \sum_i M_i P(E_i) \tag{3}$$

$$\langle C_V \rangle = \frac{1}{kT^2} \left( \langle E^2 \rangle - \langle E \rangle^2 \right) \tag{4}$$

$$\langle \chi \rangle = \frac{1}{kT} \left( \langle M^2 \rangle - \langle |M| \rangle^2 \right) \tag{5}$$

### 2.3 Phase transition

The two dimensional Ising model is able to predict a phase transition in the material. At a critical temperature $T_C$ the quantities for the material will start to behave differently. For $C_V$ and for $\chi$ the phase transition is a sharp peak when plotted against Temperature. For $|M|$ and E it can be seen, but only as a slight change in value.

A second order phase transition is characterized by a correlation length. For finite lattice the correlation length is equal to the length of the system. $T_C$ can be obtain through scaling of the results from a finite system with a infinite system:

$$T_C(L) - T_C(L = \infty) = aL^{\frac{-1}{v}} \tag{6}$$

a is an unknown constant and v = 1. For finding a we use eq. 6 with two different L. Substract the expression with $L_i$ by the expression with $L_j$ and we get:

$$T_C(L_i) - T_C(L_j) = a \left( L_i^{\frac{-1}{v}} - L_j^{\frac{-1}{v}} \right)$$

$$a = \frac{T_C(L_i) - T_C(L_j)}{L_i^{\frac{-1}{v}} - L_j^{\frac{-1}{v}}} \tag{7}$$

We combine this with eq. 6 and we get an expression for $T_C(\infty)$:

$$T_C(L) - T_C(L = \infty) = aL^{\frac{-1}{v}}$$

$$T_C(L = \infty) = T_C(L) - \frac{T_C(L_i) - T_C(L_j)}{L_i^{\frac{-1}{v}} - L_j^{\frac{-1}{v}}} L^{\frac{-1}{v}} \tag{8}$$

[2]lecture note page 420

# 3 Method

## 3.1 Metropolis algorithm

The metropolis algorithm only has a few steps. First, pick one site in the matrix of spins. This process need to be random. For that site, calculate the energy difference if the spin is flipped. Then the algorithm decide whether to flip the spin or not. This is decided based on the energy difference. If the difference is negative flip, then flip the spin. If not, then pick a random number between 0 and 1 and if this number is less then $e^{-\beta\Delta E}$ flip the spin. Else keep the spin. Finally update expectation values.

REF

### 3.1.1 Precalculate

The energy difference is expressed as an exponential function. Exponential values are expensive to calculate. In two dimensions there is a finite number of energy differences. We can precalculated the exponentials. By calculating these in advance the program will run more efficient. It can be shown that the energy difference then is:

$$\Delta E = 2Js_j \sum_{<k>} s_k$$

## 3.2 Randomness

REF hvilk random generater bruk vi.

# 4 Result & Discussion

## 4.1 Analytic 2x2

### 4.1.1 Microstates 2x2

Table 1: This shows the different microstates that is possible for a 2x2 spinmatrix. It also states the energy and magnetic moment for each microstate.

| State | Energy | Magnetic moment | State | Energy | Magnetic moment |
|---|---|---|---|---|---|
| ↑ ↑<br>↑ ↑ | -8J | 4 | ↓ ↓<br>↓ ↓ | -8J | -4 |
| ↓ ↑<br>↑ ↑ | 0J | 2 | ↑ ↓<br>↓ ↓ | 0J | -2 |
| ↑ ↓<br>↑ ↑ | 0J | 2 | ↓ ↑<br>↓ ↓ | 0J | -2 |
| ↑ ↑<br>↓ ↑ | 0J | 2 | ↓ ↓<br>↑ ↓ | 0J | -2 |
| ↑ ↑<br>↑ ↓ | 0J | 2 | ↓ ↓<br>↓ ↑ | 0J | -2 |
| ↓ ↓<br>↑ ↑ | 0J | 0 | ↑ ↑<br>↓ ↓ | 0J | 0 |
| ↓ ↑<br>↓ ↑ | 0J | 0 | ↑ ↓<br>↑ ↓ | 0J | 0 |
| ↑ ↓<br>↓ ↑ | 8J | 0 | ↓ ↑<br>↑ ↓ | 8J | 0 |

Table 2: The table shows a summary from table 4.1.1.

| Number of ↑ | Multiplicity | Energy | Magnetic moment |
|---|---|---|---|
| 4 | 1 | -8J | 4 |
| 3 | 4 | 0J | 2 |
| 2 | 2 | 8J | 0 |
| 2 | 4 | 0J | 0 |
| 1 | 4 | 0J | -2 |
| 0 | 1 | -8J | -4 |

### 4.1.2 Quantities

We will use the equations from section 2.2.2.

For energy the eq. 2 will result in:

$$
\begin{aligned}
&Z = \sum_i = e^{-\beta E_i} \\
&\mathrm{T} = \mathrm{kT/J} = 1 \\
&Z = \sum_i = e^{-\beta E_i} = 2e^{8} + 2e^{-8} + 12
\end{aligned}
$$

For energy the eq. 2 will give the result:

$$
\begin{aligned}
&\langle E \rangle = \sum_i E_i P(E_i) \\
&\mathrm{T} = \mathrm{kT/J} = 1 \\
&\langle E \rangle = \frac{1}{Z} \sum_i E_i e^{-E_i} \\
&\langle E \rangle = \frac{1}{Z} \left( -16e^{8} + 16e^{-8} \right) = -7.9839 \\
&\langle E \rangle / N = \frac{\langle E \rangle}{4} = -1.9959
\end{aligned}
$$

For energy the eq. 3 will give the result:

$$
\begin{aligned}
&\langle |M| \rangle = \sum_i M_i P(E_i) \\
&\mathrm{T} = \mathrm{kT/J} = 1 \\
&\langle |M| \rangle = \frac{1}{Z} \sum_i M_i e^{-E_i} \\
&\langle |M| \rangle = \frac{1}{Z} \left( 4 \cdot 1e^{8} + 2 \cdot 4e^{0} + 0 \cdot 2e^{-8} + 0 \cdot 4e^{0} + 2 \cdot 4e^{0} + 4 \cdot 1e^{8} \right) \\
&\langle |M| \rangle = \frac{1}{Z} \left( 16 + 8e^{8} \right) = 3.9946 \\
&\langle |M| \rangle / N = \frac{\langle M \rangle}{4} = 0.9986
\end{aligned}
$$

For $C_V$ we need to calculate $\langle E^2 \rangle$:

$$\begin{aligned}
&\langle E^2 \rangle = \sum_i E_i P(E_i) \\
&\mathrm{T} = \mathrm{kT/J} = 1 \\
&\langle E^2 \rangle = \frac{1}{Z} \sum_i E_i^2 e^{-E_i} \\
&\langle E^2 \rangle = \frac{1}{Z} \left(128 e^8 + 128 e^{-8}\right) \\
&C_V = \langle E^2 \rangle - \langle E \rangle^2 = 0.12832 \\
&C_V/N = 0.03208
\end{aligned}$$

For $\chi$ we need to calculate $\langle M^2 \rangle$:

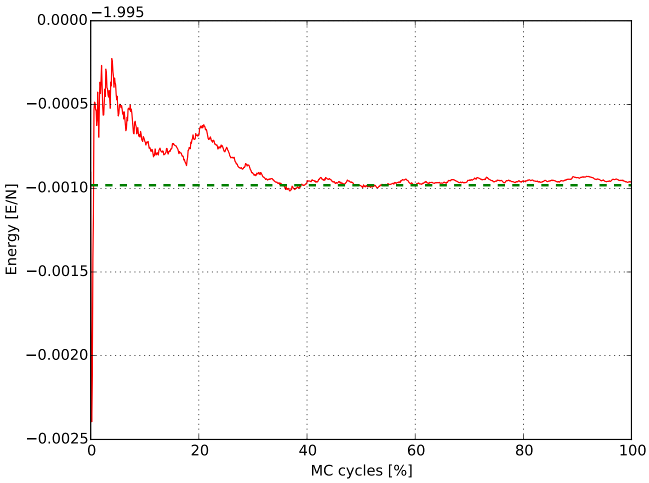
$$\begin{aligned}
&\langle M^2 \rangle = \sum_i M_i^2 P(E_i) \\
&\mathrm{T} = \mathrm{kT/J} = 1 \\
&\langle M^2 \rangle = \frac{1}{Z} \sum_i M_i^2 e^{-E_i} \\
&\langle M^2 \rangle = \frac{1}{Z} \left(16 \cdot 1e^8 + 4 \cdot 4e^0 + 0 \cdot 2e^{-8} + 0 \cdot 4e^0 + 4 \cdot 4e^0 + 16 \cdot 1e^8\right) \\
&\langle M^2 \rangle = \frac{1}{Z} \left(32 + 32e^8\right) = 15.9732 \\
&\langle \chi \rangle = 0.01604 \\
&\langle \chi \rangle / N = 0.004010
\end{aligned}$$

Below you can see a summary for the quantities:

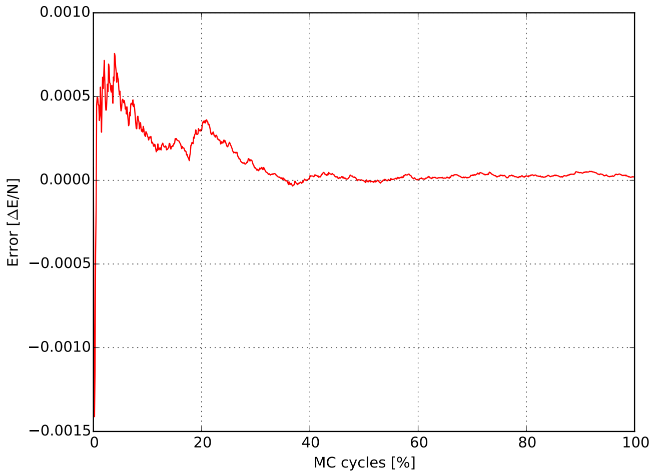
$$\begin{aligned}
\langle E \rangle / N &= -1.9959 & \qquad \langle |M| \rangle / N &= 0.9986 \\
C_V / N &= 0.03208 & \qquad \langle \chi \rangle / N &= 0.004010
\end{aligned}$$

## 4.2 Simulation 2x2

These simulations ran for $10^5$ monte carlo cycles. All the simulations were done at T=1 and for a 2x2 grid.

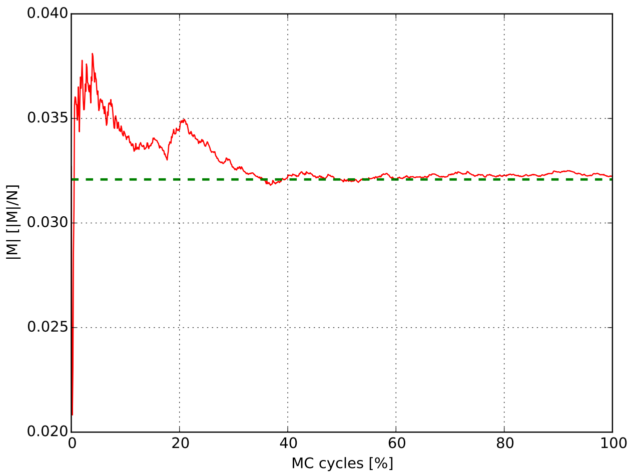



(a)

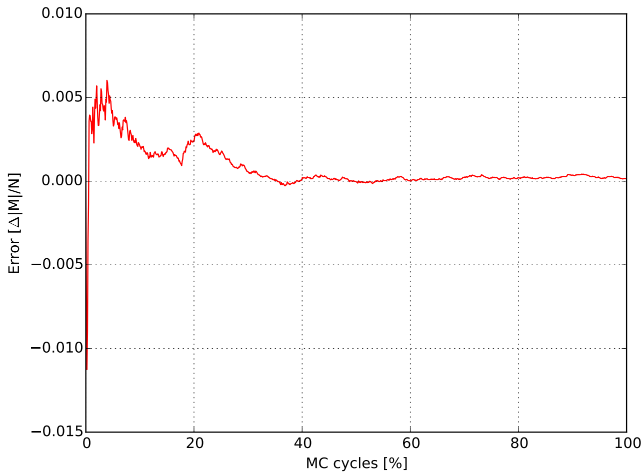



(b)

Figure 1: a)

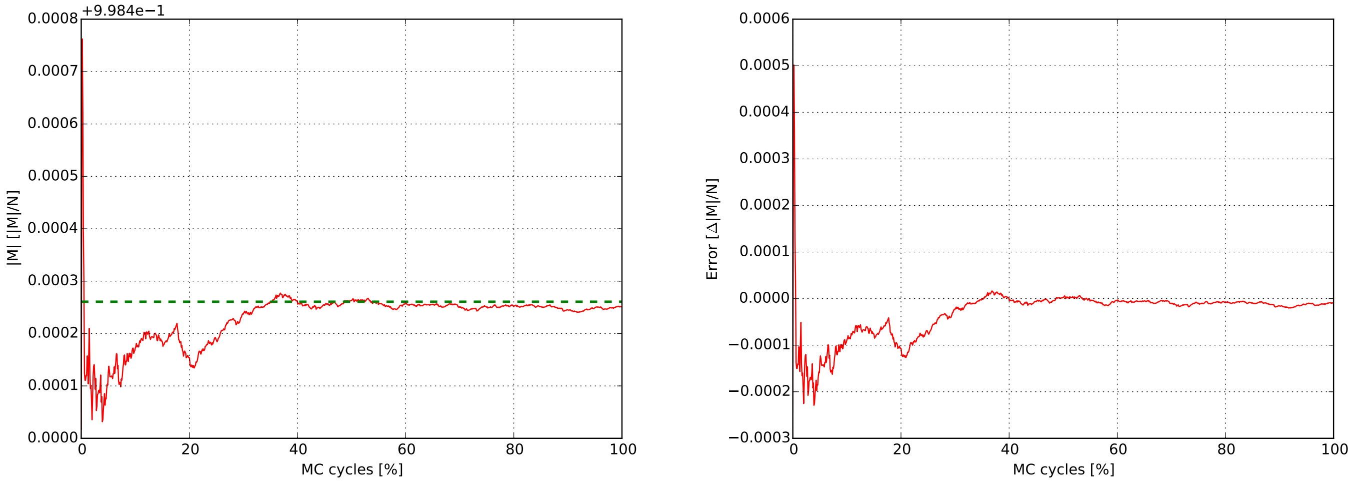



(a)



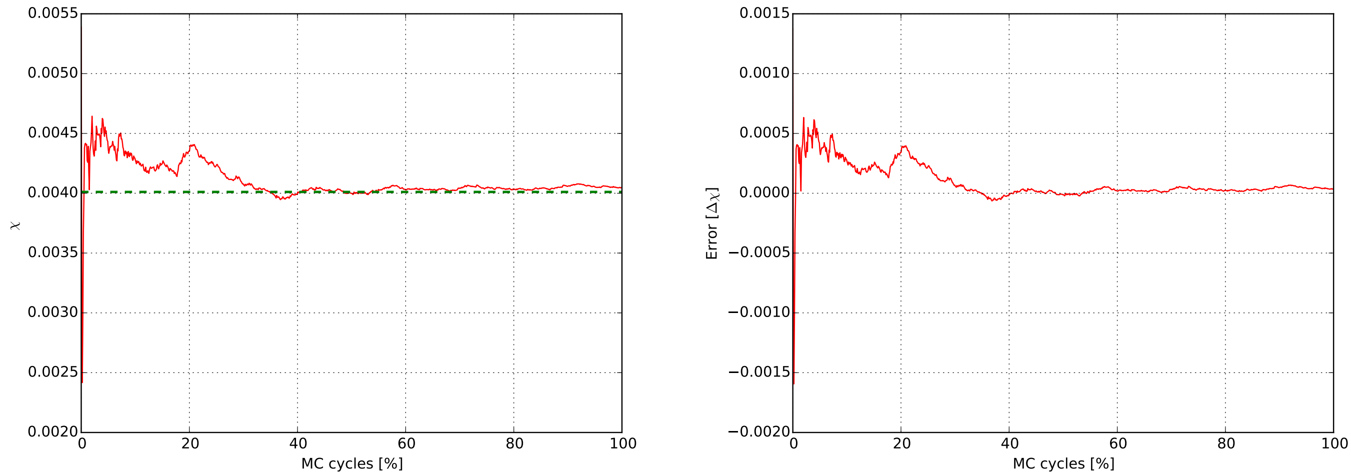

(b)

Figure 2: a)




(a) (b)

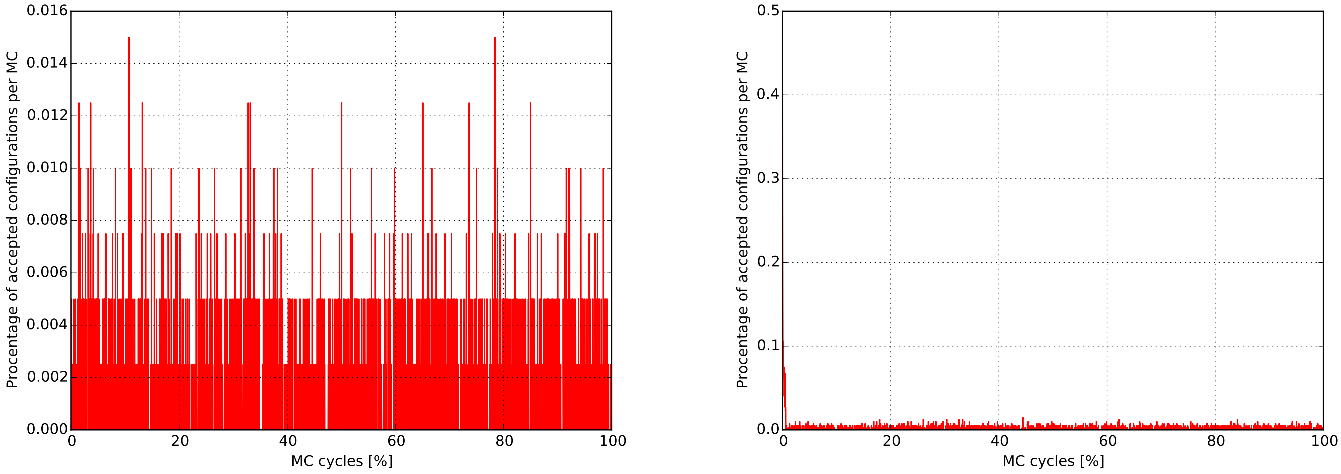
Figure 3: a)




(a) (b)

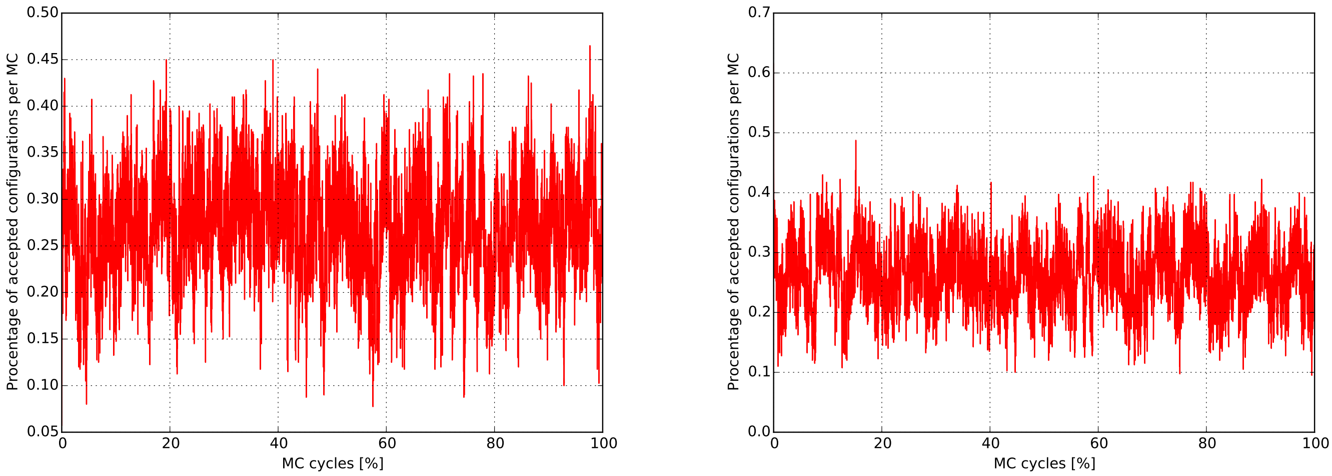
Figure 4: a)

### 4.3 Accepted configurations




(a) (b)

Figure 5: a)

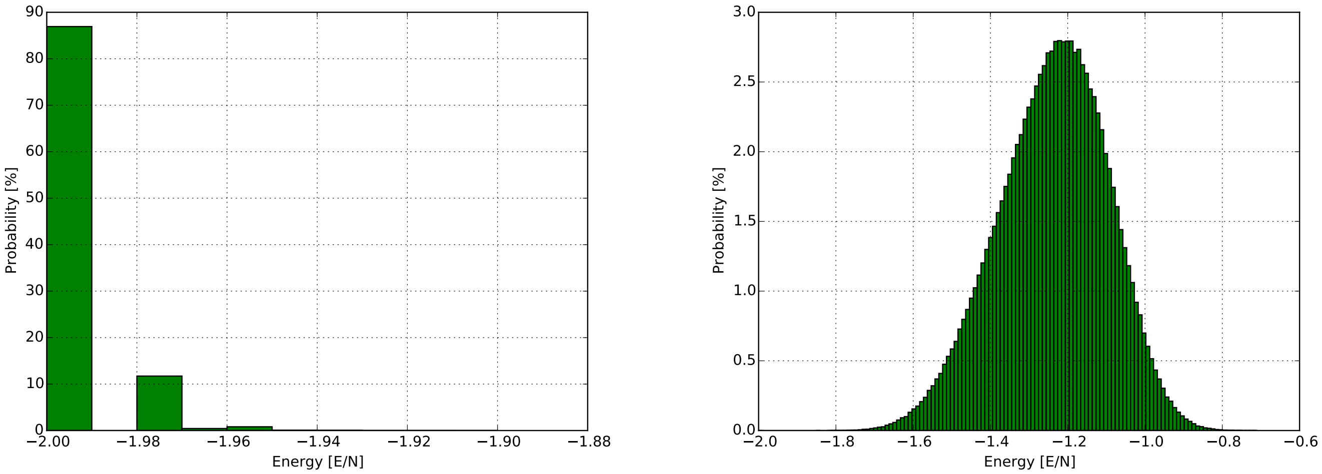



(a) (b)

Figure 6: a)

## 4.4 Probability distribution

Several simulations were made with different L. Below a selected few of these simulations are shown. All the data and figures for this section are available at my github. The figures below were created with a python script.



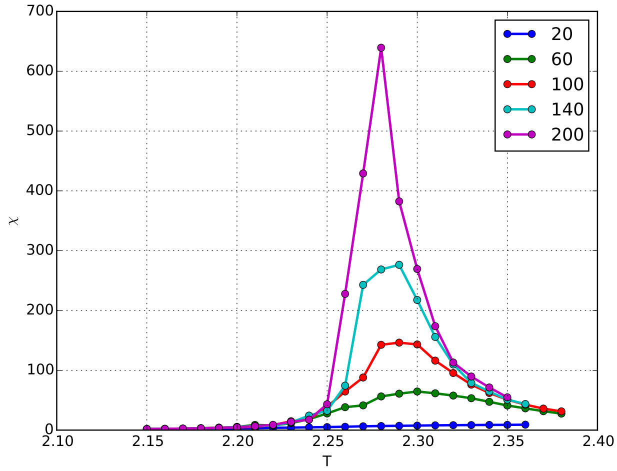

(a) (b)

Figure 7: a)

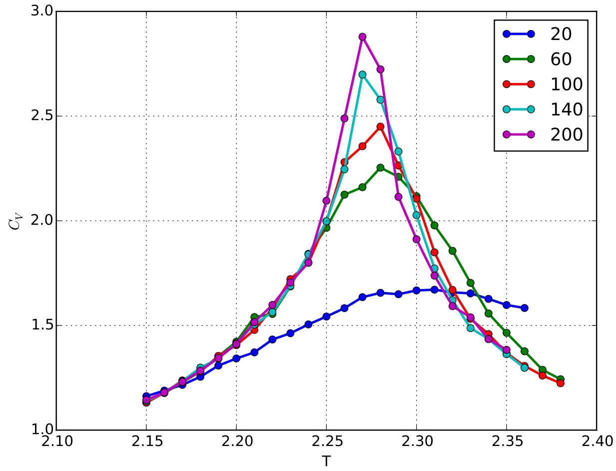
## 4.5 Phase transition

### 4.5.1 Numerical studies of phase transition

Several simulations were made with different L. Below a selected few of these simulations are shown. All the data and figures for this section are available at my github. The figures below were created with a python script.

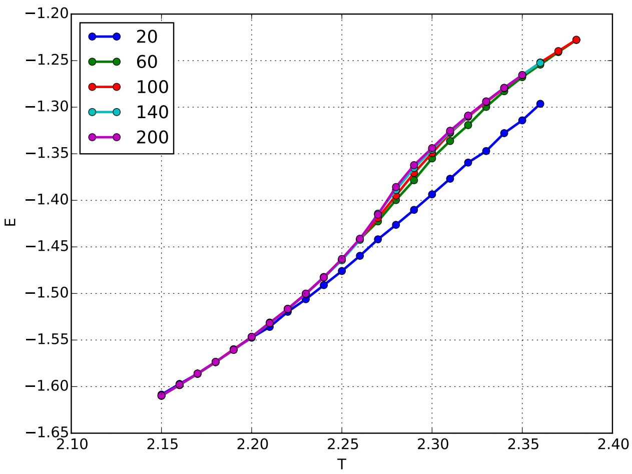



(a)

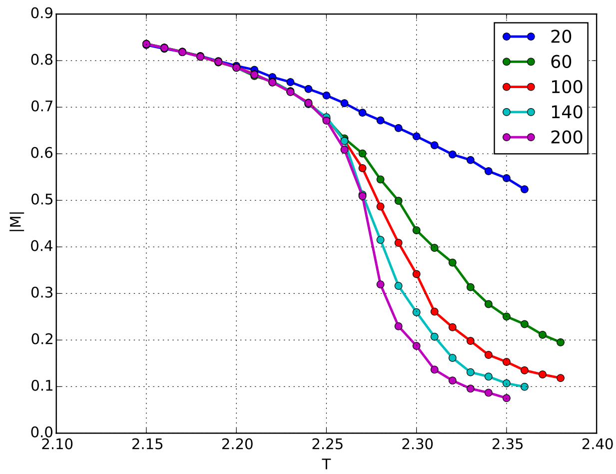



(b)

Figure 8: a)




(a)




(b)

Figure 9: a)

### 4.5.2 Extracting the critical temperature

$$T_C(L) - T_C(L = \infty) = aL^{\frac{-1}{v}}$$

$$T_C(L_i) - T_C(L_j) = a\left(L_i^{\frac{-1}{v}} - L_j^{\frac{-1}{v}}\right)$$
$$a = \frac{T_C(L_i) - T_C(L_j)}{L_i^{\frac{-1}{v}} - L_j^{\frac{-1}{v}}}$$

Table 3: The table shows how a differ for which $L_i$ and $L_j$ one uses. The values for $T_C$ were picked from figure 8 a)

| $L_i$ | $L_j$ | $T_{C_i}$ | $T_{C_j}$ | a |
|---|---|---|---|---|
| 60 | 100 | 2.30 | 2.29 | 0.00025 |
| 60 | 140 | 2.30 | 2.28 | 0.00025 |
| 60 | 200 | 2.30 | 2.27 | 0.0002142 |
| 100 | 140 | 2.29 | 2.28 | 0.00025 |
| 100 | 200 | 2.29 | 2.27 | 0.0002 |
| 140 | 200 | 2.28 | 2.27 | 0.0001666 |

From the values for a above, we can extract the average value of a. $\overline{a}$ turns out to be 0.0002218.

$$T_C(L) - T_C(L = \infty) = aL^{\frac{-1}{v}}$$
$$T_C(L = \infty) = T_C(L) - aL^{\frac{-1}{v}}$$

Table 4: The table shows how a differ for which $L_i$ and $L_j$ one uses. The values for $T_C$ were picked from figure 8 a)

| $L_i$ | $T_C(L_i)$ | $T_C(\infty)$ with $\overline{a}$ |
|---|---|---|
| 60 | 2.30 | 2.2999 |
| 100 | 2.29 | 2.2899 |
| 140 | 2.28 | 2.2799 |
| 200 | 2.27 | 2.2699 |

# 5 Conclusion

# 6 References

## References

[1] Morten Hjorth-Jensen. *Computational Physics*. Lecture notes. 2015. URL: https://github.com/CompPhysics/ComputationalPhysics/blob/master/doc/Lectures/lectures2015.pdf.

[2] Morten Hjorth-Jensen. *Computational Physics*. Project-4. 2017. URL: https://github.com/CompPhysics/ComputationalPhysics/blob/master/doc/Projects/2017/Project4/pdf/Project4.pdf.

# 7 Appendix

```
//FLOPs FOR POSITION :: EULER
// 2 FLOPs * 3 directions
x = x + t_step*Vx
//TOTAL FLOPs = 6 FLOPs
```