FYS-4150
Computational Physics
Project 4
Studies of phase transitions in magnetic systems

Fred Marcus John Silverberg

19 October 2018

Abstract

The aim of the project is to identify the critical temperature of a phase transition in a ferromagnetic material, as well as highlight the usefulness of statistical physics. The project will implement the metropolis algorithm and base the physics on the Ising model in 2D.

The projects model accurately agreed with the analytical values for $2 * 10^7$ Monte Carlo cycles. Equilibrium states for higher temperatures was building up past 10^4 cycles, allowing further investigation. The model subsequently succeed in highlighting the phase transition visually, as spikes of the specific heat capacity and magnetic susceptibility was observed. The extracted critical temperature of this phenomena was calculated to be 2.279 C, which differ by only 0.0044% from the analytical value.

Contents

1 Introduction

At a given temperature, a ferromagnetic material experience a phase transition where the magnetization dramatically drop to zero and consequently a strong reaction of the materials properties occur. This phenomena is to be investigated by implementing the idea of statistical physics, simply by averaging the effect of frequently occurring spin-flips. For this, the metropolis algorithm is to be used for simulating a phase change, and thereby highlighting the effects regarding properties such as, specific heat capacity and magnetic susceptibility. The main purpose is then to extract the critical temperature where this occur. Further, the project will give the reader an insight in how powerful a combination of numerical modelling and parallelized coding can be, for extracting such complicated information.

The Ising model, describing such electron-spin behaviour, was constructed by Ernst Ising, who found an analytical solution in 1D and later Lars Onsager extracted the solution in 2D, which allow us to calibrate our model in order to identify the critical temperature numerically.

2 Theory

2.1 Magnetization

A ferromagnetic material can align its spins such that magnetism occur. But at a certain temperature the internal energy rise and the spins vibrate in such a way that they begin to rotate, thereby breaking the alignment that produced the magnetism. Simply, a phase transition has occurred.

The material have some properties that allows us to study this phenomena:

Magnetic moment $[M]$
The magnetic moment of an object is the measurement of the objects tendency to align with a magnetic field. For an electron the magnetic moment is proportional to its spin.

Energy $[E]$
The potential energy of a material with magnetic moment.

Specific heat capacity $[Cv]$
The amount of heat needed to increase the temperature of one gram by one degree.

Magnetic susceptibility $[\chi]$
The susceptibility measure the strength of interaction by placing the material in a magnetic field.

The identification of a phase transition can be highlighted by the increase of energy, the dramatical drop in magnetization as well as highly fluctuating values of the specific heat capacity and the magnetic susceptibility.[2]

2.2 The Ising model

A model that allow us to describe the phase transition phenomena for ferromagnetic materials. In two dimensions the model configure a lattice of size LxL that represent N spins of either up $[+1]$ or down $[-1]$ values. The model limit is self to the nearest neighbour approach by applying periodic boundary condition. In detail this means that the spins on the edge of the lattice are neighbours with the represenatative spin on the other side. By this approach all spins have the same number of neighbours and the local geometry is intact over the lattice.[2]

By assuming absence of any other magnetic field, the energy can be written as:[1]

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

Where J is the coupling constant between the spins, [J=1].

Lattice example for $L = 2 \rightarrow N = LxL = 4$:
$\Uparrow \Uparrow$
$\Uparrow \Uparrow$: E=-8

2.3 Analytical solution for 2x2 lattice

For benchmarking our results the analytical expressions for the expectation energy, mean magnetization, specific heat capacity and the magnetic susceptibility will here be derived.[1]

For a canonical ensemble describing the mechanical system in thermal equilibrium, the temperature is an intensive variable and the energy follows an expectation value. Hence we need a probability distribution. Let us begin with the Boltzmann probability distribution:

$$P_i(\beta) = \frac{\exp^{-(\beta)E_i}}{Z} \tag{2}$$

So, by conclude that all probabilities summed are equal to 1:

$$\sum_{i=1}^{N} P_i(\beta) = 1 \qquad \rightarrow \qquad Z = \sum_{i=1}^{N} \exp^{-(\beta)E_i} \tag{3}$$

Where E is the energy of a certain micro-state and Z is the partition function for a canonical ensemble.

Inverse temperature is written as:

$$\beta = \frac{1}{K_b T} \tag{4}$$

Where K_b = Boltzmann constant, T = Temperature.

By defining the expectation energy, we can derive an expression for the square of expectation energy, the variance as well as the specific heat capacity.

Expectation value of energy:

$$< E >= K_b T^2 (\frac{\partial(ln(Z))}{\partial(T)}) \tag{5}$$

Take partial derivative and substitute with eq (2) gives:

$$< E >= \frac{1}{Z} \sum_{i=1}^{N} E_i \exp^{-(\beta)E_i} \tag{6}$$

Expectation value for square of energy:

$$< E^2 >= \frac{1}{Z} \sum_{i=1}^{N} E_i^2 \exp^{-(\beta)E_i} \tag{7}$$

Variance of energy:

$$\sigma_E^2 = (< E^2 > - < E >^2) = \frac{1}{Z} \sum_{i=1}^{N} E_i^2 \exp^{-(\beta)E_i} - (\frac{1}{Z} \sum_{i=1}^{N} E_i \exp^{-(\beta)E_i})^2 \tag{8}$$

Specific heat capacity:

$$C_v = \frac{\sigma_E^2}{K_b T^2} \tag{9}$$

Now, by following the same prescription for the magnetism as for the energy, we can find expressions for both the mean magnetization, its variance and the magnetic susceptibility.

Expectation value of magnetization:

$$< M >= \frac{1}{Z} \sum_{i=1}^{N} M_i \exp^{-(\beta)E_i} \tag{10}$$

Variance of magnetization:

$$\sigma_M^2 = (< M^2 > - < M >^2) = \frac{1}{Z} \sum_{i=1}^{N} M_i^2 \exp^{-(\beta)E_i} - (\frac{1}{Z} \sum_{i=1}^{N} M_i \exp^{-(\beta)E_i})^2 \tag{11}$$

Magnetic Susceptibility follows as:

$$\chi = \frac{\sigma_M^2}{K_b T} \tag{12}$$

For the analytical solution there are in total N^2 configurations. A $2x2$ lattice would then have $N^4 = 16$ configurations, however, not distinct.

Configuration examples:
⇑ ⇑ ⇑ ⇑ ⇑ ⇑
⇑ ⇑ : E=-8 ⇑ ⇓ : E=0 ⇓ ⇓ : E=+8

Possible states for a $2x2$ lattice structure is then:

Table 1: Possible configurations $2x2$ lattice

Number of spins up	Degeneracy	Energy	Magnetization
4	1	-8J	4
3	4	0J	2
2	4	0J	0
2	2	+8J	0
1	4	0J	-2
0	1	-8J	-4

From the possible energy states in table(1) there is the conclusion that for E = (-8), there is only two configurations of up and down spins, the same for E = (+8). And for E = (0) there is twelve possible configurations.

Equation (4) and the reasoning above allow us to find an analytical expression for the partition function as:

$$Z = 12exp^{0(\beta)J} + 2exp^{8(\beta)J} + 2exp^{-8(\beta)J} \tag{13}$$

Using the hyperbolic function cosh:

$$cosh(x) = \frac{exp^{x} - exp^{-x}}{2} \qquad \rightarrow \qquad Z = \frac{(cosh(8J(\beta)) + 3)}{4} \tag{14}$$

By equation (7,11) we find the expectation energy and mean magnetism $|M|$:

$$< E >= \frac{-2Jsinh(8J(\beta)}{Z} \qquad , \qquad < |M| >= \frac{0.5Jexp^{8J(\beta)} + 0.5}{Z} \tag{15}$$

By equation (9,12) we have the variances:

$$\sigma_E^2 = \frac{16J^2cosh(8J(\beta)}{Z} - < E >^2 \qquad , \qquad \sigma_M^2 = \frac{2exp^{(8J(\beta)} + 0.25}{Z} \tag{16}$$

These can be plugged into equation (10) for C_v and equation (13) for χ.

$$C_v = \frac{\sigma_E^2}{(\beta)T} \qquad , \qquad \chi = \frac{\sigma_M^2}{(\beta)} \tag{17}$$

2.4 The Metropolis algorithm for the Ising model

For calculating large sized lattices of the Ising model a numerical method is convenient. The Metropolis algorithm is here preferred, which is one form of the Monte Carlo algorithms.

First we have to decide how many iterations, or 'cycles', the algorithm will preform. For each cycle the algorithm flip one spin in the active lattice $< N = L^2 >$ times. A higher value of cycles will allow the system to converge against an equilibrium level. If the chosen cycles are to low, the expectation values will differ substantially from the analytical ones. The correct amount of cycles depends on the size of the lattice.

With an initial and evaluated configuration $[Lattice_0]$ the concept is to generate a new configuration $[Lattice_1]$ by flipping one of the spins. The difference in energy $[[E_1 - E_0] = \delta E]$ is then evaluated against the following acceptance condition:

$$A(Lattice_0 \rightarrow Lattice_1) = \begin{cases} \exp^{-\frac{\delta E}{T}}, & \text{if } \delta E > 0 \\ 1, & \text{otherwise} \end{cases}$$

Where, $exp^{-\frac{\delta E}{T}}$ is the Boltzman factor. So, simply if the new configuration has lower energy than the previous one, or if the probability is favourable, we accept the new configuration. Otherwise the iteration continuous with the old configuration. Before the above process is re-entered with either the old or new configuration, the expectation values of the situation are added. After the iteration, the average values are obtained by dividing with the number of cycles. Here is a pseudo code of the algorithm:[1]

```
Input: cycles, lattice, temperature
E = energy(lattice)
M = magnetism(lattice)
for i in range(cycles):
   for j in range(N):
      * New lattice by flipping a spin [i,j]
      * Delta energy
      * Boltzman factor
      if Delta energy < 0 or random_nr < Boltzman factor
         lattice[i,j] = -lattice[i,j]
         E += E
         M += M
   E_average /= cycles
   M_average /= cycles
Output: E_average, M_average
```

2.5 Finding the critical temperature

At this critical temperature ,T_c, the length scale, or size of a cluster of aligned spins, ξ, diverges. In detail that means that for high temperatures, the spins point randomly up or down. But for $T < T_c$ the size of these cluster begin to

grow in size. Since the fluctuation in magnetization diverges at this point, an exact calculation can never be made by a numerical method. However, Lars Onsager found the analytically by:[2]

$$T_c = \frac{2J}{log(1+\sqrt{2})} \tag{18}$$

This temperature can be obtained to a certain degree even with a finite lattice size. By mimic the behaviour at finite lattices with the result for a infinite lattice, the scaling is as:

$$T_c(L) - T_c(L=\infty) = \alpha L^{-\frac{1}{v}} \tag{19}$$

For $v = 1$ the above equation can be used to estimate the critical temperature by observing two finite lattices of size N and their indications of where T_c is. This approach allows us to find the constant α as:

$$\alpha(N_0, N_1) = \frac{T_{c0} - T_{c1}}{N_0^{-1} - N_1^{-1}} \tag{20}$$

The critical temperatures used above can be drawn from the maximum point of either the specific heat capacity or magnetic susceptibility, as functions of temperature.[2]

3 Code implementation

The calculations are to be made in python with large use of the library Numpy. Since the Metropolis algorithm is computational heavy, the library of multiprocessing are also to be used, which allow for parallel computations. In practice it will help us calculate a set of temperatures at the same time, by utilizing multiple threads in the processor.

```
Main file:
  * project_4.py
Classes:
  * None
Imported Files:
  * methods.py
    Holds all functions that are needed for the project.
  * parallelization.py
    Separate file for parallel computation for a set of temperatures.
  * plots.py
    Plot figures.
```

4 Results

4.1 Analytical comparison of values

Table 2: Analytical and numerical values

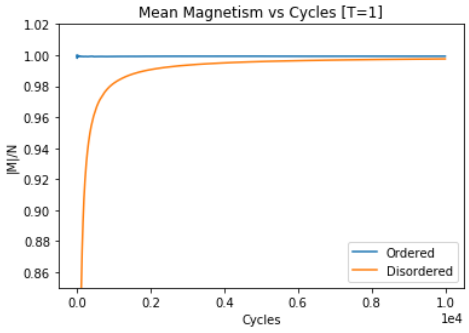
$< E/N >$	$< \|M\|/N >$	Cv/N	χ/N	$Cycles$
-2.00000	1.00000	0.00000	0.00000	$1 * 10^3$
-1.99640	0.99860	0.02874	0.00479	$1 * 10^4$
-1.99644	0.99887	0.02842	0.00321	$1 * 10^5$
-1.99613	0.99869	0.03086	0.00398	$1 * 10^6$
-1.99605	0.99868	0.03148	0.00395	$1 * 10^7$
-1.99595	0.99865	0.03231	0.00404	$2 * 10^7$
-1.99598	0.99832	0.03208	0.00401	Analytical

Table[2]: The results above where calculated for a 2x2 lattice with a random initial spins setting and with temperateure: [1 °C]. The analytical values corresponds well with the model:s numerical values. Especially for a cycle number of $2 * 10^7$.

4.2 Equilibrium state and accepted flips

Figure 1: Equilibrium mean magnetism

(a) T = 1.



(b) T = 2.4.

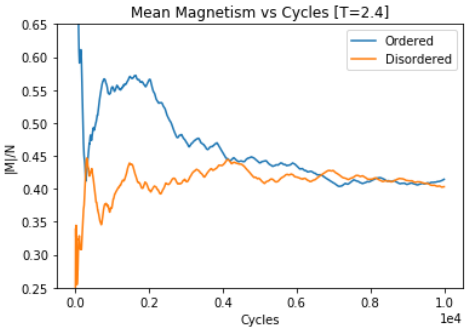
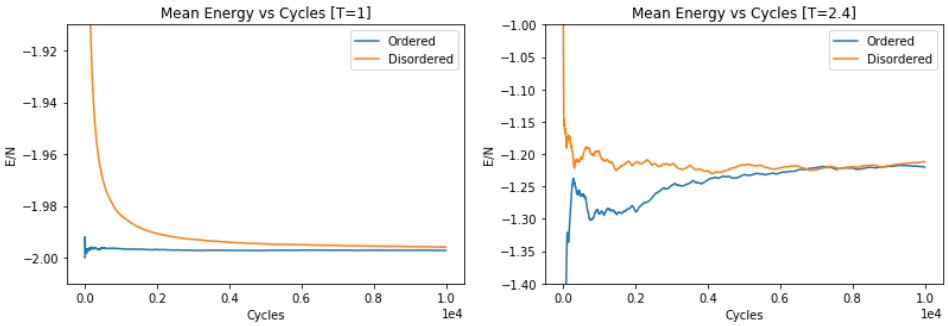


Figure 2: Equilibrium mean energy

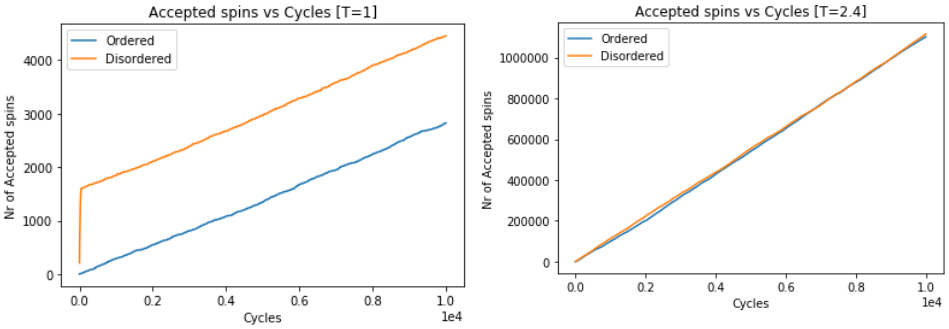
(a) T = 1. (b) T = 2.4.



Figure[1,2]: The results above where calculated for a 20x20 lattice and highlights the convergence of ordered and disordered lattices towards likely magnetization and energy values. Increasing temperature increases the variance as well.

Figure 3: Accepted flips vs cycles

(a) T = 1. (b) T = 2.4.

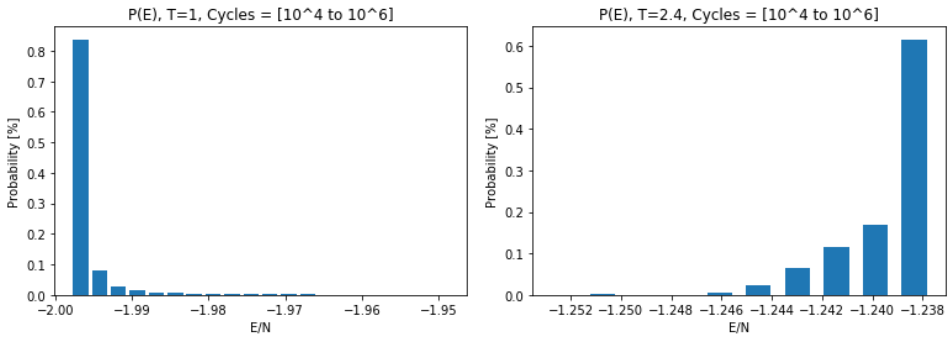


Figure[3]: The results are from a 20x20 lattice size. Notice how the disordered lattice accept substantially more configurations in the beginning. This is more visual for T = [1 °C], since the number of accepted flips escalates for T = [2.4 °C].

4.3 Analysing the probability distribution

Figure 4: Probability distributions [L = 20x20]

(a) T = 1. (b) T = 2.4.

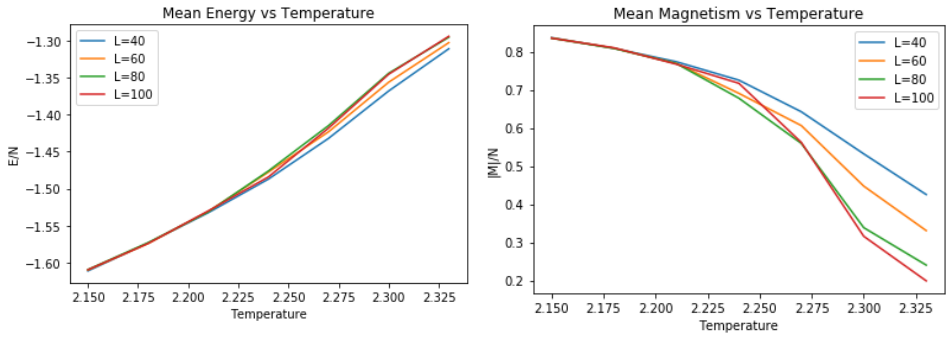


Figure[4]: The data indicate that with time a certain value is dominantly. The computed variance for T = [1 °C] was 29.77 and for T = [2.4 °C]: 3236, which highlights the effect of rising temperature in the beginning of the algorithms calculation, since above histograms correspond to variances in the order of $\sigma^2 < 10^{-4}$.[1]

4.4 Numerical studies of phase transitions

Figure 5: Phase transition interval for temperature

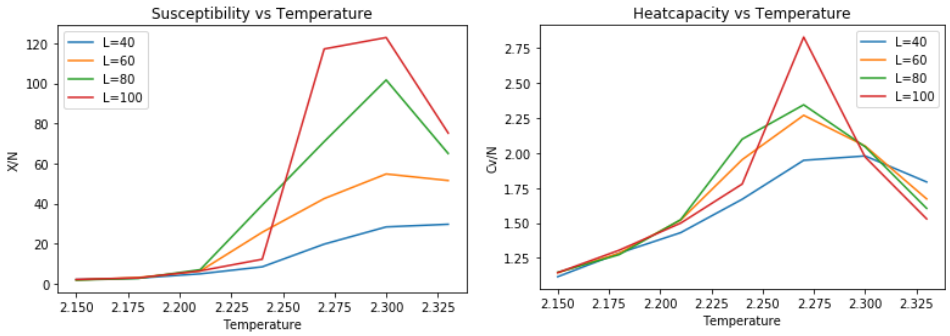
(a) Mean energy $< E >$ (b) Mean magnetisation $< |M| >$



[1] Calculated with numpy for $[10^4, 10^6]$ as $1.94*10^{-5}$ for $T = 1$ and $3.3*10^{-6}$ for $T = 2.4$

Figure 6: Phase transition interval for temperature

(a) Susceptibility χ (b) Specific heat capacity Cv



Figure[5,6]: The data was calculated with 10^5 cycles and a step-size of 0.03. The magnetism drasticly drops at the critical temperature and the energy rises, as expected. But most evident is the fluctuation in heat capacity and magnetic susceptibility, highly indicating the point of critical temperature.

4.5 Extracting the critical temperature

Table 3: Estimated critical temperatures

Extraction method	Critical temperature
By equation (20), f(χ)	2.2800 C
By equation (20), f(Cv)	2.2500 C
Average critical point, f(χ)	2.3075 C
Average critical point, f(Cv)	2.2775 C
Average critical temperature	2.2790 C

Table[3]: Even with a large step-size [0.03], the estimated temperatures are not far from the 2.269 C that Lars Onsager found. The values included in the calculations are drawn from the data in figure [6].

5 Discussion

The comparison of analytical versus numerical values for a small lattice gave encouraging feedback, table[2]. The project could progress with high confidence in the models ability to replicate the phenomena of a phase transition.

First an equilibrium point was to be found, for this kind of task it is perhaps to much to hope for. But for low temperatures the convergence narrows with time. And it seems that the oscillation around the true equilibrium value decrease in terms of amplitude for a higher temperature situation. This is at least good feedback that gives faith in the model, see figure[1,2]. So, after deciding upon a satisfied state of equilibrium, which was to be past 10^4 cycles, the probability distribution of the data could be obtained and illustrated in figure [4]. Here we find large contrasts which allow us to identify a probable energy value for both temperatures. Regarding the computed variances, they do no correspond to the histograms, the reason is that they include the high variance state in the beginning of the calculations, the data actually points to the case that T=2.4 yield a lower variance after the equilibrium state is reached and not T=1, as indicated by the total variances.

As the temperature rise, the number of new configurations that become accepted in the algorithm increases dramatically. It is expected as the energy in the system increase and a spin-flip simply become more likely. Note also the early effect of a disordered lattice, figure[3]. Both events contribute to an increase of the computational effort. The algorithm:s core is already computational heavy since it execute a double loop. This problem was partly eased by the use of parallelization, were seven temperatures were calculated at the same time and so increased the speed by a factor of 7, see appendix[1].

For identifying the phase transition , the figures [5] and [6] was constructed. A temperature interval was chosen with knowledge of Onsagers analytical value, 2.269. The hope of obtaining the dramatic drop in magnetization and highly fluctuating heat capacity was fulfilled. A phase shift can clearly be seen simply by looking at the graphs. And it is evident that a larger lattice is capable of approaching the true critical temperature. However, the analytical value is harder to extract by the eye, and after a few seconds a trained eye would recognize the weakness. The step-size can be argued as to high for such a precise determination, another range of temperatures with the same step-size would likely alter the results obtained in table [3].

6 Conclusion

The metropolis algorithm preformed as expected and could with impressive accuracy highlight and identify the phase transition for a ferromagnetic material. Visually the model clearly indicated where to expect a phase transition. A closer extraction of the critical temperature yielded an average estimation of 2.279. This number approach the analytical with increased lattice-size, increased number of cycles and decreased step-size.

The model required at least $2 * 10^7$ cycles in order to achieve close to identical values as the analytical, for a $2x2$ lattice. However, cycles above 10^4 was sufficient for the model:s ability to fulfil the purpose, even for larger lattices, as an equilibrium state was building up.

The number of accepted configurations increased with a factor of 250 between the temperatures $T = 1$ and $T = 2.4$. For the purpose of achieving results before the end of time, a parallelization of the code was highly efficient and increased the speed by a factor of 7, which was linear with the number of threads utilized.

Future investigation is recommended to focus on making the code more efficient, allowing the study of high resolution data close to the critical point. This may be implemented by focusing on another algorithm such that the Wolf algorithm, which aim at flipping multiple spins that are clustered, hence increasing the chance for acceptance.

7 Appendix

Table 4: Computational time [Cycles = 10^5]

Lattize size	Serial [min]	Parallel [min]
40x40	367	55
60x60	–	124
80x80	–	220
100x100	–	332

Table[4]: The times are from calculations of data in figure [5,6]. Due to the heavy time burden on serial calculations, only a lattice of 40x40 was tested. Note the efficiency increase of factor 7, which is linear with the number of threads utilized by the use of parallel computation.

Access to all material can be found at:
`https://github.com/silverberg89/FYS4150/blob/master/Project4/`

References

[1] Morten Hjorth-Jensen. 2018. Computational Physics Lectures: Statistical physics and the Ising Model. [ONLINE] Available at: http://compphysics.github.io/ComputationalPhysics/doc/pub/statphys/html/statphys.html. [Accessed 16 November 2018].

[2] Newman, M. and Barkema, G. (2011). Monte Carlo methods in statistical physics. Oxford: Clarendon Press, Chapter 1,3.