Computational physics
Ising Model

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1 Introduction

We will look at the Ising model using the Metropolis algorithm. The Ising model desciribes the magnetic properties of a solid body. The Metropolis algorithm is a special form of a Monte-Carlo simulation and helps us to reduce the needed computing time immensely. We will take an especially close look at the phase transition, where the system changes its magnetic properties from being magnetized to unmagnetized.
All of the used methods are described extensively in *Newman, M. & Barkema, G.; Monte Carlo Methods in Statistical Physics; Oxford University Press; 1999*

2 Ising model

The Ising model describes the magnetic properties of a solid object, by breaking it up in many small, elementary magnets. These magnets are the spins of some sub-system of the object and can point in two direction, associated with two possible spin values, $s_i = \pm 1$.
These spins are ordered in a lattice, this can be an N-d lattice, although it is usually assumed to be a 2-d one. We will only look at the 2-d lattice in the following sections. This model has been solved analytically for an infinitely large lattice, but numerically we typically assume a finite lattice of length L with periodic boundary conditions.
The energy of the system is described by the Hamiltonian

$$H = -J \sum_{\langle ij \rangle} s_i s_j - B \sum_i s_i, \tag{1}$$

where J is the coupling between spins, B an external magnetic field and $\langle ij \rangle$ denotes a sum over the nearest neighbors.
The probability to be in a state is given by the Boltzmann-distribution and depends on the temperature. Let us define $\beta = (k_B T)^{-1}$, where T is the temperature and k_B the Boltzmann-constant. Then the probability to be in a given state μ is

$$p_\mu = \frac{e^{-\beta H_\mu}}{\sum_\nu e^{-\beta H_\nu}}. \tag{2}$$

If the temperature is low, then β is very big and only the states with the lowest energy H will be populated, so all spins point in the same direction. Should the temperature be high instead,

then there will be a lot more states populated, and most of these will have the spins equally distributed. So the temperature of the system plays an important role.
To get the magnetization M from this lattice we simply have to add all the elementary magnets

$$M = \sum_i s_i, \tag{3}$$

$$m = \frac{M}{N}, \tag{4}$$

where $N = L^2$ is the number of magnets. So m is the average magnetization per lattice-site. This makes it easier to compare different lattice-sizes, since the results will all be about the same size.
One of the interesting properties of this model is the phase transition. At a specific temperature, the magnetization suddenly drops and some other quantities like the specific heat diverge. This transition can be analytically described for an infinitely large lattice and happens at the critical temperature $T_{crit} = 2.269J$.

The magnetic susceptibility χ is one of the quantities, that can be described with this model. It is defined by

$$\chi = \frac{\beta}{N}\mathrm{Var}(|m|). \tag{5}$$

Here $\mathrm{Var}(|m|)$ denotes the variance $\left\langle (|m| - \langle |m| \rangle)^2 \right\rangle$. For very low or high temperatures there is only a small range of magnetizations and energies available, so the variance and the susceptibility are quite small. But for temperatures around the phase transition there are a lot of possible states, between which the system can move, so the variance is quite big, as is the susceptibility.

Since we have a system, which is analytically described for an infinitely large lattice, we will have finite-size effects. These depend on the chosen lattice-size and will be looked at later. To make our results more scalable we will look at the finite-size scaling. This can be done by defining a new quantity ξ, which is an extension of the susceptibility χ, by

$$\xi(t) = \chi L^{-a/b}(L^{1/b}t), \tag{6}$$

where $t = (T - T_{crit})/T_{crit}$ and a, b are scaling parameters. For $a = 7/4$ and $b = 1$ this quantity ξ will be independent of the lattice size.

3 Numerical methods

To solve the Ising-model numerically we could simply Brute-force all possible states and use the probability of every state to calculate quantities like the mean $\langle m \rangle$. Since we have two possible spin-states for every lattice-site, there are 2^{L^2} possible states. So Brute-force would only work for very small lattices. Using the symmetry of the spins we can reduce our problem to only consider half the states, since the energy H is invariant to the transformation $s_i \to -s_i$, if there is no external field. There are a few more ways to reduce the number of states by realizing, that the system has some rotational invariances, but this does not reduce them sufficiently for a Brute-force method.
Because there are so many states, it makes more sense to randomly sample them. This procedure is called a Monte-Carlo-Simulation. The states get randomly sampled according to their

probability distribution, in this case according to the Boltzmann-distribution.
One of the most popular algorithms for the Ising-model is the Metropolis-algorithm. At every step we randomly choose a lattice-site and flip the spin. This changes the energy H. If the state before the flip is μ and the state after ν, then the probability to accept the flip is given by

$$P(\mu \to \nu) = \begin{cases} 1 & ,\text{for} H_\nu \leq H_\mu \\ e^{-\beta(H_\nu - H_\mu)} & ,\text{for} H_\nu > H_\mu \end{cases}. \tag{7}$$

If the flip is accepted we keep state ν and advance to the next step. If it is rejected, then we return to state μ and choose a new lattice-site.
This algorithm helps to sample all the possible states, but it also helps us to escape from a local minimum, by sometimes taking a step, that is worse in the short run, but may bring us closer to the global minimum.

Some of the quantities, that interest us are the magnetization m and the energy E. More precisely their mean and variance. They can be calculated by simply using their definition. But the autocorrelation function $\mathrm{Corr}(t)$ for the absolute value of the magnetization $|m|$ would need a lot of computing time. This can be reduced by using the Fourier-transformation (denoted by a $\hat{}$ over the quantity) and by using the definition $m'(t) = |m(t)| - \langle |m| \rangle$.

$$\hat{\mathrm{Corr}}(\omega) = \int dt\, e^{i\omega t} \mathrm{Corr}(t) \tag{8}$$

$$= \int dt\, e^{i\omega t} \int dt'\, m'(t') m'(t'+t) \tag{9}$$

$$= \int dt\, e^{i\omega t} \int dt'\, e^{-i\omega t'} e^{i\omega t'} m'(t') m'(t'+t) \tag{10}$$

$$= \int dt'\, e^{-i\omega t'} m'(t') \int dt\, e^{i\omega(t'+t)} m'(t'+t) \tag{11}$$

The second integral goes over all real numbers, and t' is just a constant offset, so we can change the integration variable to $\tau = t + t'$ and $d\tau = dt$.

$$= \int dt'\, e^{-i\omega t'} m'(t') \int d\tau\, e^{i\omega \tau} m'(\tau) \tag{12}$$

$$= \hat{m}'(-\omega) \hat{m}'(\omega) \tag{13}$$

But m' is a real function, so $\hat{m}'(-\omega) = \hat{m}'^{*}(\omega)$, where the * denotes the complex conjugate.

$$= \left| \hat{m}'(\omega) \right|^2 \tag{14}$$

So the Fourier transformed autocorrelation is the squared absolute value of the offset magnetization m'. Using FFT (Fast Fourier transform), we can calculate them quite fast. And then we simply have to use the inverse transformation to get the autocorrelation. This seems roundabout, but saves computing time in comparison to using the definition of $\mathrm{Corr}(t)$ directly.

After we found the variance, mean and autocorrelation we need a measure for the error. We can't use the standard-deviation (stdev) directly, because the the quantities depend on a lot of measurements, so the stdev of m is not the same as the stdev of $\langle m \rangle$.

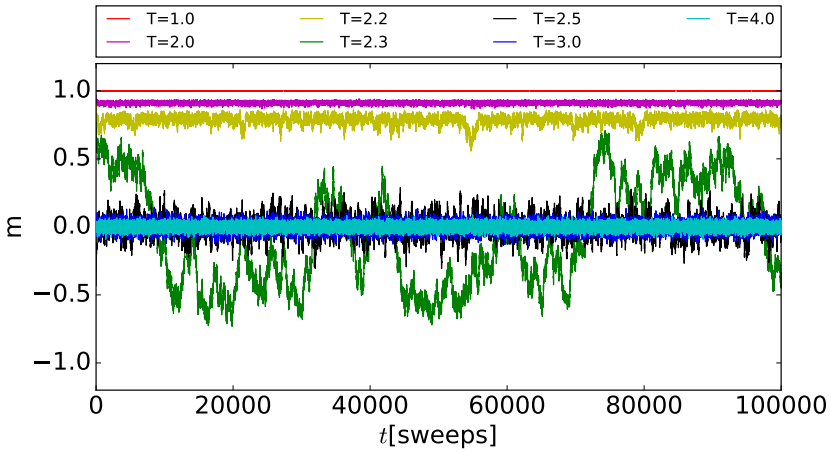


Figure 1: Time evolution for the magnetization m over time for different temperatures. The lattice length L was 100. The time is measured in sweeps, where one sweep equals L^2 steps.

We can use the bootstrap algorithm, to still get a good estimate of the error for complex quantities. First we need a quantity to look at, so let us take, for example, the susceptibility χ. To calculate it we have a dataset of a given length l. We resample this data in a new dataset of length l by randomly choosing a value of our original set. The value can be a duplicate of an element already in our new set. So in our new set we have a subset of our original data and use this to calculate the susceptibility χ. This process is repeated multiple times. Then the stdev σ of the susceptibility is given by

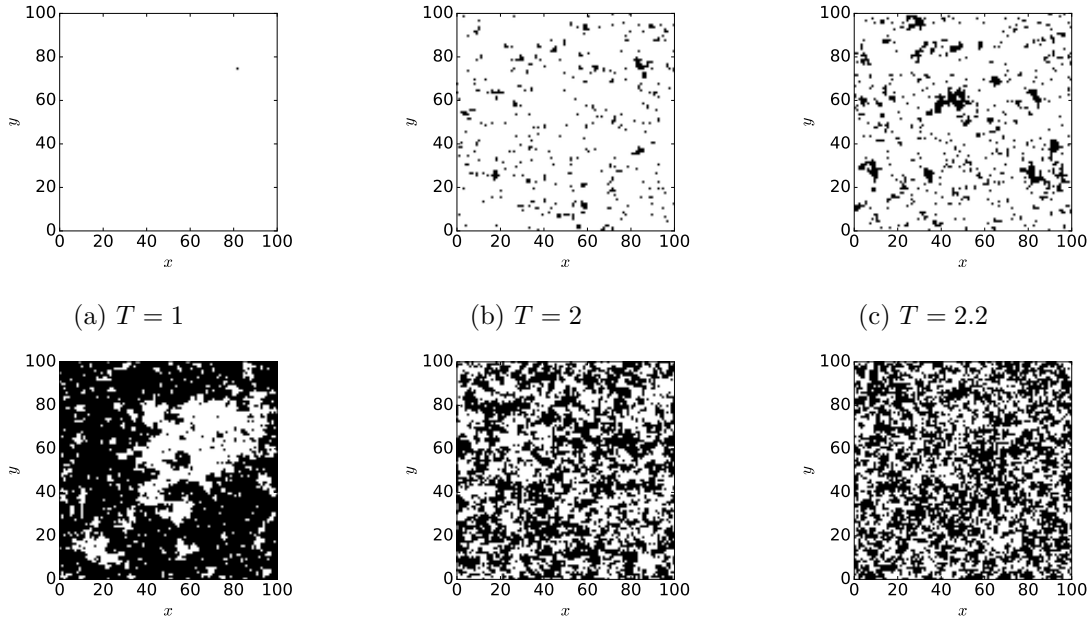
$$\sigma = \sqrt{\langle \chi^2 \rangle - \langle \chi \rangle^2}. \tag{15}$$

4 Results

For the following results we will always use that $J = k_B = 1$. A good, or lattice-size independent, timescale is a sweep. One sweep consists of L^2 steps. So for every lattice-site there is a flip. Some sites may not be chosen, but this does not concern us.

4.1 Time evolution

First of all we want to look at the evolution of the magnetization m over time and some snapshots. The time evolution for different temperatures is plotted in figure 1.
First of all we can see that the magnetization m drops with increasing temperature. We will be able to see this better in another plot. Aside from this, we see that the standard-deviation of the magnetization increases, when the temperature gets nearer to the critical temperature $T_{crit} = 2.269$. Especially for $T = 2.3$ the sign of the magnetization changes often, even though the mean is quite a lot bigger than 0.
The snapshots for some temperatures are plotted in figure 2. For low temperatures, e.g. 2a and 2b nearly all spins point in the same direction, so the magnetization is near 1.
Around the phase transition we find clusters of spins pointing in different directions. This can be seen especially well in figure 2d. And for high temperatures the spins are pointing randomly in different directions, so the magnetization tends to 0.



(a) $T = 1$ (b) $T = 2$ (c) $T = 2.2$

(d) $T = 2.3$ (e) $T = 3$ (f) $T = 4$

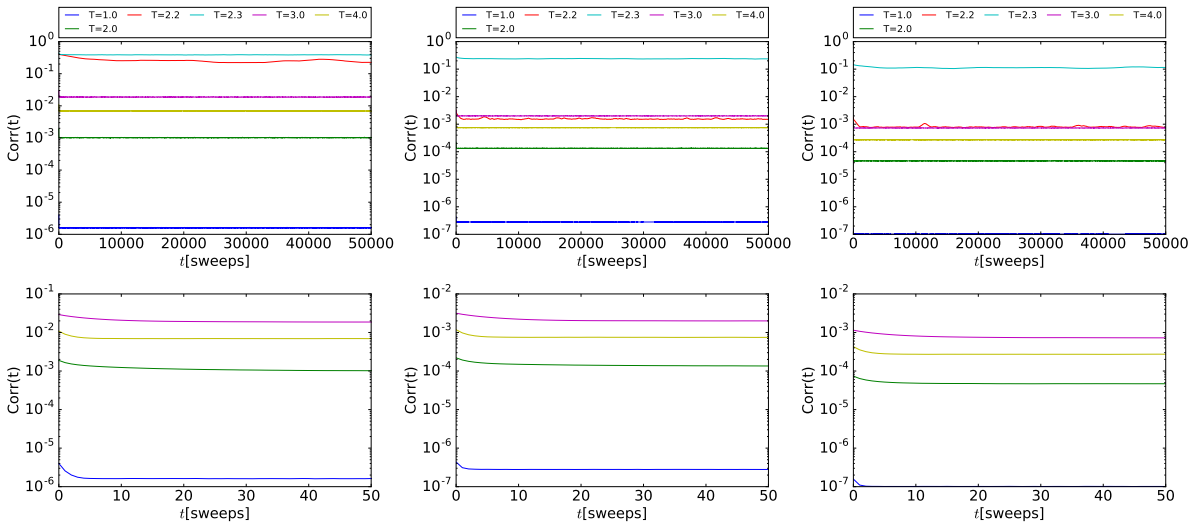
Figure 2: Snapshots of the spin states of a 100×100 lattice, for different temperatures T.

4.2 Autocorrelation

The autocorrelation function gives us an estimate for the correlation time τ, the time the system need to transition from one state to another, independent state. Generally the autocorrelation should fall of as $\text{Corr}(t) \sim e^{-t/\tau}$. So we could fit the data to find the exact correlation times. But for a qualitative observation about the system we can also look at the point, where the correlation gets constant.
The correlation is plotted in figure 3. Generally we can see that the correlation near the phase transition is the highest and also that it needs the longest time to get stationary.
For example in figure 3c the time to stationarity for $T = 2.3$ is in the order of 5000 sweeps, whereas for the temperatures $T = 1, 2, 3, 4$ it only takes about 10 to 20 sweeps. The time difference is significant. For $T = 2.2$ we have a time to stationarity of about 1000 sweeps. So even though $T = 2.3$ is just slightly closer to the phase transition it still needs 5 times as long. All these results are only qualitative, but the general idea also translates to the quantitative results. The closer we are to the phase transition, the longer our correlation time will be.

4.3 Mean

The phase transition of the Ising model happens at the temperature $T_{crit} = 2.269$ and is characterized by the sudden drop of full magnetization to no magnetization. This temperature can be analytically calculated for an infinite lattice. We will find a different temperature, since we only have a finite one.
The mean $\langle |m| \rangle$ is plotted in figure 4. Here we can observe different things. For one, we can see that we approximate the sudden drop better, if we use a bigger lattice. For $L = 20$ we can see a smooth transition and the system retains some magnetization. For $L = 100$ on the other hand we can see a relatively sharp drop and a weaker magnetization.



(a) $L = 20$ (b) $L = 60$ (c) $L = 100$

Figure 3: Autocorrelation of the magnetization $\mathrm{Corr}(t)$ for different lattice-sizes and temperatures. The time is measured in sweeps, where one sweep equals L^2 steps.

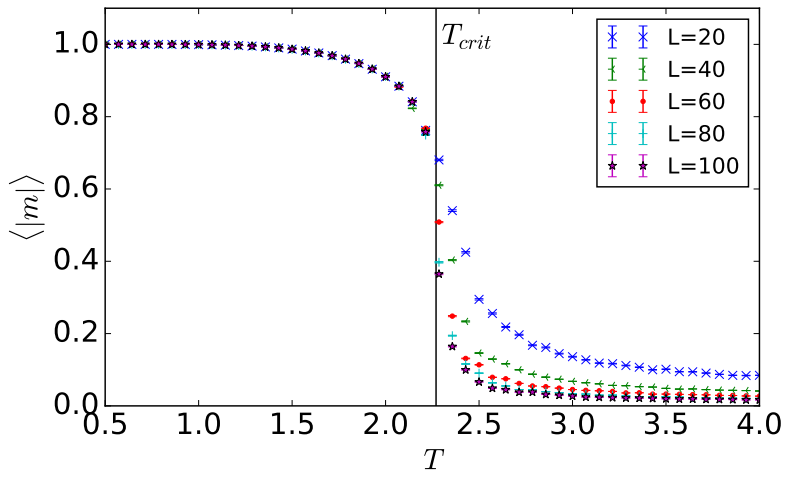


Figure 4: Mean $\langle |m| \rangle$ of the absolute value of the magnetization for different temperatures T and lattice-length L. The error of every measurement has been calculated using the bootstrap algorithm for an initial dataset of 10000 sweeps.

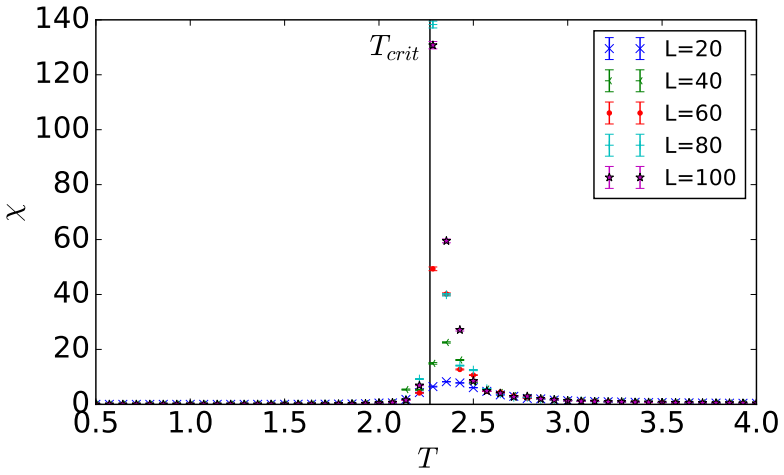


Figure 5: Susceptibility χ for different temperatures T and lattice-length L. The error of every measurement has been calculated using the bootstrap algorithm for an initial dataset of 10000 sweeps.

Because of these smooth drops there are different transition temperatures for the lattices. The smaller the lattice, the bigger the transition temperature.

What is also interesting to note is the error on the measurements. It is quite small everywhere, except at the phase transition. This could have two different origins. For one it could come from the long correlation time around the phase transition. If we take the same amount of time to average over we will have less independent states and thus a smaller sample size.
But it could also be a result of the strong fluctuations around the transition, that we have seen in figure 1.

4.4 Susceptibility

The susceptibility χ is proportional to the variance of the magnetization $|m|$ (see (5)). So using figure 4, we can assume that the susceptibility is biggest near the phase transition, if we assume the variance to be proportional to the error. We also know that the susceptibility is proportional to the lattice-size, so we can assume it to be bigger for a bigger lattice.
The susceptibility for different lattice-sizes and temperatures is plotted in figure 5. We can see that it behaves as expected. First of all it has a peak near the phase transition and it is bigger for bigger lattice-sizes.
We can also see that the peak is closer to the critical temperature, if the lattice is bigger. As for the error, we again find that it is bigger, if we are close to the phase transition. These are the same observations that we already made for the mean.

4.5 Finite-size scaling

The finite-size scaling gives the dependence of the susceptibility on the lattice-size. So if the right scaling has been found, then all points should collapse on one curve. This is plotted in figure 6. We can see that all points are very close to each other, especially far from the phase transition $t = 0$. But the nearer we get to the phase transition, the more they start to deviate

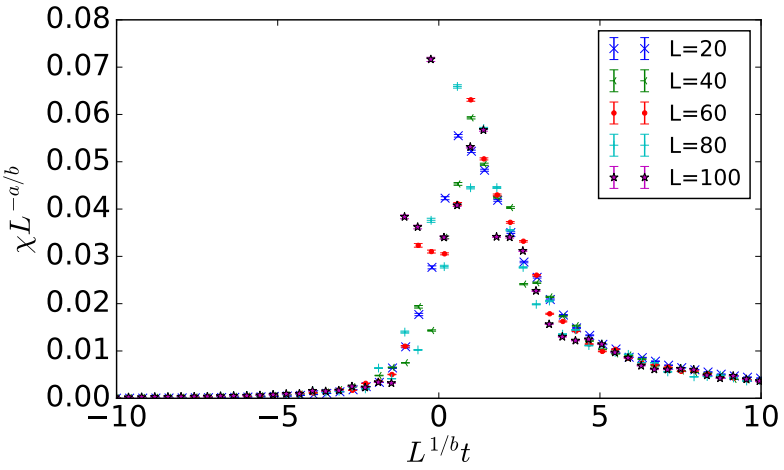


Figure 6: Finite-size scaling $\chi L^{-a/b}(L^{1/b}t)$ for different temperatures T and lattice-length L, where $t = (T - T_{crit})/T_{crit}$. The used parameters are: $a = 1.71$, $b = 1$, $T_{crit} = 2.27$. The error of every measurement has been calculated using the bootstrap algorithm for an initial dataset of 10000 sweeps.

from a line. This is to be expected, since we have seen before that the errors around the phase transition are big. Otherwise they collapse quite nicely.
If we compare the fitted parameters to the literature ones $a = 1.75$, $b = 1$, $T_{crit} = 2.269$, we find that they are quite close to each other. This is as much as can be expected, for noisy data and a fit by hand.

5 Conclusion

We have looked at the Ising model and its phase transition by investigating the properties of the mean $\langle |m| \rangle$, the susceptibility $\chi \sim \mathrm{Var}(|m|)$ and the autocorrelation $\mathrm{Corr}(t)$.
We have found, that big lattices of $L = 100$ approximate the analytical solutions for the phase transition quite nicely, but we have also seen, that the Metropolis algorithm is not as efficient close to T_{crit} as he is far from it. This is because of the long correlation time.