Ising model: an investigation into the effect of temperature on different cluster properties

Mara Brandsen, Lotte Gritter

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This article will discuss a simulation of the two-dimensional Ising model. We will use the simulation to study cluster size and compare our results to published research. We found that both the cluster size and the number of clusters can accurately be modeled by an exponential fit independent of the spin.

1 Introduction

A small fridge magnet may weigh only a few grams but contains more than 10^{22} atoms. Ferromagnetisation is caused by the alignment of these atoms in the object, giving it a net magnetisation. Some materials have to be magnetised by applying an external field, but ferromagnetic materials magnetise by themselves at sufficiently low temperatures. To study this, we will model the behaviour of a (relatively) small amount of atoms in the material in 2D. The atoms are in contact with a heat bath with temperature T. At sufficiently low temperatures and after the system has evolved for some time (and is in thermal equilibrium with the heat bath), we should see clusters form of aligned atoms. We will analyse the size of these clusters. *We will investigate the relation between the temperature of the heat bath and the average cluster size as well as the number of clusters.* Cluster size has been studied before to find out more about the properties of matter, amongst them Jae Dong Noh et al [Noh et all, 2011], who used it to study percolation in different system sizes. In these studies, the first step is to create a simulation to analyse cluster sizes. Our research question is thus a crucial topic to understand how to move deeper into other topics such as percolation.

2 Theory

The Ising model was proposed by physicist Wilhelm Lenz and solved in one dimension by his student Ernst Ising. In this article, we will only discuss the 2D model. This version consists of a lattice of N particles, each with spin up ($S_i = +1$)or spin down ($S_i = -1$). These spins lead to the magnetic moment of the particles. When spins are aligned the net magnetic moment will lead to magnetic properties of the material. Some materials need an external field to be magnetised, other materials will magnetise by themselves at sufficiently low temperatures. This is because aligned spins will lead to the lowest possible energy of the system. If the external field $H < 0$ anti-aligned spins are favourable, if $H > 0$ aligned spins will lower the system energy. In our model, the spins only interact with their nearest neighbours. The energy of the system can be described using the following Hamiltonian:

$$\mathcal{H} = -\frac{J}{2}\sum_{i=1}^{N}{\sum_{j}}' S_i S_j - H\sum_{i=1}^{N} S_i$$

Where J is the coupling between spins and H is an external field. If $J > 0$ interaction is minimised when neighbouring spins align, if $J < 0$ interaction is minimised if spins are anti-aligned.

There is no external magnetic field in the simulation, therefore we can use simplified expressions to build our model.

Firstly, we will need the interaction energy between two atoms.

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

The total energy of the system is the sum of all the interaction energies of the spins in the lattice.

$$E = -J\sum_{<i,j>} s_i s_j \tag{2}$$

The system will evolve and get closer to equilibrium with the heat bath at temperature T. More aligned spins will lead to lower system energy, but thermal variations will lead to spins aligning randomly. In the next section, we will discuss how to implement this theory to write a simulation.

In the system, the atoms can only have spin up or down, and therefore only be aligned or anti-aligned with its nearest neighbours. At sufficiently low temperatures, particles are very likely to align with the majority of their nearest neighbours. However, since we start with a random configuration, this leads to the formation of clusters with aligned spins. Some cluster shapes are more likely than others because they are more stable. One of these rather stable states occurs when the particles form bands of aligned spin. This is a very stable pattern because it minimizes the length of the border - particles within a cluster are the least likely to change spin - and because the particles that are at the border are aligned with three neighbouring spins, and only anti-aligned with one. The chances of it flipping (at these low temperatures) are slim. We want to research the mean cluster size in our system, and whether the clusters have approximately

the same size.

The expectation is that the cluster size and the number of clusters will both follow the same relation for each spin, because it does not matter for the interaction energy, only for the net magnetisation. See eq. (2). Thus we can consider these properties for all clusters together, not making the distinction between the different spins. As well as that as temperature increases the alignment will be more random and thus have a larger number of clusters and a small, approaching 1, cluster size. Both the number of clusters and the cluster size compared to the temperature are predicted to follow an exponential fit as different sources refer to exponential functions when talking about clusters [Tamayo P., 1990].

To simulate complex systems in statistical physics, it can be convenient to use Monte Carlo simulations. Big systems with lots of particles can be difficult to simulate. As this relies on lots of random samples and are governed by probability, instead of trying to design a deterministic simulation. The probability distribution used is a Boltzmann distribution, because we are describing the microstates of an isolated system with a fixed number of particles. This section will briefly discuss the general idea behind the model but will focus on the way we calculated the cluster size. See the course instructions for more details [Van der Heijden].

3 Method

The basics of the model are based on the theory described before. The lattice is created by taking n arrays of length n. The entries of these arrays are randomly generated and take values -1 and 1, see figure 1.

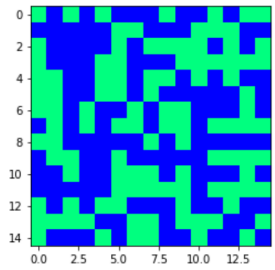

Figure 1: *An example of the randomly generated lattice created at the beginning of each run of the algorithm. Blue and green indicate spin down and up respectively.*

Then we will implement the algorithm with inputs($n = 15, i = 200, j = 6, k = 10^5$):

1. The model chooses a random particle and flips it. Then it calculates the energy associated with that flip using (1).

2. If this energy is negative, it will reduce the system energy and the flip is accepted. If the change in energy $\Delta E > 0$, we accept the change with probability $p = exp[-\frac{\delta E}{k_B T}]$. It generates a random number R in $[0, 1]$. If $R < p$ we also accept the flip. If the flip is not accepted, it will be reversed to its original state.

3. It repeats this process k times, it is import to repeat it until the system stabilizes. You can check this by plotting the (net) magnetisation or energy of the configuration over time to see whether it stabilizes.

4. After k accepted or rejected flips, the algorithm will group each spin by the cluster it is in. Then both the number of clusters and the size of each cluster are recorded per magnetisation. This is then plotted against temperature to see the relationship.
   The spins are grouped in clusters by the following algorithm:

   (a) First for all n^2 spin, it is checked which neighbours have the same magnetisation. The spin and its matching neighbours are recorded in a list.

   (b) Then if two lists include the same spin, the lists are merged. This is done such that the output will be a list which includes a list for every cluster, which then holds all the coordinates of the spins within that cluster.

5. The above process is repeated j times per i different temperatures between 0K and 20K.

4 Results

To check the validity of the simulation, the average energy of the final lattice as well as the average magnetisation is plotted against the temperature, see figure 2 and 3. This is in line with theory as discussed, as well as the theory this article builds

on [van der Heijden]. Thus we accept the model.

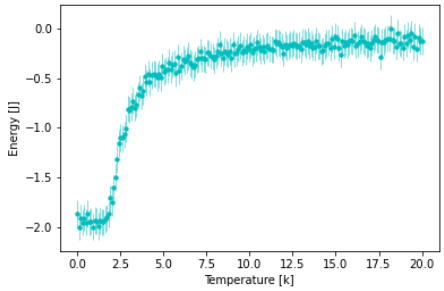

Figure 2: *Temperature [K] vs Energy [J] showing that with temperature the energy increases from -2J and from around 10K starts to converge to 0J. With a steep increase around 3K.*

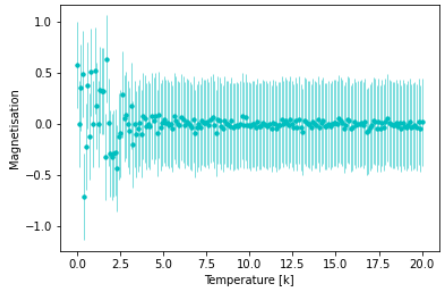

Figure 3: *Temperature [K] vs Magnetisation, where until around 3K the magnetisation jumps sporadically in between 1 and -1. Afterwards it quickly starts to continuously move around 0.*

Now we can investigate the cluster properties. A curiosity is if this depends on the spin. See figure 4 and 5. We see that there is a slight variation for the different spins. For the cluster size, spins that are positive seem to start at significantly lower than the negative spins and sooner stay close to 0. For the number of clusters, the different spin values stay a lot closer except for a slight downward shift of the positive spins relative to their negative counterpart at the beginning before the data increases around 2.5K. Initially, as the difference is only ever so small, this might be caused by the initial configuration of the lattice. In order to test this, the simulation was run with 2 other seed values, see the results in the appendix. From this we can see that similar graphs appear, do note that for a different seed we can see that for both graphs the spin which starts lower occasionally switches. The fact that this is random suggests it doesn't matter if the spin is taken separately or not.

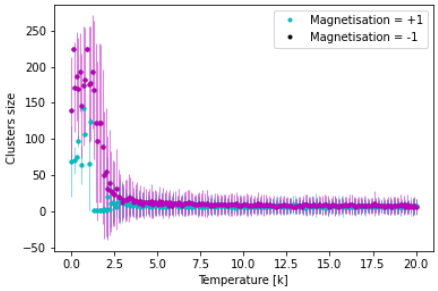

Figure 4: *Temperature [K] vs Cluster size per up and down spin. Before about 3K each clusters is quite large but steeply decreasing until afterwards where it stays close to 1. The up-spin particles start slightly lower.*

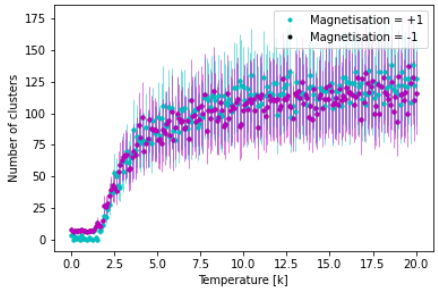

Figure 5: *Temperature [K] vs number of clusters per up and down spin, we can see that until about 3K there are close to 0 clusters. Afterwards, it quickly increases until around 10K where it flattens around 125 clusters.*

With this, we can now look at all particles without making the distinction between their spins. Using the predicted function for the cluster size compared to temperature, both graphs were fit as the number of clusters also seemed to follow an exponential fit.

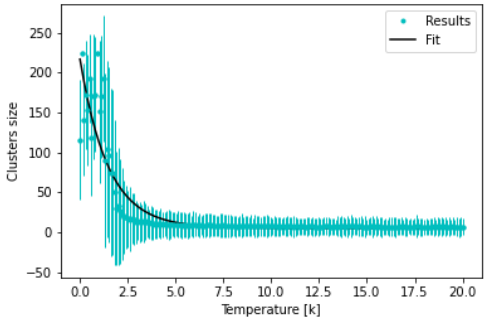

Figure 6: *Temperature [K] vs Cluster size. Before about 3K each clusters is quite larger but steeply decreasing until afterwards where it stays close around 1. The up-spin particles start slightly lower.*

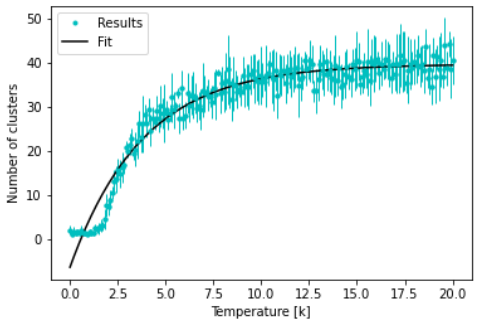

Figure 7: *Temperature [K] vs the number of clusters, we can see that until about 3K they are close to one big cluster. Afterwards, it quickly increases until around 10K where it flattens around 125 clusters.*

Variable vs Temperature [K]	**The fit**	r^2 **value**
Cluster size	$5.44 + 30.79 \cdot e^{(-0.68T+1.93)}$	0.84
Number of clusters	$39.73 + 5.20 \cdot e^{(-0.26T+2.19)}$	0.95

The r^2, correlation coefficient values, indicate that the fit is extremely strong for the number of clusters and fairly strong for the cluster size. We can see that the data agrees with the proposed exponential fit.

Looking at Figure 7 we see that there is a slight indent around 1K that does not follow the fit. This is explained by that underneath a certain temperature, the critical temperature, the system behaves differently and will form bands instead of clusters. This explains the indent as well as the indent in figure 2. This also explains the significant difference between the different spins when looking at figure 4.

5 Discussion

The figures show relatively large error bars, especially figure 5. This makes sense because at higher temperatures, the clusters are very small. Therefore the diference in number of clusters between runs can vary a lot. We only run the simulation six times per temperature, running it more often would reduce the standard deviation of the mean. Our results match our expectations and the theory because clusters form at sufficiently low temperatures, but the system behaves mostly randomly at higher temperatures. We are confident in our conclusion because the correlation coefficient is close to one. At first the script took a few hours to run, which meant we had to wait to see our results. We optimalised the script at the end, but we should have done this while coding to reduce the wait time during the process. Our system is 2D, but real-world problems are often 3D. One could modify the simulation to model 3D systems by adding more neighbours.

6 Conclusion

We determined that the cluster size vs temperature as the theory suggests follows an exponential fit, with the exact parameters as described above. We can see that as the temperature increases the cluster size decreases indeed suggesting at higher temperatures the lattice will all randomly align. From this we also found that the number of clusters vs temperature also is described by an exponential fit. In this case, we see that the number of clusters as well supports this by increasing in value. Both eventually flatten out around 10 Kelvin indicating the most random state has been reached. In future research, one could do the same for an n-dimensional model as this would model the real (3D) world better. It would add to the validity of our conclusion to do a separate investigation into the difference of these cluster properties per spin. Noticeable as well is that for each graph there is a significant change both around 3K and 10K, this will have to do with the critical temperature but as it is not part of this investigation, this definitely holds an interesting topic for future research.

7 Bibliography

Blundell, K., Blundell, S. (2006). Concepts in thermal physics. Oxford. pp. (?)
Fillion, L. (2023), Notes on the Ising model Van der Heijden, N. (2023) Numerical Experiments on the Ising model
Noh, J. D., Lee, H. K., & Park, H. (2011). Scaling of cluster heterogeneity in percolation transitions. Physical Review E, 84(1). https://doi.org/10.1103/physreve.84.010101
Tamayo, P., Brower, R.C. & Klein, W. Single-cluster Monte Carlo dynamics for the Ising model. J Stat Phys 58, 1083–1094 (1990). https://doi.org/10.1007/BF01026564
Van der Heijden, N., Numerical Experiments on the Ising Model

8 Appendix

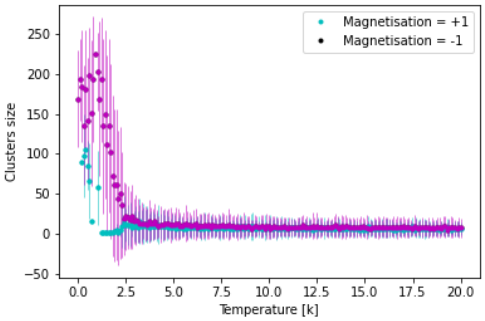

Figure 8: Temperature [K] vs Cluster size per spin-value for seed 12. At low temperatures the clusters are big, but above 3K the clusters get very small. The clusters with magnetisation -1 are bigger.

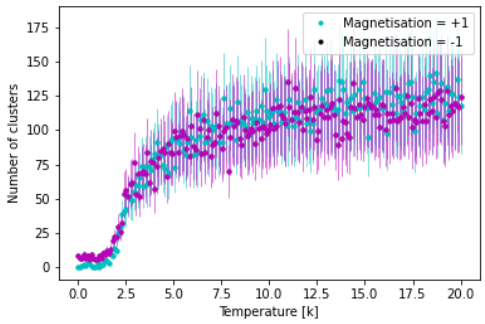

Figure 9: Temperature [K] vs Cluster size per spin-value for seed 6. At low temperatures, there are very few clusters, most of them have spin -1. But above 3K there is a rapid increase in number.

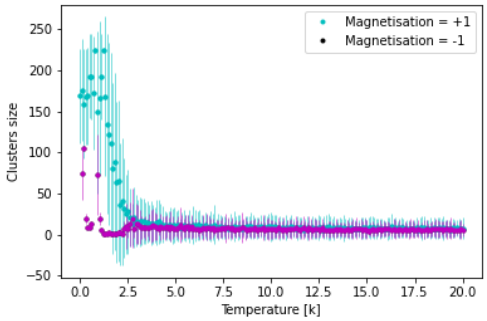

Figure 10: Temperature [K] vs number of clusters per spin-value for seed 12. The figure is almost the same as *figure 8*, but the biggest clusters have spin +1.

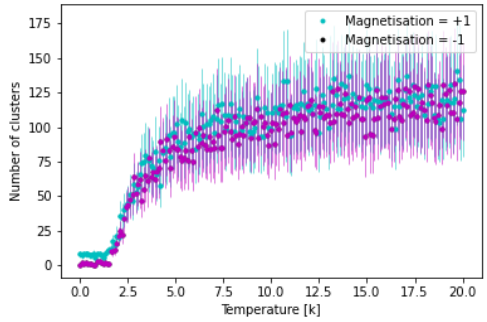

Figure 11: Temperature [K] vs number of clusters per spin-value for seed 6. The figure is almost the same as *figure 9*, but at temperatures below 3K most clusters have spin +1.