Monte Carlo Simulation of the Ising Model

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Abstract

Ising model is one of the most simple models of ferromagnetism in statistical mechanics. This work is devoted to study two-dimensional square lattice Ising model via Monte-Carlo chains to explored effect of order-disorder phase transition which occurs in freezing-melting process of a nanoparticle.

Github repo: MC-Ising-model

1. Introduction

Ising model was first exploited for investigating spontaneous magnetization in ferromagnetic film and appeared to be an accurate and simplified explanation of phase transitions in ferromagnetics. The model is very general an can be applied for a variety of tasks, for example, lattice-based liquid-gas model (Lee & Yang, 1952), lattice model of liquid, various binary mixtures and alloys, adsorption on the surface, DNA "melting" and other systems.

Here we will investigate the 2-dimentional Ising model for enclosed nanoparticle (no interaction with outer) of different scales.

The main contributions of this report are as follows:

1. Desription of Ising model.
2. Baseline for Monte-Carlo modelling of Ising model.
3. Experiments with melting and freezing processes.

2. Ising model

Ising model can be taken into consideration for different dimensions, but all of them will have the same Hamiltonian:

$$H = -J \sum_{<i,j>} \vec{S}_i \vec{S}_j - \vec{h} \sum_i \vec{S}_i, \tag{1}$$

where $\vec{S}_i$ – n-component is spine vector (for Ising model n=1, for XY model n=2, for Heizenberg model n=3), $< i, j >$ – means that summation is conducted throw i spin and for each i only throw its nearest neighbours j, – is external magnetic field (which in this paper is considered as zero) and J – integral of exchange interaction, which is a measure of the force of interaction between the nearest neighboring spins. So if $J > 0$ the minimum energy of the system will be in the configuration, when the neighbouring spines are in the same direction and the system is named ferromagnetic. Alternatively, if $J < 0$ the minimum energy of the system will be in the configuration, when the neighbouring spines are in the same direction, such system is named antiferromagnetic. For simplicity it was assumed equal to 1 in this paper.

Ising model is one of the most widespread models of phase transition in statistical physics. It describes phase transition from a paramagnetic to a ferromagnetic state at a temperature T_c with the appearance of spontaneous magnetization on the lattice at. The investigation of this model in the absence of an external magnetic field (Kramers & Wannier, 1941) accurately determined the phase transition temperature

$$\frac{kT_c}{J} = \frac{2}{\ln(1+\sqrt{2})} = 2.269, \tag{2}$$

where k – Boltzman constant and J – integral of exchange interaction.

2.1. Physical quantities used for modelling

To produce modelling the following physical quantities were used. The Hamiltonian was simplified to have a from of:

$$H_i = -\sum_{j_{nn}} s_i s_j, \tag{3}$$

where s_i equals 1 or -1 as it is spin.

Energy is estimated as a sum throw all of the spins in a nanoparticle:

$$E = \frac{1}{2} < \sum_i^N H_i > \tag{4}$$

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Magnetisation:

$$M = N_{up} - N_{down} = \sum_{i}^{N} s_i \tag{5}$$

3. Monte-Carlo modelling

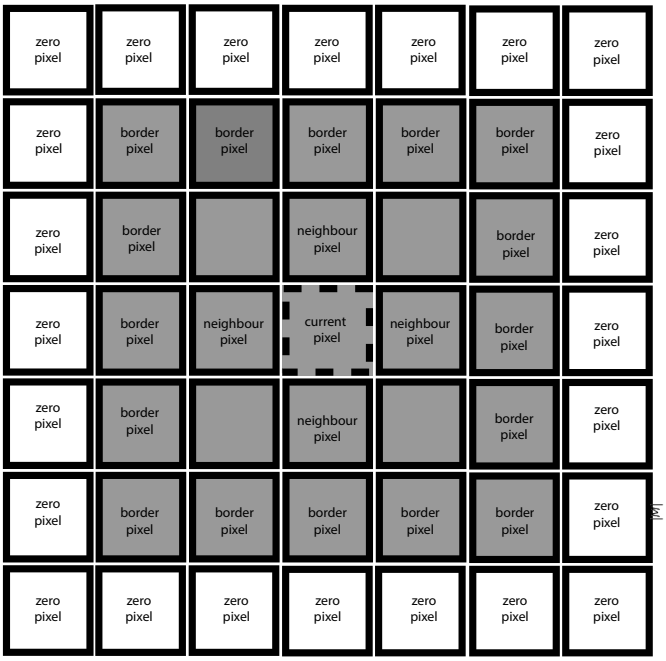

Figure 1. The picture of a nanoparticle 7×7 which might have been used for numerical experiment. All pixels on the border *(zero pixels)* are zeros which doesn't change while computation. Also for *current pixel* the neighbouring cells are marked as *neighbour pixels.*

The Metropolis Algorithm was implemented to perform Monte-Carlo modelling. Here are the steps of the algorithm:

First of all we need to initialize the lattice. This can be done in two ways: random – disordered state (high temperature, should be used for freezing simulation) or filled – completely equally oriented state (low temperature, should be used for melting simulation). On figure 1 you can see the border conditions and details about neighbours for each spine.

Then decide with step (size and sign) for changing temperature and perform a Monte-Carlo loop for each temperature step.

Monte-Carlo loop:

1. Pick random spine and check the change in energy that it will produce if it swaps the direction of its alignment.
   - If $dE < 0$, change the alignment of the spine.
   - Else generate a random number ξ between 0 and 1. If $\xi < e^{-\frac{dE}{kT}}$, also change the alignment of the spine.
2. Go to the previous step while the equilibrium is not reached (check energy convergence)

4. Experiments

The computational program for this paper was written on Python with the use of Numba accelerator.

4.1. Melting

Melting is an equilibrium process for such a system. Melting was calculated from random initial lattice. T was changing from 6 to 0.01 with 0.06 step size. On the pictures you can see average values obtained form 10 simulations of a lattice 64×64.

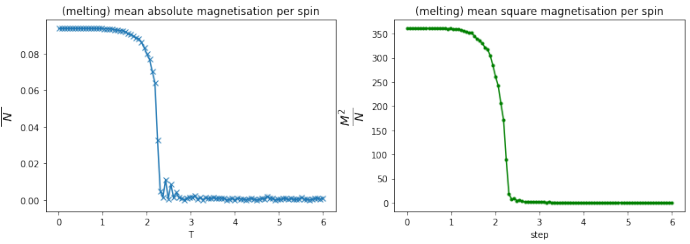

Figure 2. Absolute magnetization averaged over 10 runs per spin VS Temperature for nanoparticle 64×64 in melting process on the left. Square magnetization averaged over 10 runs per spin VS Temperature for nanoparticle 64×64 in melting process on the right.

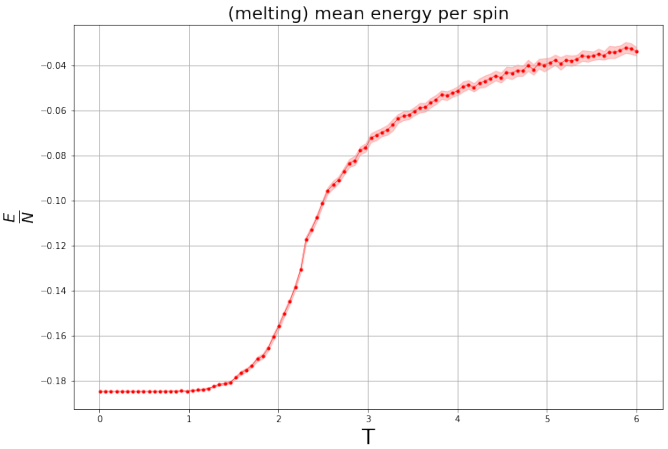

Figure 3. Energy averaged over 10 runs per spin VS Temperature for nanoparticle 64×64 in melting process on the right.

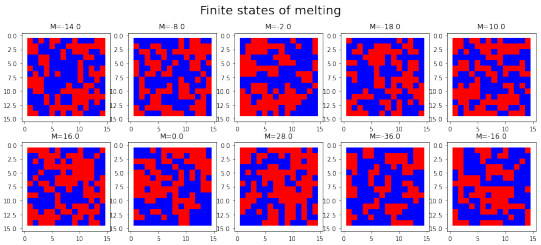

Figure 4. Finite states which were reached at the end of melting process

4.2. Freezing

Freezing is an non-equilibrium process for such a system. Freezing was calculated from fully oriented initial lattice. T was changing from 0.01 to 6 with 0.06 step size. On the pictures you can see average values obtained form 10 simulations of a lattice 64×64.

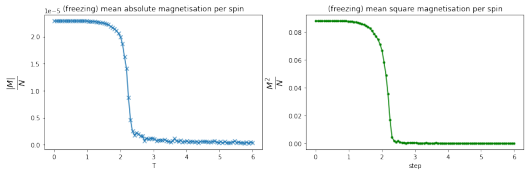

Figure 5. Absolute magnetization averaged over 10 runs per spin VS Temperature for nanoparticle 64×64 in freezing process on the left. Square magnetization averaged over 10 runs per spin VS Temperature for nanoparticle 64×64 in freezing process on the right.

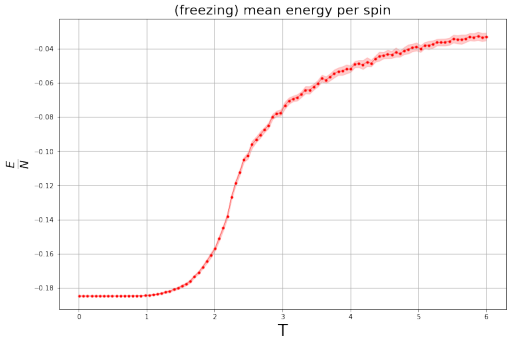

Figure 6. Energy averaged over 10 runs per spin VS Temperature for nanoparticle 64×64 in freezing process on the right.

4.3. Curi Temperture

To evident the value of T_C from theoretical section and compare it with graphs of order parameter the following graphs were created.

We can see that increasing the scale brings us closer and closer to the theoretical analogue of this graph and the theoretical value of the Curie temperature, this might be connected to the boundary conditions which are used for our nanoparticles. Also we can observe that graphs for larger scale are more smooth (less noisy).

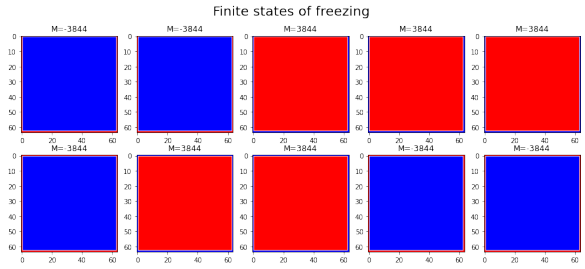

Figure 7. Finite states which were reached at the end of freezing process

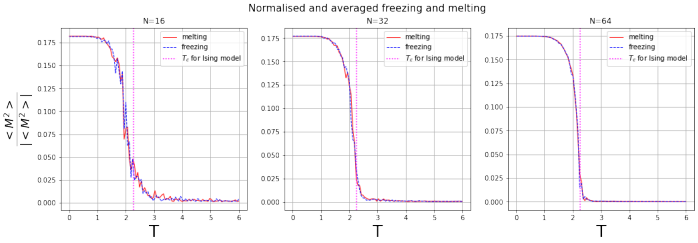

Figure 8. Normalised and averaged square magnetization VS Temperature for nanoparticles of different scale in freezing (blue) and melting (red) processes. Theoretical value for T_C is vertical line on all graphs.

4.4. Hysteresis

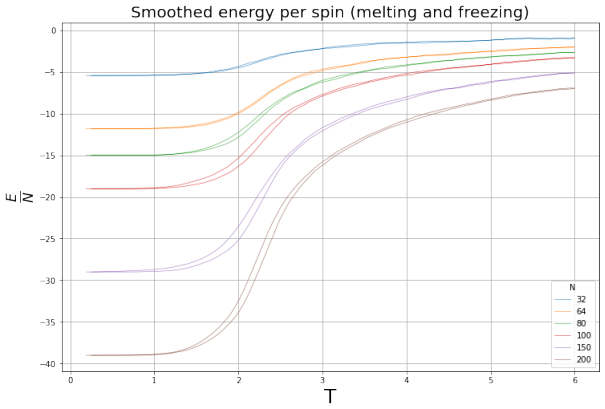

Figure 9. Smoothed energy per spin VS Temperature for nanoparticles in freezing and melting process for different scales of nanoparticle

To accurately draw combination of graphs and hysteresis there were simulations in which temperature was rising from

the lowest value to the largest and returned. Here are the corresponding graphs.

On the figure 9 we can see how hysteresis gradually appears with an increase in the size of the nanoparticle. The plots on the graph are smoothed with the moving average of the scale 8.

4.5. Order parameter graphs

To compare the behavior of order parameter for different scales of nanoparticles let's look at the figures 10, 11. The upper line on each graph corresponds to melting part of the simulation. We can observe, that this part in quite stable throw all of the cases. The lower line corresponds to freezing part. We can observe that for smaller scales (3 upper plots) its behafiour is more stable, than for larger scale (3 lower plots).

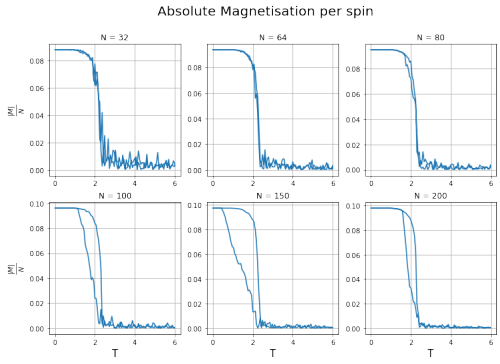

Figure 10. Absolute magnetization per spin VS Temperature for nanoparticles in freezing and melting process for different scales of system.

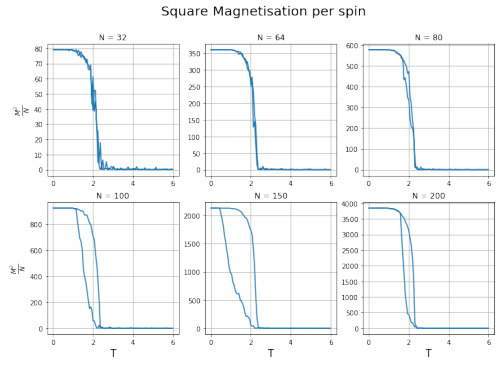

Figure 11. Square magnetization per spin VS Temperature for nanoparticles in freezing and melting process for different scales of system.

5. Conclusion

This work can be considered as an overview of 2-D Ising model for nanoparticles. Melting and freezing processes were studied to investigate order-disorder phase transitions, observed stability of melting and instability of freezing (especially for large scales of nanoparticle). We observed the appearing of hysteresis with increasing nanoparticle scale and checked the theoretical value of Curie temperature T_C.

The work on this field can be proceeded. Interesting would be to try different shapes of nanoparticles (rectangular and hexagonal(investigate two-dimensional percolation)), extend the dimensions and simulate 3-D model. Also a nice idea would be to add some non-changing spins which might be corresponding to irregularities of a real ferromagnetic tissure.

References

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Lee, T. D. and Yang, C. N. Statistical theory of equations of state and phase transitions. ii. lattice gas and ising model. *Phys. Rev.*, 87:410–419, Aug 1952. doi: 10.1103/PhysRev.87.410. URL https://link.aps.org/doi/10.1103/PhysRev.87.410.