Computational physics 2, Project work, Ising model

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What is the Ising model?

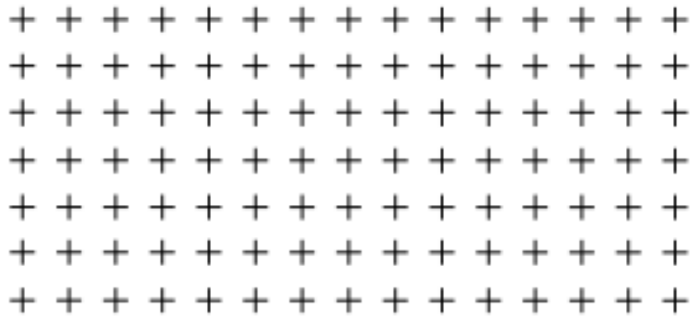
Ising model is a mathematical model describing a ferromagnet in statistical physics.

Let us assume a set of atoms arranged on a regular lattice (2D in this project) and assume further that each atom can be in one of only two states, which we will denote by the values +1 and −1, corresponding to their spin states up and down, respectfully.

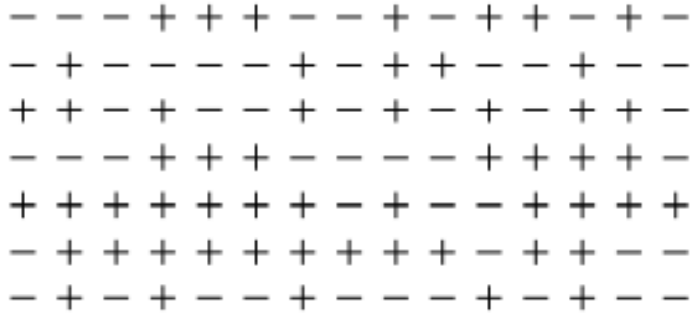
Let us also assume that it is energetically more efficient for an atom to be in the same state as its nearest neighbours. This would mean that the most efficient configuration is when all the spins are +1 or -1 (ordered). Given the fact that the number of lattice atoms is usually quite large, it is much more probable for the system to be in disordered configurations with half the sites +1 and the other half -1.

Equilibrium is achieved by minimizing the Hemholtz function

$F = E - TS$, where E is the internal energy, T is the temperature and S entropy. Meaning that in low temperatures E dominates the F, favouring the ordered configuration. In high temperatures F is dominated by -TS, so maximizing the S is energetically efficient, favouring the disordered configuration.



Ordered states



Disordered state

Project setup

With these assumptions in mind the energy E(s) of the Ising model on a specific microstate s is given as

$$E(s) = -\sum_{i,j} J_{i,j} s_i s_j$$

where the sum is taken over the spin values of nearest-neighbour sites i and j. J is interpreted as the exchange constant in magnetism. J > 0 corresponds to ferromagnetic interactions (all the spins line up), while J < 0 corresponds to antiferromagnetic interactions (neighbouring spins are oppositely aligned).

In this project we assume a 2D lattice with ferromagnetic interaction and compare model with only nearest neighbour interactions to model with nearest neighbour and next nearest neighbour interactions.

We will also study how the size of the regular lattice effects the measured observables.

Monte-Carlo method

The number of distinct configurations of the Ising model for a N*N lattice is 2^{N^2}, which grows rapidly with N, making the calculation of the partition function for a system of this size by hand quite toilsome. This problem can be solved with computational methods, namely Metropolis Monte Carlo algorithm in this project.

Let us choose a random site in the lattice and flip the spin. If this change lowers the total energy of the system we leave it as flipped. If it raises the energy by an amount ΔE, the state is returned to its original state with a probability $\mathrm{e}^{-\beta\Delta E}$ or leave it flipped with a probability $1 - \mathrm{e}^{-\beta\Delta E}$. After this we pick another spin and repeat the process. Utilizing this we can sample spin configurations from probability density function P(s), which we then use to calculate observables from the system.

The measure of acceptance is given as

$$q(s - s') = \min\left(e^{-\beta[E(s')-E(s)]}, 1\right)$$

Where s is the old state before the flip and s' is the new flipped state, β = kT, where k is the Boltzmann constant and T is the temperature.

Calculating observables

$$\langle E \rangle = \sum_s E(s)P(s) \qquad C_V = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_B T^2}$$

$$\langle M \rangle = \sum_s M(s)P(s) \qquad \chi = \frac{\langle M^2 \rangle - \langle M \rangle^2}{k_B T}$$

Different observables can be calculated from a thermodynamical system. In this project we will compare energies, magnetizations, heat capacities and susceptibilities.

Nearest neighbour model: $E(s) = -J_1 \sum_{\langle i,j \rangle} s_i s_j$,

where j is the nearest neighbour of i.

Nearest neighbour and next nearest neighbour model:

$\mathrm{E}(s) = -J_1 \sum_{\langle i,j \rangle} s_i s_j - J_2 \sum_{\langle i,k \rangle} s_i s_k$,

Where j is the nearest neighbour of i and k is the next nearest neighbour of i and the nearest neighbour of j)

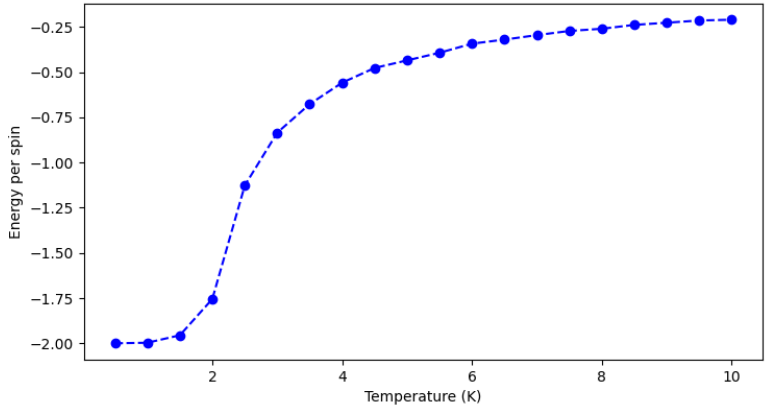
$M(s) = \Sigma_i s_i$ (sum of the spin values)

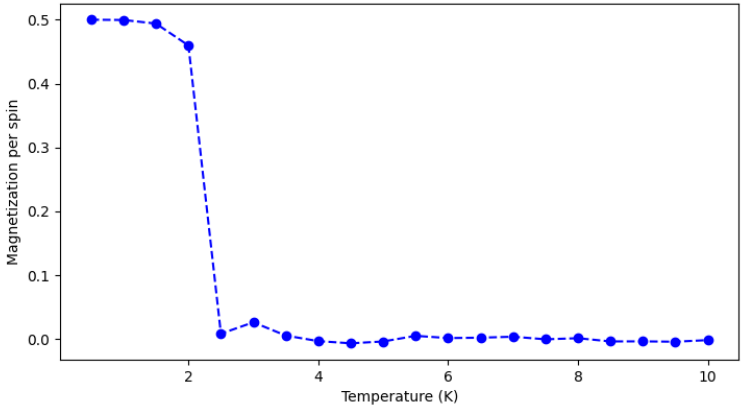
Results, nearest neighbour model (nn)

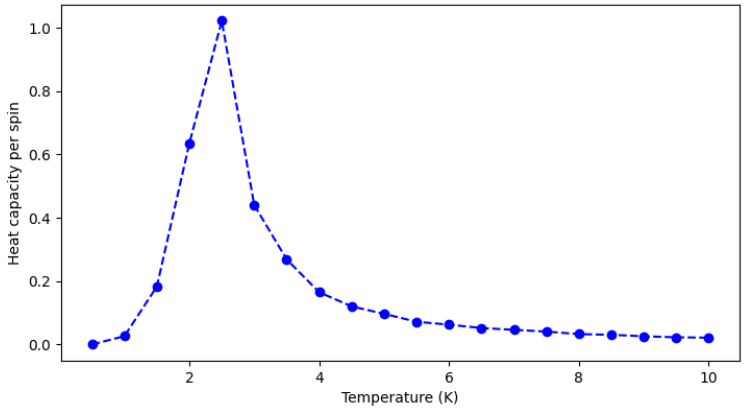
10*10 sized regular lattice was used alongside of 200 blocks and 1000 iterations in the Monte Carlo simulation.

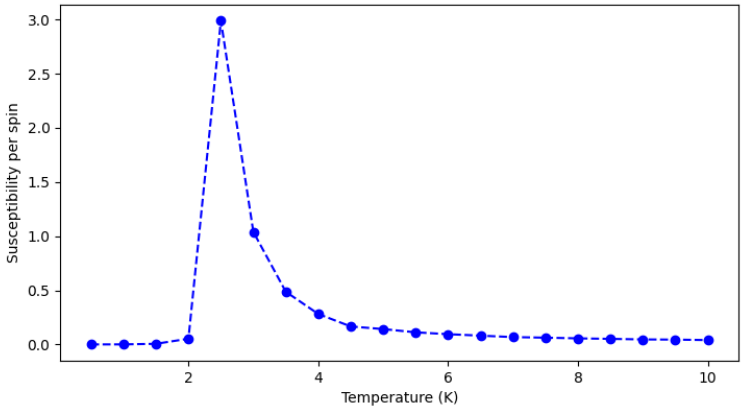
From top left to bottom right: energy, magnetization per spin, heat capacity and susceptibility (per spin)

We can recognize transition temperature to be in the range of 2-3 K from the sudden change in the figures.







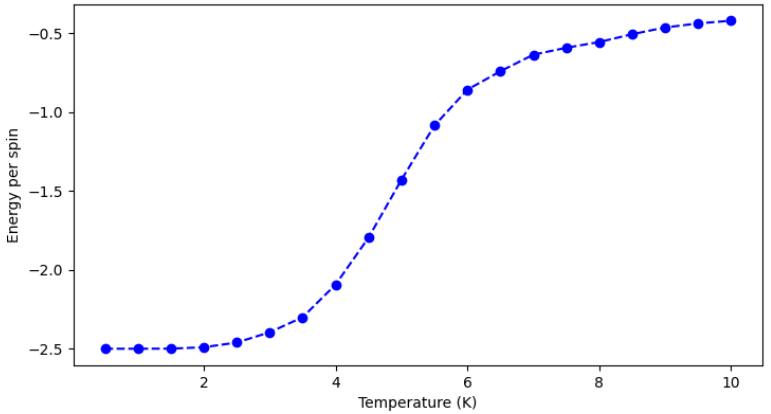


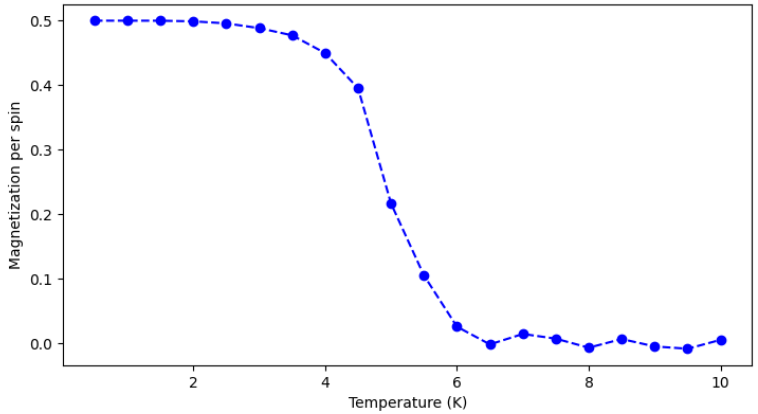
Results, next nearest neighbour model (nnn)

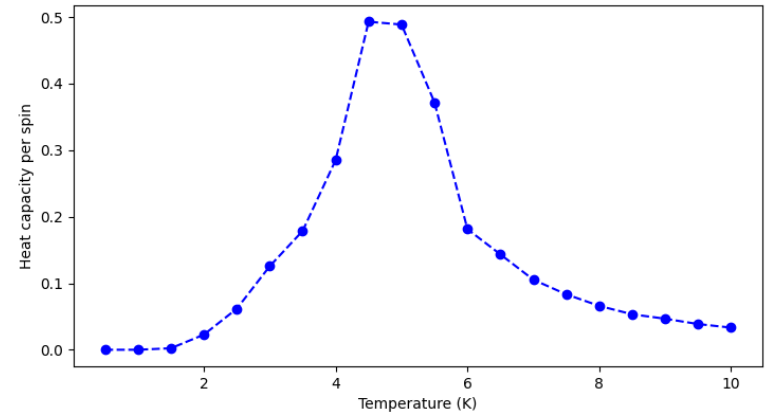
10*10 sized regular lattice was used alongside of 200 blocks and 1000 iterations in the Monte Carlo simulation.

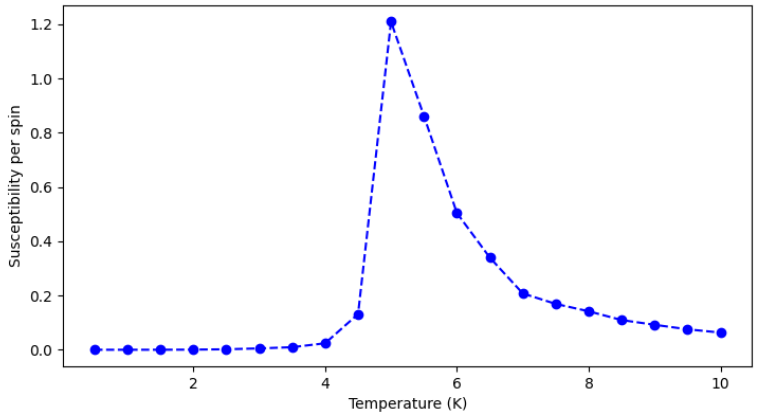
We can recognize that the transition temperature has shifted to a higher temperature in the range of 4-6 K from the sudden change in the figures.

We see that the energy is greater in nnn model than in nn model. This seems reasonable, since the nnn takes into consideration more interactions between lattice ions. Magnetization does not change noticeably. Heat capacity and susceptibility are both smaller during the peak in nnn than in nn model, but the equilibrium value is relatively the same.





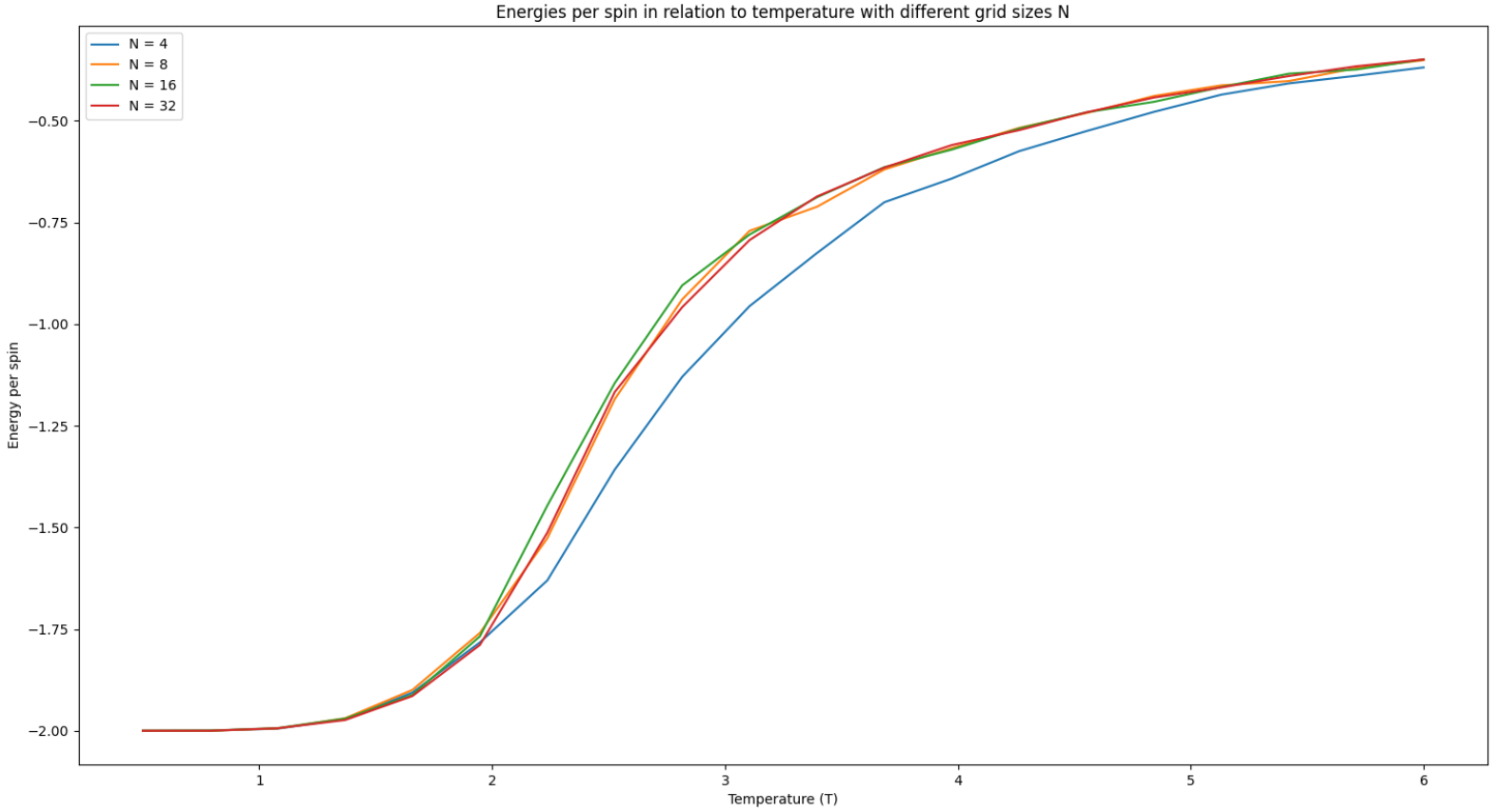




Finite size effects, energies

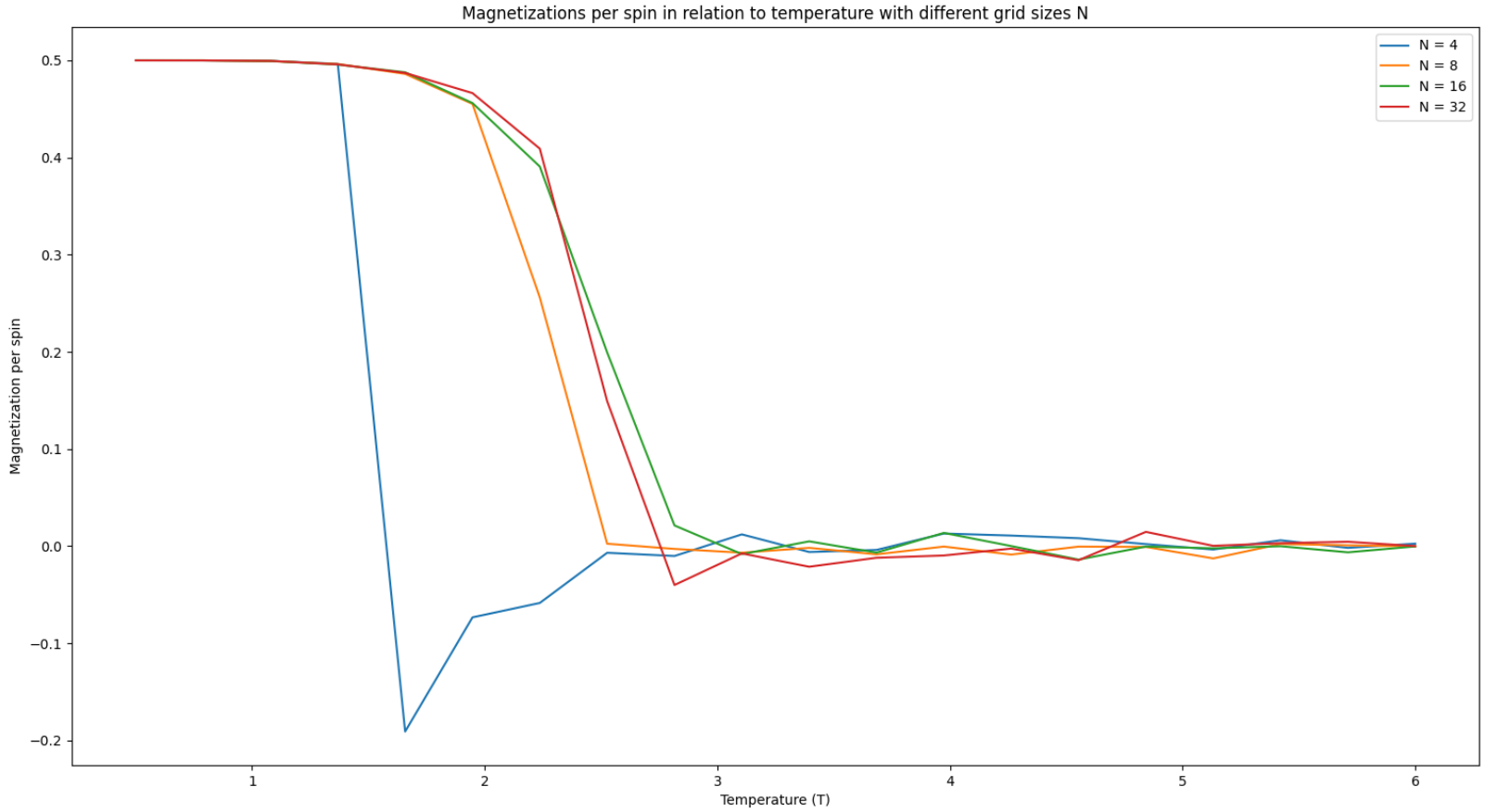
Observables where counted using different grid sizes to see how that would affect the results.

Energies all have the same shape and are relatively close to each other.



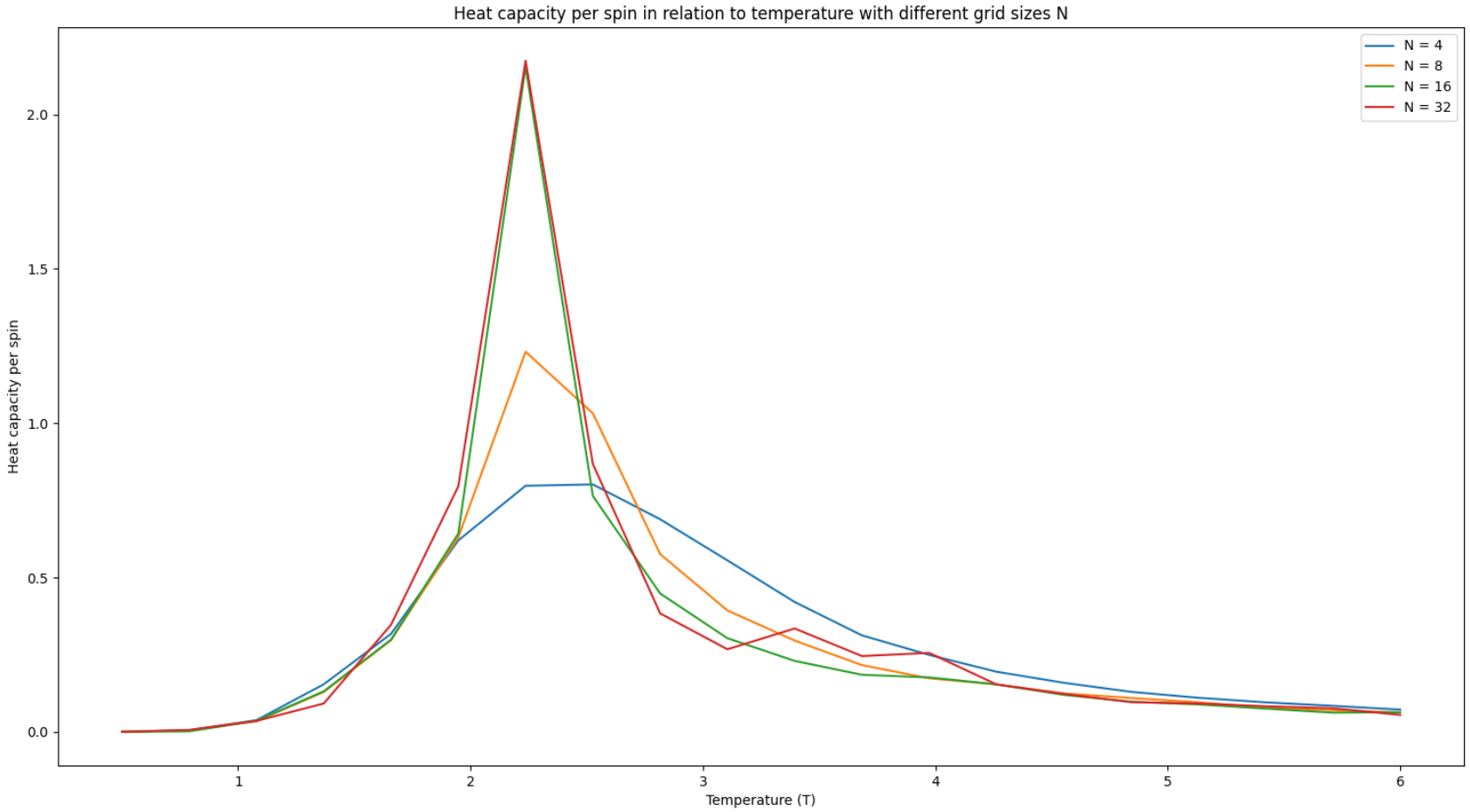
Finite size effects, magnetization

Magnetizations also have the same shape. Interestingly with the smallest grid size the dip is more negative than with the others. The dip also starts in lower temperature



Finite size effects, heat capacity

Heat capacities are relatively close to each other. The peak related to transition temperature seems to be smaller when the grid is smaller.



Finite size effects, susceptibility

Susceptibilities also have the same form regardless of the grid size. Interestingly this seemed to vary the most of all the observables from simulation to simulation. According to literature the peak value should be higher the bigger the grid, but in this particular simulation the 16*16 grid is actually smallest.