Ferromagnetic phase transition: the Ising model
Solution and guidelines for grading

May 12, 2024

The aim of this document is two-fold. At first, it will provide details on the implementation of the Monte Carlo simulation that was provided to the students. Hence, the first part is for information purposes only. The second part of this document provides a model solution of the experimental tasks, as well as guidelines for grading. The task was designed by Tudor Mocioi (Ecole Polytechnique), with significant debugging help from Victor Dumbravă (Ecole Polytechnique). Many details of the implementation as well as some optimization ideas are based on the course of Lauren Hayward (Perimeter Institute) presented during Perimeter Institute's PSI Summer Program.

1 Implementation of the Monte Carlo simulation

The simulation software is written in Python 3. Below, we introduce the basic building blocks of this software. At first, we introduce the relevant modules onto which the simulation software is based, as in the code block below.

[47]:
```
import matplotlib.pyplot as plt
import matplotlib.colors as colors
import numpy as np
import time
import pandas as pd
from scipy.optimize import curve_fit
from IPython import display

bw_cmap = colors.ListedColormap(['black', 'white'])
```

For efficiency purposes, the spin configurations will be stored as bidimensional numpy arrays. First, we implement a function that, given a spin configuration as well as the value of the coupling parameter J, in an external field H, returns the energy of the spin configuration.

[3]:
```
def get_energy(spins, J, H):
    energy = -H*np.sum(spins)-J*np.sum(spins*np.roll(spins, 1, axis = 0) +
                                       spins*np.roll(spins, 1, axis = 1))
    return energy
```

Next, we implement the function that performs one step of the Monte Carlo simulation. Given a spin configuration, the procedure is the following

- First, choose an arbitrary position in the spin lattice, and flip its sign. All positions are chosen with an equal probability.

- If the resulting spin configuration has a lower energy, accept the new spin configuration.
- If the resulting spin configuration has an energy that is higher than before, by a value ΔE, randomly choose whether to accept the new spin configuration, with a probability $\exp\left(-\frac{\Delta E}{k_B T}\right)$.

For convenience, note that our implementation operates with temperatures expressed in units of energy, *i.e.* the corresponding value of $k_B T$.

[4]:
```
def monte_carlo_step(spins, J, T, H):

    L = np.shape(spins)[0]
    N_spins = L*L
    i = np.random.randint(0,N_spins) # randomly choose which spin to consider␣
↪flipping
    i_row = i//L # row corresponding to i
    i_col = i%L  # column corresponding to i

    # look at the four nearest neighbours to calculate the change in energy for␣
↪this proposed move:
    deltaE = 2*H*spins[i_row,i_col]+2*J*spins[i_row,i_col] * (␣
↪spins[(i_row+1)%L,i_col] + spins[(i_row-1)%L,i_col] + spins[i_row,(i_col+1)%L]␣
↪+ spins[i_row,(i_col-1)%L] )

    if (deltaE <= 0) or (np.random.rand() < np.exp(-deltaE/T)):
        spins[i_row,i_col] = -spins[i_row,i_col] #accept the spin flip

    return spins
```

Now, we implement the function which performs one Monte Carlo simulation, for a given set of J, T and H, with a number of steps N, for a square lattice of size L.

[5]:
```
def monte_carlo_simulation(L, J, T, H, N, animate):
    spins = 2 * np.random.randint(0, 2, size=((L,L))) - 1 # start from a random␣
↪spin configuration

    # first, perform the equilibration steps
    N_eq = N//10
    for _ in range(N_eq):
        spins = monte_carlo_step(spins, J, T, H)

    # then, perform further Monte Carlo steps and record the corresponding␣
↪magnetizations
    Ms = []
    for _ in range(N):
        spins = monte_carlo_step(spins, J, T, H)
        Ms.append(np.sum(spins))
        if animate:
            #Display the current spin configuration:
```

```
            plt.clf()
            plt.imshow( spins.reshape((L,L)), cmap=bw_cmap, norm=colors.
↪BoundaryNorm([-1,0,1], bw_cmap.N), interpolation='nearest' )
            plt.xticks([])
            plt.yticks([])
            #plt.title('%d x %d Ising model, T = %.3f' %(L,L,T))
            display.display(plt.gcf())
            display.clear_output(wait=True)
            plt.pause(0.01)

    # finally, compute the average magnetization per spin and its standard␣
↪deviation
    magnetization = np.average(Ms)/(L*L)
    std_magnetization = np.std(Ms)/(L*L*np.sqrt(len(Ms) - 1))

    return (magnetization, std_magnetization)
```

Finally, we implement a function that performs the Monte Carlo simulations for ranges of values for J, T and H.

[6]:
```
def simulations(L, Js, Ts, Hs, N, N_repeat, animate):
    dict = {'J':[], 'T':[], 'H':[], 'M':[], 'M_err':[]}
    for J in np.nditer(Js):
        for T in np.nditer(Ts):
            for H in np.nditer(Hs):
                for _ in range(N_repeat):
                    M, M_err = monte_carlo_simulation(L, J, T, H, N, animate)
                    dict['J'].append(J)
                    dict['T'].append(T)
                    dict['H'].append(H)
                    dict['M'].append(M)
                    dict['M_err'].append(M_err)
    results = pd.DataFrame(dict)
    return results
```

The final step of the implementation, which we omit in this document, is to package the above functions into the graphical user interface that was provided to the participants.

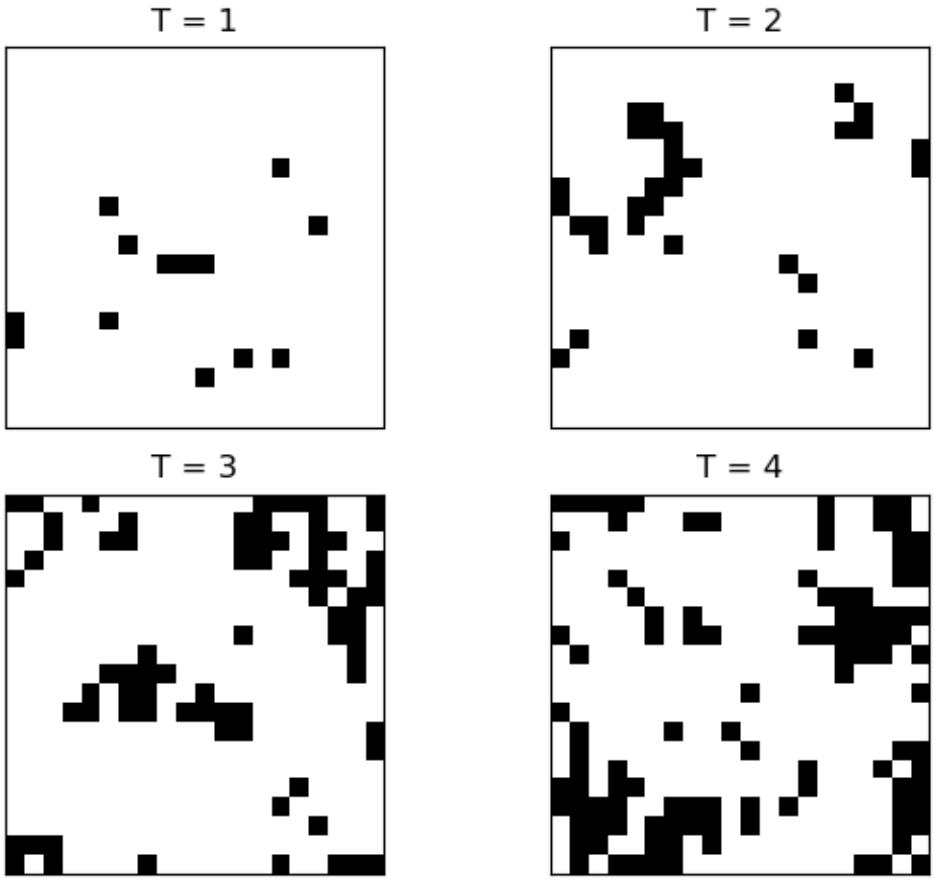
2 Model solution and guidelines for grading

A. Phase transition and the critical temperature

Question A.1. We notice that the behaviour of the spin system is qualitatively different for the temperatures $T = 3$ and $T = 4$ than for $T = 1$ and $T = 2$. Indeed, for the lower temperatures there is a well-defined ordered state of the spins, with some random fluctuations around this order. The fluctuations are more frequent as the temperature increases. For the two higher temperatures, one cannot distinguish any sort of order between the spins, which just seem to randomly flip at all times. Furthermore, for the higher temperature it seems like the spin flips happen more and

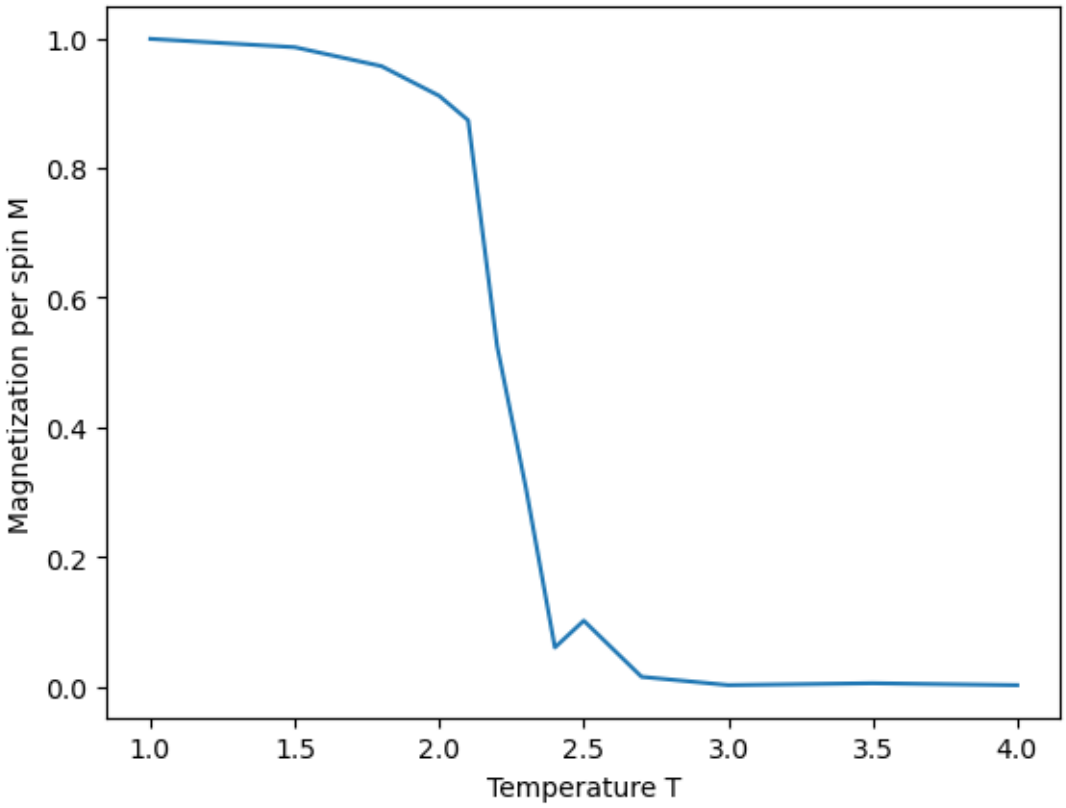
more frequently, with less and less order. A diagram showing typical spin configurations for the four temperatures is shown below.

Note for graders: depending on the initial seed of the random simulation, the students might not observe just one direction of alignment, but perhaps several "domains", each pointing either up or down. Full marks may also be given for such remark, as long as the concept of ***order*** *is clearly stated in the answer.*



Question A.2. The figure below shows, for the given lattice size and number of Monte Carlo steps, at $J = 1$, the dependence of the system magnetization on temperature. One notices a very sharp drop around $T \approx 2.2 \pm 0.1$, which indicates that it is the temperature at which the phase transition takes place.

Note for graders: accept results within ± 0.2 *of the value above. It is important that, around the phase transition, the participants go in finer steps (say* 0.1*), so as to detect the transition correctly. Deduct marks for answers that miss the phase transition due to the steps being too coarse, as well as for answers not presenting an error bar.*



Question A.3. We redo the experiment for several values of J. We always focus on a temperature range around $2.2T$. The results of our analysis are included in the table below. The analysis shows that the dependence of the transition temperature T on the exchange parameter J is very well described by a line passing through the origin, with slope 2.29 ± 0.03.

Note: an exact solution, in the thermodynamic limit (infinite lattice size), leads to $\frac{T}{J} = \frac{2}{\ln\left(1+\sqrt{2}\right)} \approx 2.26$. *Such solution is outside the scope of the exam.*

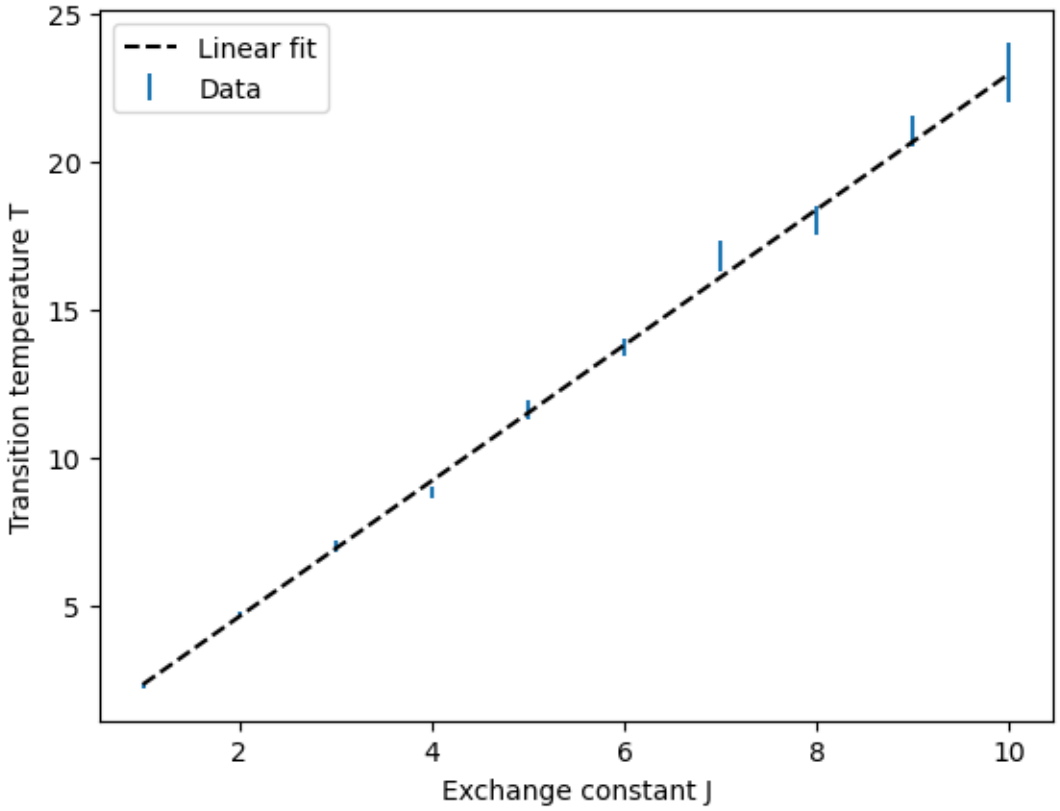
Note for grading: for full marks, accept linear dependencies roughly passing through the origin, with slopes between 2.2 *and* 2.4. *At least 10 different data points need to be presented, deduct points for less. All values (critical temperatures, slopes) need to be presented with error bars.*

[36]:

	Exchange constant J	Phase transition temperature Tc	Temperature errorbar
0	1	2.3	0.1
1	2	4.7	0.1
2	3	7.0	0.2
3	4	8.8	0.2
4	5	11.6	0.3
5	6	13.7	0.3
6	7	16.8	0.5
7	8	18.0	0.5
8	9	21.0	0.5
9	10	23.0	1.0

****

```
slope =     2.2914 +/-  0.0325
intercept =     0.0383 +/-  0.0997
********************
```



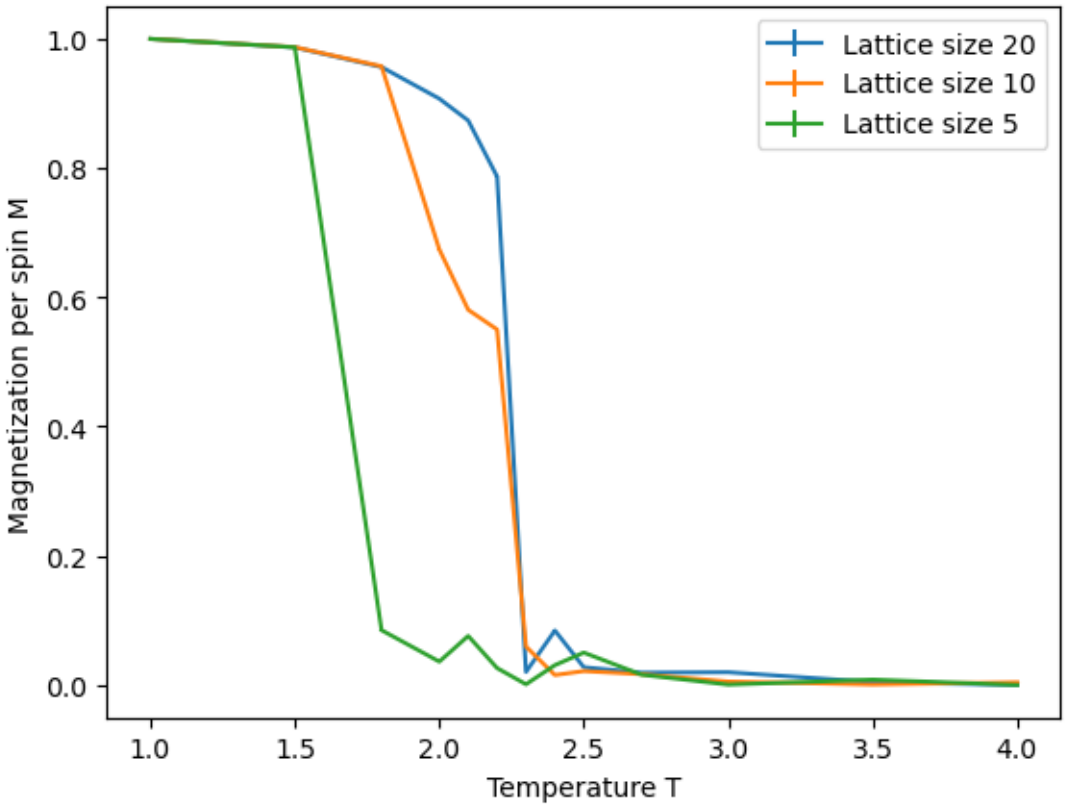
Question A.4. To assess whether one direction of magnetization is preferred in the ferromagnetic regime, we run an experiment for $J = 1$ and $T = 1$ for 100 repeats, at zero external magnetic field, each time recording the direction of the magnetization. Our simulations show that, out of 100 runs, 48 of them have a positive magnetization (pointing 'up') and 52 of them have a negative magnetization (pointing 'down'). This allows us to reasonably conclude that there is no preferred direction of magnetization, and that the system randomly chooses a direction along which it spontaneously magnetizes.

Note for graders: award full marks for similar remarks based on at least 20 repeats.

B. The crossover regime

Question B.1. The figure below shows the magnetization versus temperature curve for the three specified lattice sizes, for $J = 1$. One notices that as the lattice size decreases, the transition stays sharp, but that there is more variability in its outcome. The transition temperature also seems to be effectively shifted.

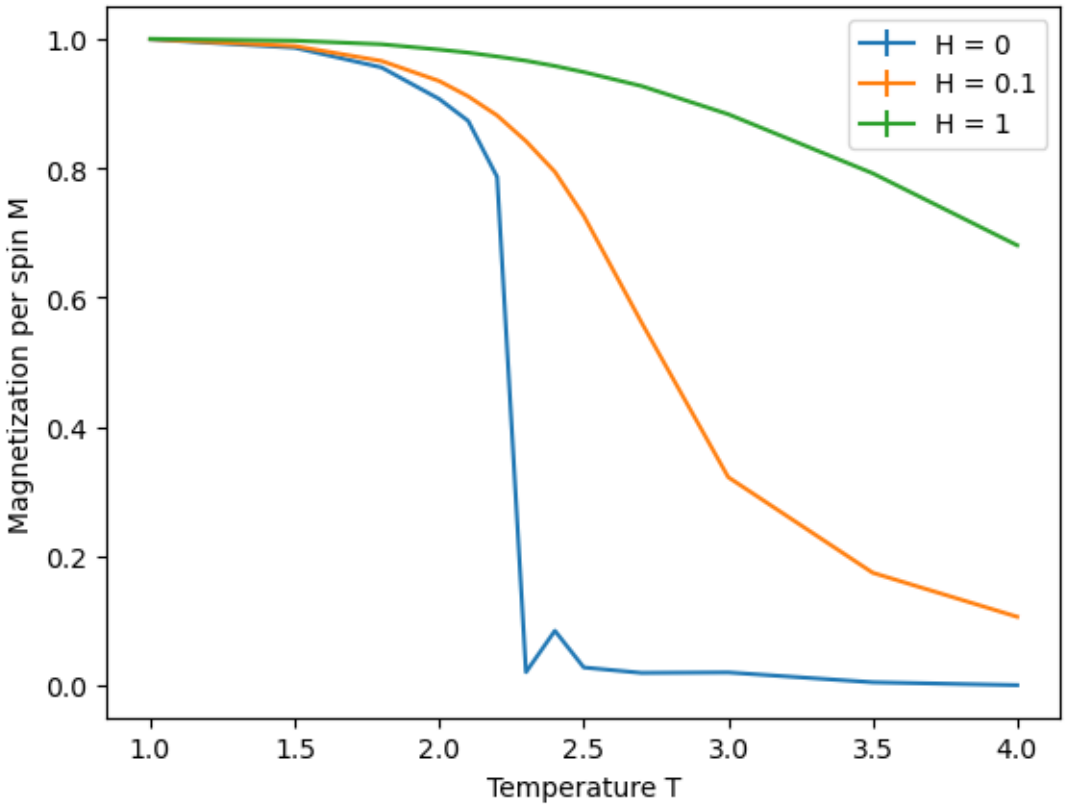
Note for graders: award full marks for similar observations, based on a plot similar to the one presented here.



C. Lattice in an external field

Question C.1. The figure below compares the magnetization versus temperature curves in the presence and in the absence of an external field. One can notice that, below the ferromagnetic phase transition temperature, the magnetization remains saturated at its maximum regardless of the external field. Above the transition temperature, the system starts to demagnetize, but still preserves some magnetization which, at a given temperature, is stronger as the external field increases. As the temperature increases, the magnetization decreases for each value of the external field. The field also "smoothens out" the phase transition, making it less obvious to detect. Still, one notices similar effects at similar temperatures so one could assert that introducing an external field does not affect the temperature of the phase transition.

Note for graders: award full marks for answers specifying all of the above explicitly, based on an appropriate plot.

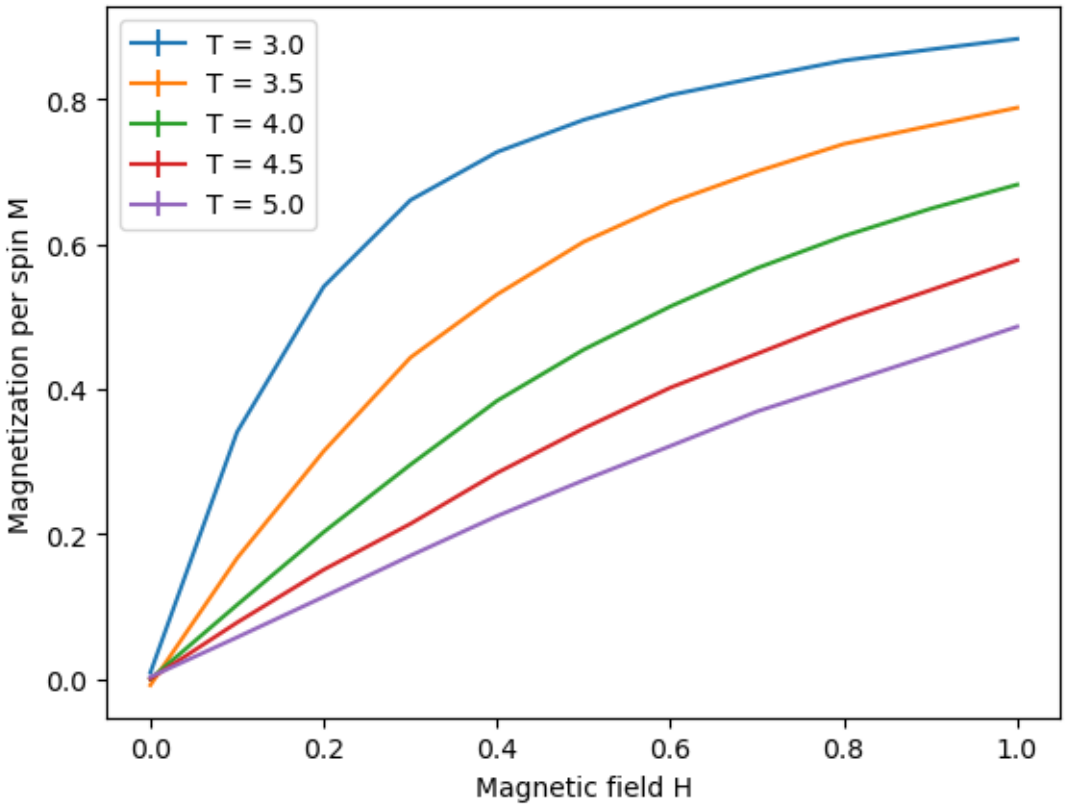


Question C.2. For this question, we set $T = 1$, and we perform 100 runs each for each of the external fields $H = 0.1$ and $H = 1$. For $H = 0.1$, after 98 of the 100 runs, the spins were aligned on the same direction with the external field (positive magnetization). For $H = 1$, all 100 runs led to a positive magnetization. Thus, we conclude that indeed the direction oriented along the field is preferred in this case.

Note for graders: award full marks for similar observations made on at least 20 runs for each field.

Question C.3. The plot below shows the magnetization-applied field dependences at five different temperatures. One notices that the magnetization increases with the applied field, and that after an initial linear increase regime, the magnetization tends to saturate. As the temperature increases, the dependences become less and less saturated.

Note for graders: award full marks for a similar plot with the same remarks, for five different temperatures.



Question C.4. The above dependences allow us to extract the susceptibilities. In the table below we show the obtained susceptibilities at the different temperatures. To compare with the Curie-Weiss law, we study a linearized dependence $\chi^{-1}(T)$, shown in the figure below. The data is very well fit by a line. From the slope and the intercept of the line, we obtain the Curie temperature $T_c = 2.58 \pm 0.16$. This value is in line with the ones obtained previously but it is slightly larger, showing that the Curie-Weiss model of paramagnetism does not quantitatively reproduce the results of the Ising model. Still, such a model yields impressively many of the same qualitative features.

Note for graders: for full marks, the participants need to show a data table with at least five susceptibilities. All results need to be presented with error bars. Any reasonable comparison with the Curie-Weiss law is acceptable. The takeaways of the discussion need to be those mentioned above.

[124]:

	T	chi	chi err
0	3.0	3.405652	0.170283
1	3.5	1.664007	0.083200
2	4.0	1.019137	0.050957
3	4.5	0.774814	0.038741
4	5.0	0.570666	0.028533

```
********************
slope =     0.6864 +/-  0.0270
intercept =    -1.7711 +/-  0.0886
Tc = 2.580218391369748 +/- 0.16431716852133216
********************
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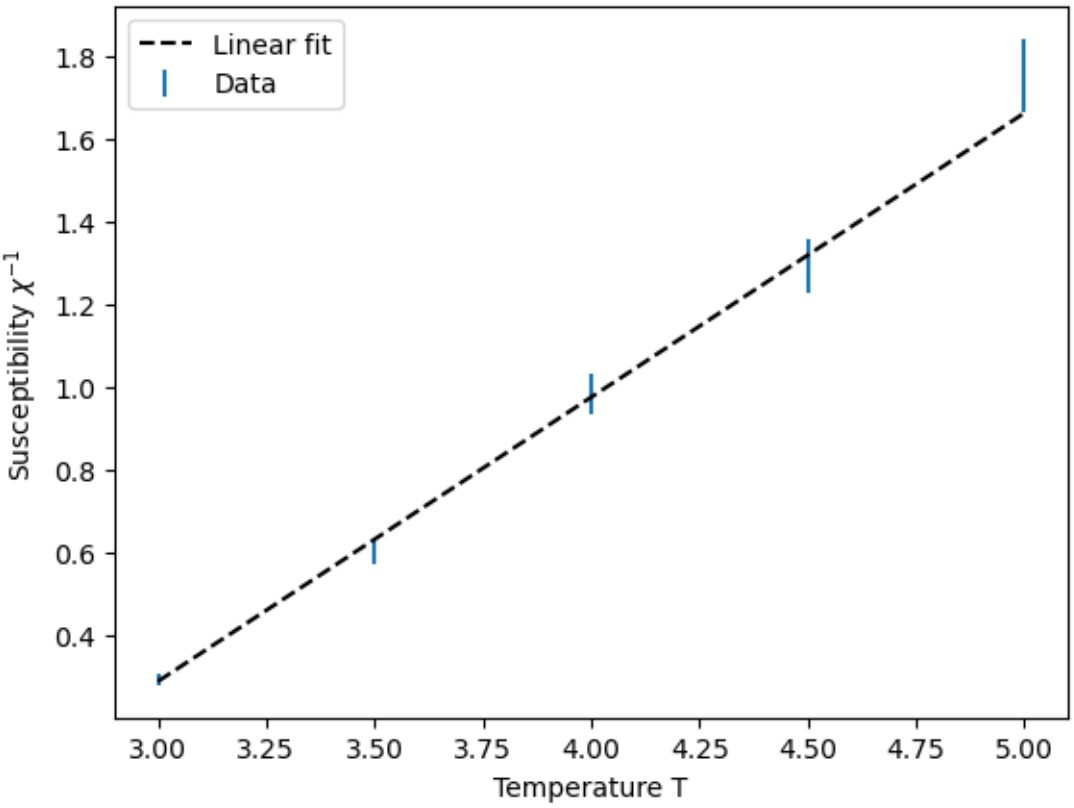

D. Antiferromagnetism

Question D.1. The behaviour remains largely the same: there is still a phase transition and it occurs around a similar temperature. The only change is how the ordered state looks like: rather than the spins being all aligned in the same direction, they form a checkerboard pattern, where each spin tends to align in the opposite directions of its neighbors.

Note for graders: award full marks for answers including all of the above.

Question D.2. Magnetization is no longer the relevant order parameter as, regardless of whether the system is in an ordered or an unordered state, the magnetization will still be equal to zero. In particular, there will be no sharp change in magnetization upon the phase transition. An alternative order parameter could be, for example

$$A = \frac{1}{L^2} \sum_{(i,j)} (-1)^{i+j} \sigma_{ij}$$

which takes into account the tendency of neighboring spins to oppose each other through the factor $(-1)^{i+j}$. Another order parameter could be the energy of the system, that jumps from a (significantly) nonzero value to zero upon the phase transition.

Note for graders: award full marks for any of the two suggestions above.