Ferromagnetic phase transition: the Ising model

Depending on the external parameters imposed on a physical system, its properties can vary drastically. One only needs to think of water at usual temperatures and pressures to see how, within a temperature range of about 100 K, it can change from solid to liquid, and finally onto gas. These three different states are examples of what is more generally called a *phase of matter*. The different phases of matter are characterized by differing physical properties, that undergo an abrupt change at a *phase transition*. The phase transitions are characterized by the external temperatures and pressures at which they can occur. One notes that phase transitions are *emergent phenomena*, meaning that they are specific to thermodynamic systems, which exhibit a very large number of microscopic degrees of freedom. When reducing the number of constituents of a system, the transition smoothens out. In such cases, one rather talks about *regimes* of matter and their *crossovers*.

The concept of a phase transition is not limited to the solid, liquid and gas states. Depending on the physical properties taken into account, one can distinguish further states of matter. More generally, we can associate to a phase transition with any process that involves a sudden change in the "order" of a system. Such order can be characterized by a well-chosen parameter of the system which allows to distinction between the ordered and the unordered phases.

For example, the magnetic state of a material is also subject to a phase transition. A material is in a *ferromagnetic state* when it exhibits a large, nonzero magnetization even in the absence of any external magnetic field. For example, iron at room temperature is in a ferromagnetic state. On the contrary, a material is in a *paramagnetic state* when it exhibits a zero net magnetization in the absence of a magnetic field, and applying an external magnetic field gives rise to a (small) colinear nonzero magnetization. This justifies that, in this case, the magnetization of the system is a possible order parameter describing the phase transition.

Before going forward, one must note that most solids at room temperature are paramagnetic, with few exceptions. One also distinguishes a third class of materials, called diamagnetic, that also have zero net magnetization in the absence of an external field, and which respond with a magnetization that opposes an external applied field. In this problem, we only consider transitions between ferromagnetic and paramagnetic states.

At a given temperature, most substances will either be in a ferromagnetic or in a paramagnetic state. At very low temperatures, a substance will always be ferromagnetic, and above a certain temperature T_c, called the *Curie temperature*, it will suddenly lose its magnetization and transition to a paramagnetic state. In this problem, we will investigate the Ising model of ferromagnetism. The system described by this model is simple enough to give an intuition of the physical situation, yet powerful enough to yield many qualitative features of real ferromagnets. Furthermore, it allows to explore the influence of the number of constituents on the phase transition.

In the Ising model, we consider a two-dimensional $L \times L$ lattice of *spins*, which can each either point *up* or *down*. The state of the spin at position (i, j) in the lattice is encoded by the number σ_{ij}, as follows

$$\sigma_{ij} = \begin{cases} +1 \text{ if the spin } (i,j) \text{ points up} \\ -1 \text{ if the spin } (i,j) \text{ points down} \end{cases} \tag{1}$$

The main assumption of this model is that neighboring spins in the lattice interact by a mechanism called *exchange interaction*. The parameter describing the exchange interaction for a ferromagnet is denoted by $J > 0$. If two neighboring spins point the same way (either both up or both down), the state is energetically favorable and contributes $-J$ to the energy of the system. When two neighboring spins point opposite ways, the state is energetically unfavorable and contributes an energy $+J$ to the system. Furthermore, one assumes for simplicity *periodic boundary conditions*: the spins on row L are assumed

to neighbor those on row 1 (as well as those on column L neighbor those on column 1). Then, the total energy of a given system of spins is given by

$$E = -\frac{J}{2} \sum_{u} \sum_{v \text{ neighbor of } u} \sigma_u \sigma_v \tag{2}$$

In such a system, the distinction between the ferromagnetic and the paramagnetic state can be done by choosing the *magnetization per unit spin* M as an order parameter. Its definition is

$$M = \frac{1}{L^2} \sum_{(i,j)} \sigma_{ij} \tag{3}$$

The absolute value of M will be very close to one in a ferromagnetic phase, whereas it will be almost zero in a paramagnetic phase.

The thermal description of the Ising model relies on Boltzmann statistics. In this description, two states α and β of a given system at temperature T, having energies E_α and E_β, will arise with probabilities p_α and p_β whose ratio is

$$\frac{p_\alpha}{p_\beta} = \exp\left(-\frac{E_\alpha - E_\beta}{k_B T}\right) \tag{4}$$

In order to compute the expectation values of thermodynamic parameters in the Ising model, one needs to consider all the possible spin configurations, compute their associated probabilities, and then average over all the different states with their corresponding probabilities. Given that there are 2^{L^2} possible configurations of an $L \times L$ spin-lattice, for N as low as 10, this already becomes a formidable task.

One can mitigate this limitation by noting that most of these states will yield a negligible contribution to the expected values. In fact, only a few of these most likely states will make a significant contribution. Selecting the relevant states, however, is also a non-trivial task. The solution that we take in this case is a *Monte Carlo simulation*. This approach relies on random sampling of states according to wisely chosen probability distributions, following Boltzmann statistics. Starting from a randomly chosen initial state, one evolves it through random spin flips, occurring with probabilities chosen by Boltzmann statistics. After a certain number of steps N_{eq}, the system can be considered as *equilibrated*, meaning that it will only be evolving among the most likely states mentioned before. Then, the system continues to evolve according to the same random procedure for a further number of steps N_{MC}. The expectation of a thermodynamic parameter is then obtained by computing its value for each of the states obtained during the Monte Carlo procedure and averaging over all the obtained values.

We provide an implementation of the said Monte Carlo algorithm. The adjustable parameters are the lattice size L, the exchange constant J, the temperature T of the system, as well as the number of steps in the Monte Carlo procedure N_{MC}. The number of equilibration steps is always chosen as $N_{eq} = N_{MC}/10$. The algorithm returns the expectation of the average magnetization per spin with its error bar, as obtained from the algorithm. The algorithm may also generate, for visualization purposes, a graphical representation for a thermal equilibrium configuration of spins. The purpose of this problem is to investigate the behavior of the average magnetization M as the three adjustable parameters vary.

One notes that the results generated by the algorithm correspond to the thermodynamic limit only asymptotically, ie. upon considering a very large system of spins undergoing a very high number of Monte Carlo steps. In practice, the algorithm is still quite time-consuming, and a single run can last up to several minutes. As such, for time efficiency reasons, you must limit the number of spins as well as the number of iterations. In doing so, you must be careful with the following trade-off: reducing these values too much might lead you to obtain non-relevant thermodynamics, and you might not be able to observe the required phase transitions! The strategy we suggest is the following: first, read through the entire problem to get a feeling of the questions you need to study. Then, take a while to play with the algorithm and get a feel of its typical runtime. Start with small lattices and small numbers of Monte Carlo steps, and increase the values steadily up until you get clear phase transitions in a reasonable runtime. Always mention the lattice size and the number of steps you use on your answer sheet.

You will need to produce several graphs and plots: you can either create them on your computer, using an available software of your choice (such as Excel), or using millimeter paper provided to you. If you create a digital graph, make sure to save it and hand it in, and explicitly mention the file name on your answer sheet. Also, hand in all of the data files on which your solution is based, and always mention the file name where the corresponding data is located. Your answers will not be graded if the graphs and data files are not handed in or not appropriately referenced in your solution.

A Phase transition and the critical temperature

In this section, work with a lattice size $L = 20$. Select an appropriate number of iterations so as to reach thermodynamic equilibrium.

A.1. (1 point) Set $J = 1$ and toggle the animation on. Observe the system at the temperatures $T = 1$, $T = 2$, $T = 3$ and $T = 4$. Qualitatively describe the results. Do you observe a phase transition? In what temperature range?

A.2. (2 points) Set $J = 1$ and plot the resulting (absolute value of) magnetization versus temperature. Present your data in a table. Obtain an estimate for the phase transition temperature.

A.3. (4 points) Repeat the experiment for several values of J. Plot the dependence of the critical temperature on the exchange parameter J and suggest a reasonable fit.

A.4. (1 point) In the ferromagnetic regime, is there a preferred direction of magnetization? Perform a sufficient number of experiments to draw a conclusion.

B The crossover regime

B.1. (3 points) Repeat the experiment for a small $L = 10$ and $L = 5$. How does the phase transition change?

C Lattice in an external magnetic field

Here, we introduce an additional term in the energy, accounting for an external magnetic field H, having the form

$$E_H = -H \sum_{(i,j)} \sigma_{ij} \tag{5}$$

Work again with a lattice size $L = 20$. Fix the value of $J = 1$.

C.1. (2 points) Repeat the experiment for $H = 0.1$ and $H = 1$. Plot the magnetization versus temperature curves and compare them with the curve obtained in the absence of a magnetic field. Does the external field influence the temperature of the phase transition?

C.2. (1 point) Focus on the ferromagnetic regime. Is there a preferred direction of magnetization in this case? Study both cases $H = 0.1$ and $H = 1$.

C.3. (2 points) Focus on the paramagnetic regime. Plot the dependence of the magnetization on the external field $0 < H < 2$ for five different temperatures. Compare these dependences and discuss.

For small enough external fields, one can assume that the magnetization responds linearly to the applied field. In that case, one can define the susceptibility of the system as

$$\chi = \frac{M}{H} \tag{6}$$

For paramagnetic substances, the susceptibility strongly depends on the temperature, according to the *Curie-Weiss* law

$$\chi(T) = \frac{\chi_0}{T - T_c} \tag{7}$$

where χ_0 is a fitting constant and T_c is the Curie temperature at which the phase transition occurs.

C.4. (2 points) Compute the susceptibilities from the previous question and investigate their temperature dependence. Compare with the Curie-Weiss law and comment.

D Antiferromagnetism

Setting a negative value for the exchange parameter $J < 0$ results in qualitatively different behavior, usually called *antiferromagnetism*.

D.1. (1 point) Set $J = -1$ and describe the resulting states for different temperatures. What are the phases of this system?

D.2. (1 point) Explain why magnetization is no longer the relevant parameter to describe the phase transition. Propose an alternative order parameter.