

## Session 1: key concepts and background

## 1 Introduction to the laboratory

In this laboratory we shall explore the basic physics of the *Ising model*. This is a simple theoretical model describing magnetism. While the model is simple to state and can be solved in some simple situations, it is still impossible to solve in general. Instead of exact mathematical solutions, the best way to understand the model is to simulate it numerically. The *Monte Carlo* method is a powerful numerical technique, using random numbers to sample statistically states out of a huge number of possible configurations. The aim of the laboratory is to use Monte Carlo simulation to model magnetism in the Ising model, extracting key physical information about the magnetic phase transition.

The laboratory is not intended as a programming exercise, but a 'computing laboratory', in which we use the computer as a sort of experimental tool. Using a simple numerical technique we will simulate the model, and calculate its various physical observables. Ultimately we will explore in detail the region of parameters close to the phase transition,  $T_c$ , looking for the remarkable properties of **scaling** and **critical phenomena**. We shall be mainly concentrating on the case of the Ising model on a square lattice in two dimensions. This is the simplest case which exhibits a true phase transition of **spontaneously-broken symmetry** type. We shall explore the theoretical methods used to study this sort of problem, both mathematically and numerically.

The laboratory is intended to be rather open-ended and depending on time students can explore one of a number of extensions and variations of the model. For example time permitting we can look at the exact solutions of the model in one dimension. Or, time permitting, students can use the computer to look at related models such as the Potts or XY models in two dimensions.

You are free to do the simulations in whatever programming language you prefer. I will provide an example simulation code written in python, which is freely available from the internet. But if you prefer to conduct the simulation in another language, such as C or Fortran I may be able to provide a basic code for you to use. I may or may not be able to help if you prefer any other languages. The lab is not a programming exercise, but you will be expected to understand the example code given to you and make small

modifications as needed, for example to extract and measure new observables during the simulation.

Given the covid restrictions I will be assuming that most of you will be working from home on your own laptops or desktop computers. But if you do not have access to a suitable computer at home, then we may be able to arrange for some of you to use the computers in the laboratory room 2.20. Alternatively some of you may wish to learn how to use larger high performance computers, such as the university's bluecrystal HPC system. There is some additional overhead in learning how to run simulations on this system, but the machine is more powerful than a single desktop or laptop, enabling larger and more accurate simulations to be run. But a successful simulation is not just about the size of the simulation, the best marks are for understanding how to extract important physics from the simulation data. It is a laboratory *in silico*, where we use the computer as a laboratory apparatus, and "experimental" tool.

## 2 Background introduction to phase transitions

The idea of a *phase transition* is a familiar one in everyday life, from water boiling in the kettle to snow or ice melting. What is occurring is a change of *phase* of a medium, which occurs at a specific and precisely defined temperature,  $T$ , pressure  $P$  etc. In the theory of thermodynamics we describe a system by an *equation of state*, such as the ideal gas law

$$PV = Nk_B T, \quad (1)$$

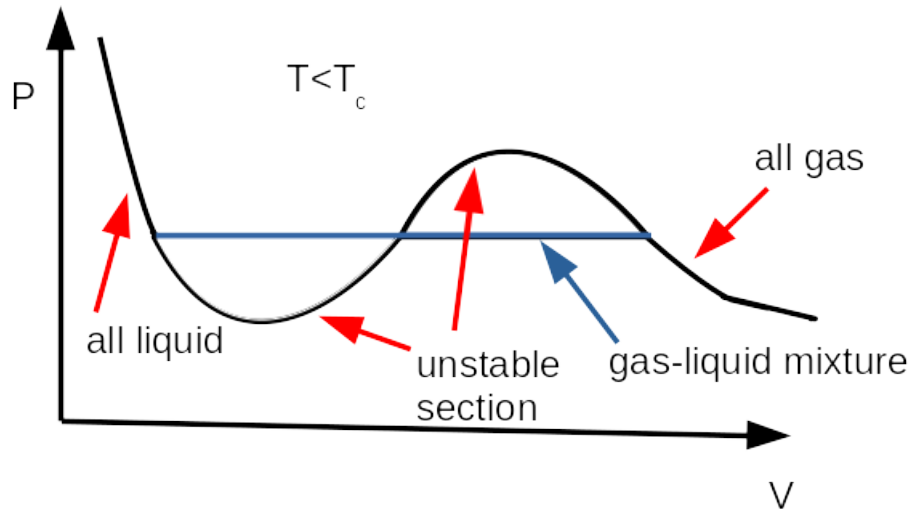
where  $N$  is the number of molecules and  $k_B$  is Boltzmann's constant. For a more realistic description of a gas we can use the van der Waals equation

$$\left( P + a \frac{N^2}{V^2} \right) (V - Nb) = Nk_B T. \quad (2)$$

The two new constants,  $a$  and  $b$  represent the effect of interactions between the molecules, which were neglected in the original ideal gas law. The constant  $a$  represents a long range force of attraction between molecules, while the constant  $b$  represents the fact that molecules have a finite size, and so we cannot compress the gas beyond a certain limit.

The effect of these two new terms is negligible if the density of molecules,  $N/V$  is small, but as the density is increased these begin to have some significant effects. At fixed temperature  $T$ , the curve  $P(V)$  develops a point of inflection, or *critical point*  $(P_c, V_c)$ , at some *critical temperature*  $T_c$ . A typical  $P(V)$  curve is shown below for the

case when the temperature  $T$  is below the critical temperature  $T_c$ .



In the van der Waals equation, as in the example shown above, at temperatures below the critical temperature  $T_c$ , the  $P(V)$  curve has some sections with positive slope, as shown above. The gas in the positive slope sections is *unstable*. We can see this because if we compress the gas here, decreasing volume  $V$ , the pressure goes down not up, and so the gas does not resist being compressed. In contrast, with the usual ideal gas law the *compressibility* of the gas is always negative:

$$\frac{\partial P}{\partial V} < 0.$$

This ensures stability, since if you try to compress a gas into a smaller volume the pressure will increase and resist the change. The instability coming from the van der Waals equation of state tells us that there must be a *phase transition*.

What happens in this region is that the gas separates into two parts, a liquid phase and a gaseous phase. So we have a *phase transition*. Starting at low density, to the far left part of the line shown in the figure, all of the molecules are in the gas phase. But decreasing the volume at constant temperature (isothermal) we eventually get to the point shown by the horizontal blue line. Here some of the gas condenses into droplets, and so we no longer have a pure single phase, but a mixture of the gas and liquid phases (a saturated vapour). Continuing to compress the gas the pressure  $P$  stays constant, but more and more of the gas condenses into the liquid droplets. Eventually, at the far

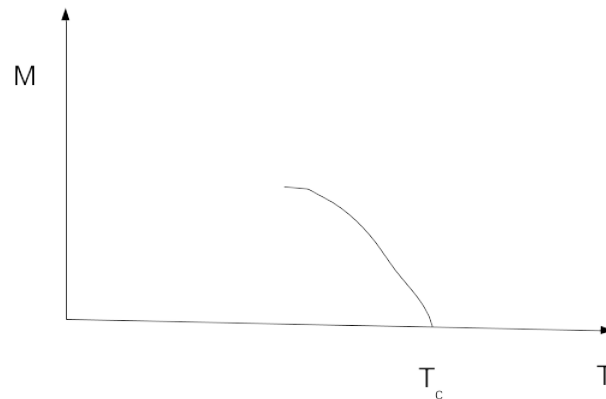
left of the blue line, all of the gas has condensed and we have a pure liquid.

Exercise 1: Use implicit differentiation (or otherwise) to find the critical temperature  $T_c$  where there is a point of inflection in the van der Waals  $P(V)$  curve at the critical pressure and volume  $(P_c, V_c)$ .

Magnetism is another very familiar phase transition, and this is the phase transition that the Ising model is designed to explain theoretically. In this case we consider the *magnetization* of a crystal,  $M$ , as a function of external magnetic field,  $B$ , and temperature  $T$ . We can assume each atom in the crystal has a spin, for example  $S_z = \pm\hbar/2$ , which can point in either of two directions, “up” or “down”. Neighbouring atoms like to point on the same direction as each other so at absolute zero temperature we have two possible, equivalent, ground states, either all of the spins are “up” or all of them “down”. These are magnetic states with a finite magnetization  $M$ . If all the spins are all “up”  $M$  would be positive, and if all of them are “down”  $M$  would be negative. This describes a simplified picture of a typical *ferromagnet*, such as iron.

Raising the temperature above absolute zero, entropy favours the spins become random. At very high temperatures each spin would randomly be up or down with equal probability, and so on average there would be as many “up” as “down” and the total magnetization  $M$  is zero (in zero external magnetic field). Changing the temperature continuously from absolute zero we will find there is a critical temperature,  $T_c$ , above which the magnetization  $M$  becomes zero, when equal numbers of spins point in each

direction. This is the classic magnetic phase transition, as shown below.

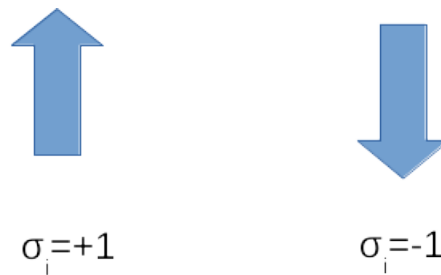


There are very many other phase transitions known in physics. Another example, in the case of *superconductivity* a condensate of Cooper pairs appears at a given temperature,  $T_c$ , which changes a normal metal into a superconducting one, leading to zero resistance and expulsion of magnetic flux.

The Ising model has a central place in mathematical physics and the theory of phase transitions. It was introduced as a model of the magnetic phase transition, eg as in iron at the Curie temperature,  $T_c$ . By studying this model it is possible to learn a great deal about many different types of phase transitions, as well as magnetism. Even more than that, by studying properties of the model it has provided a framework which led to a general approach applicable to considering many other types of phase transitions in physics, ranging from magnetism, to superfluids, superconductors. In turn, these insights led to the Higgs mechanism in particle physics. Such phase transitions are examples of **spontaneously-broken symmetry**, namely that the symmetry of the system changes as the temperature passes through a critical temperature  $T_c$ . In a very analogous way in particle physics the Higgs mechanism for generating mass is based on the idea that a Higgs field is present everywhere in the vacuum, changing its symmetry. The Ising model provides the simplest model known in which this occurs. Therefore by studying the Ising model we can explore many of these types of phenomena theoretically.

### 3 Statement of the Ising Model

The beauty of the Ising model is that it is very easy to state. Consider a lattice of atoms for example in a crystal. The example of a square lattice in two dimensions is illustrated below. Each atom is assumed to have a magnetic moment or spin, which can have only two possible values, which we shall denote as  $\sigma_i = \pm 1$ .



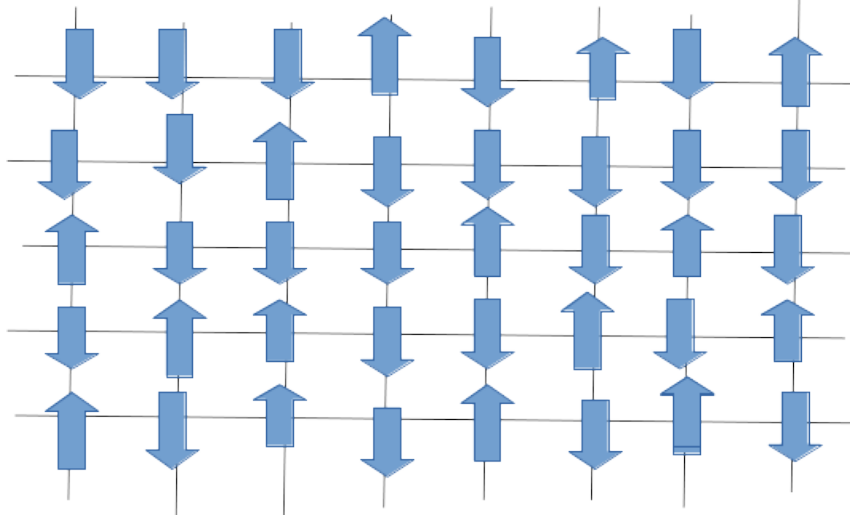
The spin on each atom will have an energy which depends on both an external magnetic field,  $B$ , and also on the values of the spins of the nearest neighbour atoms. The energy for the system can then be represented as

$$H = - \sum_{\langle ij \rangle} J \sigma_i \sigma_j - \sum_i B \sigma_i \quad (3)$$

We use the symbol  $H$  for the energy because this is a Hamiltonian. But it is not a quantum mechanical one, like you saw in 2nd year quantum physics, but a classical one of the type as you will see later this year if you do Analytical Mechanics course. Using classical physics we can measure each atomic spin without any quantum measurement problems. But even the classical Hamiltonian above is a mathematically hard problem, since if there are  $N$  spins in our lattice there are  $2^N$  possible configurations of the whole lattice. It is impossible to count all of these exactly, except in some special cases!

The notation  $\langle ij \rangle$  used above means that we sum over all the nearest neighbour bonds in the lattice, i.e. that sites  $i$  and  $j$  are next to each other. Each bond is counted only once in the sum. For example in the square lattice each site has four nearest neighbours, so we sum over the four bonds, between site  $i$  and its neighbours  $j$  in the

sites above, left, right and below.



In the Hamiltonian the constant  $J$  is the **exchange energy**, which (because of the minus sign in front ) favours having neighbouring spins pointing in the same direction (assuming that here  $J > 0$ ). This is therefore a model of a **ferromagnet**. The case  $J < 0$  would describe an **anti-ferromagnet** in which neighbouring spins like to be opposite.

Note that here we are not using SI units for the spin or magnetic field. If necessary it would be trivial to go back to SI units by making the spins  $S_z = \pm\hbar/2$  instead of  $\pm 1$ , but this would just lead to a redefinition of the exchange constant  $J$  and the magnetic field  $B$  by the appropriate constants. In fact it greatly simplifies the derivations later to use the units which are more natural to describe the mathematics of the problem. The most natural unit of energy here is the exchange energy  $J$ . Taking this as our unit of energy, this can be compared naturally to the energy of the spin in the magnetic field  $\pm B$ . Effectively we are defining both  $J$  and  $B$  by the energies they lead to.

We shall not attempt to 'derive' the Ising model, since it is a model and not necessarily specific to any real physical system. But perhaps it is helpful to note that in a real magnetic system the atomic spins can point in any direction, but the crystal structure usually leads to some preferred directions aligned with the crystal lattice. This is a result of **spin-orbit coupling**. But here we will be using the two states 'up' and 'down' spins as merely mathematical labels on the two possible states, and these have no particular link to the orientations in space of the model lattice. In fact the Ising model could

be used to model any other physical system where each lattice site has two possible states. For example it can be used to model an alloy where each lattice site might be occupied by one of two types of atom, such as say, a copper or nickel atom. Here it is the mathematical nature of the model which we wish to explore, especially what it tells us about phase transitions.

## 4 Key Principles of Statistical Physics

You have been introduced to the key concepts of thermodynamics and statistical physics in 2nd year. Here we just restate the main concepts which we will need here.

Here we wish to consider the system at a fixed temperature,  $T$ . The Boltzmann law states that at a given temperature  $T$  each *microstate* of a system occurs with probability

$$p = \frac{1}{Z} \exp(-H/k_B T) \quad (4)$$

where  $H$  is the Hamiltonian, or energy, of that microstate,  $k_B$  is Boltzmann's constant, and  $Z$  is the **partition function**,

$$Z = \sum \exp(-H/k_B T) \quad (5)$$

summed over all possible microstates.

Exercise 2: In our “theorist” units we took the exchange energy  $J$  as our unit of energy. If we also measure temperatures in the same units, then the Boltzmann constant,  $k_B$  becomes equal to 1. Energy and temperature are effectively the same thing dimensionally, it is only for historical reasons that we measure one in Joule and the other in Kelvin. Find the temperature in Kelvin corresponding to an energy of 1 electron volt (1eV).

We will leave the constant  $k_B$  in the formulas below, to keep them looking like the textbook formulas. But note that in our simulations we will measure temperature in units of  $J$  and therefore not need the Boltzmann constant.

In our case a microstate, or **configuration** of the model is any specific set of values  $\sigma_i = \pm 1$  for each spin in the system. So if we have  $N$  spins altogether there are  $2^N$  such configurations in the sum. Clearly if we have more than a very small number of spins, we cannot examine all possible configurations. The method we will use to study this numerically will make use of a computer algorithm, called the Metropolis algorithm, which will generate configurations with probabilities given by the above Boltzmann law.



The above probabilities can be used to calculate statistical averages of all physical quantities. For example the average energy is

$$U = \langle H \rangle = \frac{1}{Z} \sum H \exp(-H/k_B T) \quad (6)$$

and the average value of the spin on atom  $i$  is

$$\langle \sigma_i \rangle = \frac{1}{Z} \sum \sigma_i \exp(-H/k_B T). \quad (7)$$

The entropy is another important quantity, which we can find using Shannon's formula

$$S = -k_B \sum p \ln(p) \quad (8)$$

where again the sum is carried out over all  $2^N$  possible configurations.

Another useful quantity is the (Helmoltz) Free energy

$$F = U - TS. \quad (9)$$

This is useful when we consider systems at a given temperature  $T$  as we are doing here (called the canonical ensemble). We can consider  $F$  a natural function of temperature  $T$  and the other external parameters, eg here magnetic field  $B$ . Differentiating gives us a relationship analogous to the 1st law of thermodynamics

$$dF = dU - SdT \quad (10)$$

and so we can find the entropy  $S$  by differentiating

$$S = \frac{\partial F}{\partial T} \quad (11)$$

The total magnetization,  $M$ , of the sample is

$$M = \sum_i \langle \sigma_i \rangle = \frac{1}{Z} \sum \sigma_i \exp(-H/k_B T) \quad (12)$$

which for our Ising Hamiltonian can be conveniently rewritten as

$$M = \sum_i \langle \sigma_i \rangle = \frac{\partial \langle H \rangle}{\partial B}. \quad (13)$$

or in terms of the free energy

$$M = \frac{\partial F}{\partial B}. \quad (14)$$

implying that

$$dF = -SdT + MdB. \quad (15)$$

This implies we can consider the free energy as a natural function of the  $T$  and  $B$  variables,  $F(T, B)$ , as discussed above. For comparison this is similar mathematically to with the usual 1st/2nd laws for a gas where the total energy changes as  $dU = TdS - PdV$  and the free energy as  $dF = -SdT - PdV$ .

Finally some elegant relations relate the total energy,  $U$ , and free energy,  $F$ , to the partition function  $Z$ . So if we can find  $Z$  as a function of temperature  $T$  and magnetic field  $B$  all of the other observable quantities are easy to find mathematically.

Writing  $\beta = 1/k_B T$  it can easily be shown that

$$U = -\frac{\partial \ln(Z)}{\partial \beta} \quad (16)$$

and

$$F = -k_B T \ln(Z). \quad (17)$$

So in principle all thermodynamic quantities we would wish to calculate can be found solely from knowledge of the partition function  $Z$ .

Exercise 4: Derive the last two equations given above. Hint: use the equations provided earlier in this section for  $S$  and  $U$  to find  $F = U - TS$ .

## 5 Exact solution for a single spin

First consider a single spin only. The Hamiltonian is simply

$$H = -B\sigma \quad (18)$$

where the allowed values of  $\sigma$  are just  $\pm 1$ . There are only two microstates and their energies are given by  $\pm B$ . Therefore the partition function is simply

$$Z = \exp(-B/k_B T) + \exp(B/k_B T) \quad (19)$$

The average value of the spin is easily found to be

$$\langle \sigma \rangle = \tanh(B/k_B T) \quad (20)$$

Exercise 5: Plot the function  $\langle \sigma \rangle$  as a function of  $B$ . Indicate on your sketch how different temperatures change the curve. Using the formulas given above evaluate the total energy  $U$ , free energy,  $F$ , entropy  $S$ , and specific heat ( $C = TdS/dT$ ) for this system.

## 6 Mean-field Theory

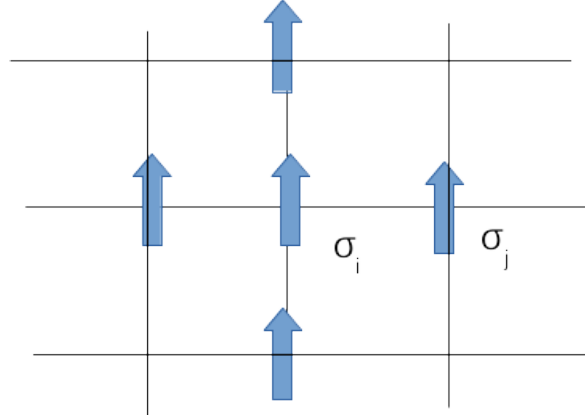
The results from the previous section can be exploited to find a much more interesting answer. This is the **mean-field** solution.

Assume that in the lattice, each spin  $\sigma_i$ , is experiencing the effects of its neighbours as an average effective energy. So in the Hamiltonian we make the approximation

$$\begin{aligned}
 H &= - \sum_{\langle ij \rangle} J \sigma_i \sigma_j - \sum_i B \sigma_i \\
 &= - \sum_{\langle ij \rangle} J \sigma_i \langle \sigma_j \rangle - \sum_i B \sigma_i \\
 &= - \sum_i B_{eff} \sigma_i
 \end{aligned} \tag{21}$$

where the effective magnetic field on spin  $i$  is a sum of both the external field and the average effect of the neighbouring spins  $j$

$$B_{eff} = B + J \sum_{\text{neighbours } j} \langle \sigma_j \rangle. \tag{22}$$



Each spin is equivalent, on average, and so the neighbouring spins will all have the same average spin  $\langle \sigma_j \rangle$ . If there are  $z$  neighbours (eg 4 for the square  $2d$  lattice), we get

$$B_{eff} = B + zJ\langle \sigma_i \rangle. \quad (23)$$

Combining this with the single site results obtained earlier we get the following **self-consistent** equation for the average value of spin  $i$

$$\langle \sigma_i \rangle = \tanh((B + zJ\langle \sigma_i \rangle)/k_B T) \quad (24)$$

This is now an interesting result. To see why let us consider the simplest case where there is no external magnetic field,  $B$ . This gives us

$$\langle \sigma_i \rangle = \tanh((zJ\langle \sigma_i \rangle)/k_B T). \quad (25)$$

We cannot solve this equation directly, it is a *transcendental* equation. But we can easily see if it has any solutions by plotting the graphs for both the left and right hand sides.

If the graphs intersect we have a solution.

Exercise 6: Plot yourself both sides of this equation as a function of  $\langle\sigma_i\rangle$  looking for points where the left and right hand sides are equal, giving a solution of the transcendental equation. Notice that all the physical constants can be combined into a single dimensionless variable, say  $x = zJ/k_B T$ , so we only need to plot graphs for a few different values of this dimensionless  $x$  to see the whole range of possible solutions.

Notice that whatever the values of the parameters there is a trivial solution  $\langle\sigma_i\rangle = 0$ . This corresponds to the non-magnetic phase.

But if the parameters are such that  $zJ/k_B T > 1$  then you should see that in addition to the trivial solutions there are two others, one with  $\langle\sigma_i\rangle > 0$  and one with  $\langle\sigma_i\rangle < 0$ . The system will *spontaneously* choose one or other of these two solutions. In other words we have a **ferromagnet** with a spontaneous magnetic moment. The temperature when this happens in our approximate solution is

$$T_c = zJ/k_B. \quad (26)$$

(The fact that the system spontaneously chooses to have a single spin direction out of the two equivalent alternatives is called *spontaneous symmetry breaking*. It is essentially like the Higgs field spontaneously breaking symmetries in particle physics).

## 7 Summary

- We have reviewed basic ideas about *phase transitions* with examples from the van der Waals gas and a ferromagnet.
- We revised some key concepts from *statistical physics*, such as partition function and free energy.
- We defined the Ising model and its approximate solution in *mean field theory*, showing the existence of a magnetic phase transition at temperature  $T_c = zJ/k_B$ .

In the next session we will examine the Monte Carlo algorithm to solve the Ising model, and see that the exact solution has some important differences from the simple mean-field results found above.