

Figure 1: A plot of the magnetisation of nickel (Ni) (in rather old units, sorry) as a function of temperature. The magnetisation of Ni goes to zero at its Curie temperature of 627K.

1 The Paramagnet to Ferromagnet Phase Transition

The magnetic spins of a magnetic material, e.g., nickel, interact with each other: the energy is lower if the two spins on adjacent nickel atoms are parallel than if they are antiparallel. This lower energy tends to cause the spins to be parallel and below a temperature called the Curie temperature, T_c , most of the spins in the nickel are parallel, their magnetic moments then add up constructively and the piece of nickel has a net magnetic moment: it is a ferromagnet. Above the Curie temperature on average half the spins point in one direction and the other half in the opposite direction. Then their magnetic moments cancel, and the nickel has no net magnetic moment. It is then a paramagnet. Thus at T_c the nickel goes from having no magnetic moment to having a magnetic moment. See Fig. 1. This is a sudden qualitative change and when this happens we say that a phase transition has occurred. Here the phase transition occurs when the magnetic moment goes from zero to non-zero. It is from the paramagnetic phase to the ferromagnetic phase.

Another example of a phase transition is when water freezes to ice, here we go from a liquid to a crystal with a crystal lattice. The lattice appears suddenly. Almost all phase transitions are like the paramagnet-to-ferromagnet phase transition and are driven by interactions. Here we will study the Ising model. This is pretty much the simplest model which shows how interactions, in this case between the spins, can bring about a sudden qualitative change — a phase transition.

When there are interactions we almost always have to make approximations in order to calculate the values of the properties, e.g., T_c , that we are interested in. Here we will introduce a very popular approximation in physics: the mean-field approximation.

1.1 The Ising model of a ferromagnet

The Ising model is a very simple model of a magnetic material, i.e., a material like nickel that is ferromagnetic at low temperatures. At high temperatures, magnetic materials are paramagnetic. Recall that a ferromagnet has a non-zero magnetic moment even when it is not in a magnetic field, whereas a paramagnet only has a magnetic moment when it is in a magnetic field. So, if we take a hot magnetic material which is not in a magnetic field it will not have a magnetic moment. But if we cool the magnetic material then at Curie temperature, T_c , the material suddenly goes from not having a magnetic moment to having a magnetic moment. This is an example of a *phase transition*. The Ising model has a phase transition, below which it has a magnetic moment, above which it does not. For simplicity we choose to study it in 2 not 3 dimensions. The Ising model in 2 dimensions consists of a square lattice with each lattice site occupied by a model spin. Note that the model is classical, there is no quantum mechanics involved. For simplicity this spin can only point up or down. Adjacent spins interact with each other. By adjacent sites we mean that a spin interacts with the 4 spins north, south, east and west of it. A schematic of the 2-dimensional Ising model is shown in Fig. 2. If 2 adjacent

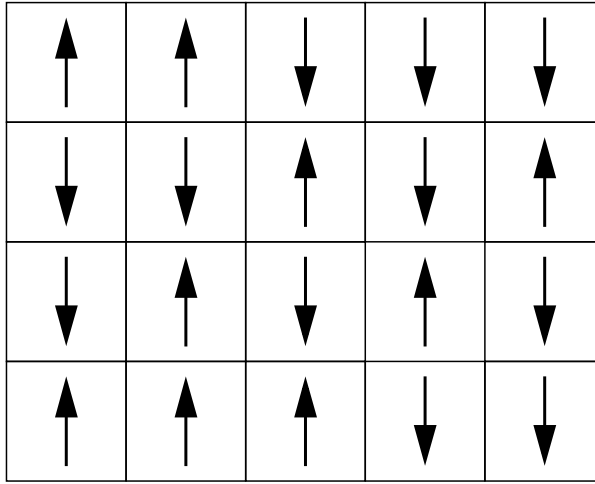


Figure 2: A schematic of the 2-dimensional Ising model. Only a small part of a lattice is shown. The squares represent the lattice and the up and down arrows the up and down spins.

spins are parallel then the energy of interaction is set equal to $-J$, if they are antiparallel the energy is set to J . If J is positive then the energy is lower for a pair of parallel spins than for a pair of antiparallel spins — the interaction is like that in a ferromagnet, it acts to align the spins so they all point in the same direction. Here we will always take J to be positive and so our model is a very simple model of a ferromagnet.

If we have N spins then we need N numbers, one to tell us whether each spin is point up or down. We denote these numbers s_i , $i = 1, 2, 3, \dots N$. If spin i points up, $s_i = +1$, and if it points down $s_i = -1$,

$$s_i = \begin{cases} 1 & \text{if the } i\text{th spin is pointing up} \\ -1 & \text{if the } i\text{th spin is pointing down} \end{cases}, \quad (1)$$

Then if the two spins s_i and s_j are adjacent the interaction energy is

$$\text{interaction energy} = -Js_i s_j = \begin{cases} -J & s_i = s_j = 1 \text{ or } s_i = s_j = -1 \\ J & s_i = 1 \ s_j = -1 \text{ or } s_i = -1 \ s_j = 1 \end{cases} \begin{matrix} \text{spins parallel} \\ \text{spins antiparallel} \end{matrix} \quad (2)$$

At 0K the model will be in the lowest energy state possible: the ground state. As the energy is lower for parallel than for antiparallel spins this corresponds to all the spins parallel. There are two such states, one with all the spins pointing up and one with all the spins pointing down. As all the spins are pointing in the same direction at 0K the Ising model is in a ferromagnetic state. A ferromagnetic state is defined as being one in which the spins, on average, point either up or down. If we define S as

$$S = \sum_{i=1}^N s_i, \quad (3)$$

then the model is ferromagnetic if and only if $S \neq 0$. At 0K, S is either $+N$ or $-N$.

In the opposite limit, that of $T \rightarrow \infty$ then the interactions are irrelevant. Then adjacent spins are as likely to be antiparallel as parallel and so are as likely to point up as down. So half the spins will point up and half down. Therefore, S , Eq. (3), is a sum of $N/2$ from the 50% of the spins that point up and $-N/2$ from the other 50% of the spins which are point down: $S = N/2 - N/2 = 0$. At high temperatures the model is not ferromagnetic. As it is ferromagnetic at low temperatures and not at high temperatures there must be a point, a temperature T_c , at which the model goes from being ferromagnetic to not being ferromagnetic: this point is a phase transition. At this point S goes from being nonzero to being 0. Locating this phase transition is one of the tasks of an approximate theory.

1.2 Mean-field theory

The average value of S , call it $\langle S \rangle$, will be zero in a paramagnet but non-zero in a ferromagnet. As will the average value of the spin at a single site $\langle s \rangle = \langle S \rangle / N$. So, if we can calculate $\langle s \rangle$ we can find at what temperature it

becomes non-zero, which is the temperature of the phase transition. This is tough to evaluate exactly so we will resort to an approximation called a mean-field approximation (the reason for the name will become clear later on). Consider just one spin, with a spin of $s = \pm 1$. It interacts with its four neighbours, we denote the spins north, south, east and west by s_N, s_S, s_E and s_W . Then the interaction energy of our single spin with these four surrounding spins is

$$\text{energy} = -J [s s_N + s s_S + s s_E + s s_W] = -sJ [s_N + s_S + s_E + s_W] \quad (4)$$

The central spin has two states $s = \pm 1$ but as we don't know the values of s_N, s_S, s_E and s_W , we cannot calculate the probabilities of these two states. So we make an approximation, we approximate the sum of the four surrounding spins by four times the mean spin $\langle s \rangle$

$$s_N + s_S + s_E + s_W = 4\langle s \rangle \quad \text{mean-field approximation} \quad (5)$$

Note that at the moment we do not know the value of $\langle s \rangle$, but we will calculate it below. Now, the energies of the two states of the central spin are

$$\begin{aligned} s = +1 & \quad \text{energy} = -4J \langle s \rangle \\ s = -1 & \quad \text{energy} = +4J \langle s \rangle \end{aligned}$$

and so the Boltzmann weights, $\exp(-\text{energy}/kT)$, of the two states are $\exp(+4J \langle s \rangle /kT)$ and $\exp(-4J \langle s \rangle /kT)$. Thus the partition function of the central spin is

$$z = \exp(4J \langle s \rangle /kT) + \exp(-4J \langle s \rangle /kT) \quad (6)$$

and the probabilities of the two states are

$$\begin{aligned} \text{probability of spin-up state} &= \frac{\exp(4J \langle s \rangle /kT)}{\exp(4J \langle s \rangle /kT) + \exp(-4J \langle s \rangle /kT)} \\ \text{probability of spin-down state} &= \frac{\exp(-4J \langle s \rangle /kT)}{\exp(4J \langle s \rangle /kT) + \exp(-4J \langle s \rangle /kT)} \end{aligned}$$

Thus the mean value of the spin

$$\begin{aligned} \langle s \rangle &= \frac{1 \times \exp(4 \langle s \rangle J/kT) + (-1) \times \exp(-4 \langle s \rangle J/kT)}{\exp(4 \langle s \rangle J/kT) + \exp(-4 \langle s \rangle J/kT)} \\ \langle s \rangle &= \tanh(4 \langle s \rangle J/kT). \end{aligned} \quad (7)$$

Solutions of this equation occur when the two curves, $y = \langle s \rangle$ and $y = \tanh(\langle s \rangle 4J/kT)$ cross. In Fig. 3 we have plotted $y = \tanh(\langle s \rangle 4J/kT)$ at $4J/kT = 0.5$ as a dot-dashed curve, as well as $y = \langle s \rangle$. We see that the two curves $y = \langle s \rangle$ and $y = \tanh(\langle s \rangle /2)$ only cross at $\langle s \rangle = 0$. So here the only solution is one with zero magnetic moment: a paramagnet. So at a temperature such that $4J/kT = 0.5$, i.e., at $T = 8J/k$, the Ising model is in the paramagnetic state.

However, when $4J/kT = 2$, i.e., at a temperature $T = 2J/k$, then the two curves are $y = \langle s \rangle$ and $y = \tanh(2 \langle s \rangle)$ (dotted curve). These curves also cross at $\langle s \rangle = \pm 0.96$. There are ferromagnetic solutions, solutions with non-zero $\langle s \rangle$ at this temperature: the Ising model is in the ferromagnetic state. Thus the Curie temperature must lie between $2J/k$ and $8J/k$.

Now we would like to find the Curie temperature, the temperature of the paramagnet-to-ferromagnet phase transition. Just above the transition temperature we have a paramagnet so $\langle s \rangle = 0$, so just below the transition we expect that $\langle s \rangle$ will be small, only a little above or below 0. Then we can use the Taylor expansion of \tanh . This is

$$\tanh(x) = x - \frac{1}{3}x^3 + \dots, \quad (8)$$

$\tanh(x)$ is an odd function of x so only odd powers of x appear. If we expand the \tanh function of Eq. (7) like this we get

$$\langle s \rangle = (4J/kT) \langle s \rangle - \frac{1}{3}(4J/kT)^3 \langle s \rangle^3 + \dots \quad (9)$$

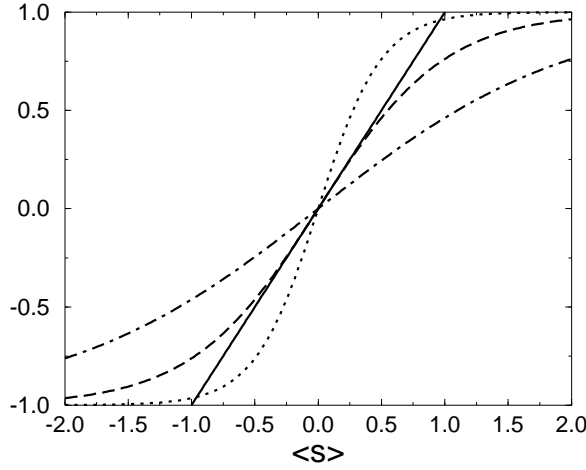


Figure 3: The tanh function. The solid line is the curve $y = \langle s \rangle$, the dashed curve is $y = \tanh(\langle s \rangle)$, the dotted curve is $y = \tanh(2 \langle s \rangle)$, and the dot-dashed curve is $y = \tanh(\langle s \rangle / 2)$.

Now, very very slightly below the Curie temperature $\langle s \rangle \ll 1$ and so we can neglect the $\langle s \rangle^3$ term. It is the cube of a very small number and so is extremely small. But then we have an equation for the Curie temperature, T_c ,

$$\langle s \rangle = 4(J/kT_c) \langle s \rangle \quad \text{or} \quad T_c = \frac{4J}{k}. \quad (10)$$

When $\langle s \rangle$ is not very small we have to solve the full equation.

I have done so and the resulting $\langle s \rangle$ as a function of temperature is plotted in Fig. 4. Compare this theoretical curve we have calculated with the measured curve for Ni in Fig. 1. We see that there is good agreement between the two. We can see that $\langle s \rangle$ is zero above the Curie temperature and non-zero below. At low temperatures it tends to 1, all the spins are parallel. Note that there is another, equivalent, solution which is the negative of the one plotted in Fig. 4. it is the solution with most of the spins pointing down not up. Also remember that the mean-field theory we are using is approximate not exact and so our Curie temperature, Eq. (10), is not the exact value but an approximation. The true Curie temperature of the Ising model is actually a little lower than our approximate theory predicts.

Returning to Eq. (9), for small $\langle s \rangle$ we retain the cubic term. Then we can cancel one power of $\langle s \rangle$ to obtain

$$1 = (4J/kT) - \frac{1}{3}(4J/kT)^3 \langle s \rangle^2. \quad (11)$$

Using the definition of the Curie Temperature, T_c , this becomes

$$1 = \frac{T_c}{T} - \frac{1}{3} \left(\frac{T_c}{T} \right)^3 \langle s \rangle^2. \quad (12)$$

We can rearrange this equation to get an equation for $\langle s \rangle^2$,

$$\langle s \rangle^2 = \frac{T_c/T - 1}{(1/3)(T_c/T)^3} = 3 \frac{1 - T/T_c}{(T_c/T)^2} \quad (13)$$

where to get the second expression we multiplied top and bottom by T/T_c . Now we define a distance along the temperature axis from the Curie temperature $t = 1 - T/T_c$, which close to T_c is $\ll 1$. As we are close to T_c T/T_c is close to one, we set the factor of $(T/T_c)^2$ equal to one. Then we have

$$\langle s \rangle^2 = 3t \quad \langle s \rangle = \sqrt{3t}^{1/2}, \quad (14)$$

the mean spin, and hence the magnetic moment of the ferromagnet, increases as the square root of t the amount by which we are below the Curie temperature. To put it another way t^2 is proportional to $\langle s \rangle$ and so if you view t as a function of $\langle s \rangle$ in Fig. 4 then the function is a parabola.

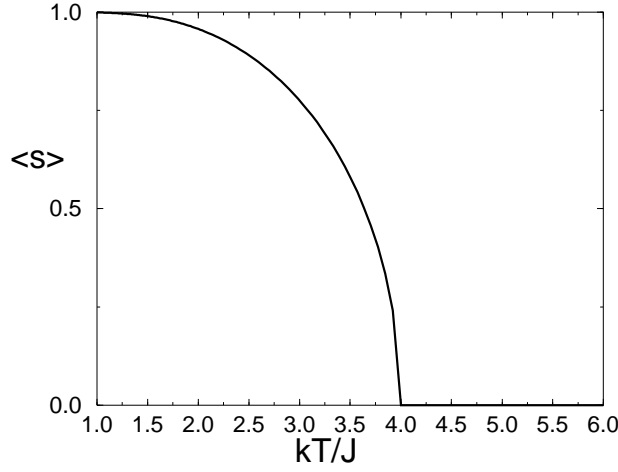


Figure 4: The mean value of the spins, $\langle s \rangle$, as a function of temperature. $\langle s \rangle$ becomes zero at the Curie temperature $kT_c/J = 4$.

It is simple to calculate how $\langle s \rangle$ varies with temperature just below the Curie temperature, we simply take the derivative of Eq. (14),

$$\frac{d \langle s \rangle}{dT} = \frac{\sqrt{3}}{2} t^{-1/2}, \quad (15)$$

and so as we approach the Curie temperature from below t tends to 0 and so the derivative of $\langle s \rangle$ with respect to the temperature diverges. This is seen in Fig. 4 where we see that the curve of $\langle s \rangle$ is vertical at the Curie temperature.

1.3 Fluctuations and response

Here we will look at and compare the fluctuations in the total spin $S = \sum_i s_i$, with its response, i.e., how its value changes, when an magnetic field h is applied. Applying a magnetic field to our system of spins, changes the energy of the states. Each spin s_i interacts with the magnetic field and so when the field h is non-zero there is an energy of the interaction between the i th spin and the field, which is equal to $-hs_i$. Thus, the total energy of all N spins in a magnetic field, which we call ϵ_h , is

$$\text{energy of spins in magnetic field} = \epsilon(s_1, s_2, \dots, s_N) - \sum_{i=1}^N hs_i = \epsilon(s_1, s_2, \dots, s_N) - hS \quad (16)$$

where $\epsilon(s_1, s_2, \dots, s_N)$ is the energy of the interactions between the spins, the sum over all the $-Js_i s_j$ terms. Above, we used definition of the total spin S , Eq. (3).

Just as in the section ‘Fluctuations’ where we started with the expression for the average energy, we will start from the expression for an average value. There it was the average of the energy but here it is the average value of the total spin, $\langle S \rangle$. Now, the average of the total spin $\langle S \rangle$ is, by definition,

$$\langle S \rangle = \frac{\sum_{\text{all states}} S \exp(-\epsilon/kT + hS/kT)}{\sum_{\text{all states}} \exp(-\epsilon/kT + hS/kT)} = \frac{\sum_{\text{all states}} S \exp(-\epsilon/kT + hS/kT)}{Z} \quad (17)$$

where the Boltzmann weights contain the total energy of Eq. (16) which has two parts: one from the interactions between the spins (which is ϵ and which we don’t need to worry about) and one from the interaction of the spins with the magnetic field. The denominator is of course just the partition function Z . Let us take the derivative of the average value of the total spin, with respect to the magnetic field h ,

$$\left(\frac{\partial \langle S \rangle}{\partial h} \right)_T = \frac{1}{Z} \sum_{\text{all states}} \frac{S^2}{kT} \exp(-\epsilon/kT + hS/kT) - \frac{1}{Z^2} \left(\frac{\partial Z}{\partial h} \right)_T \sum_{\text{all states}} S \exp(-\epsilon/kT + hS/kT)$$

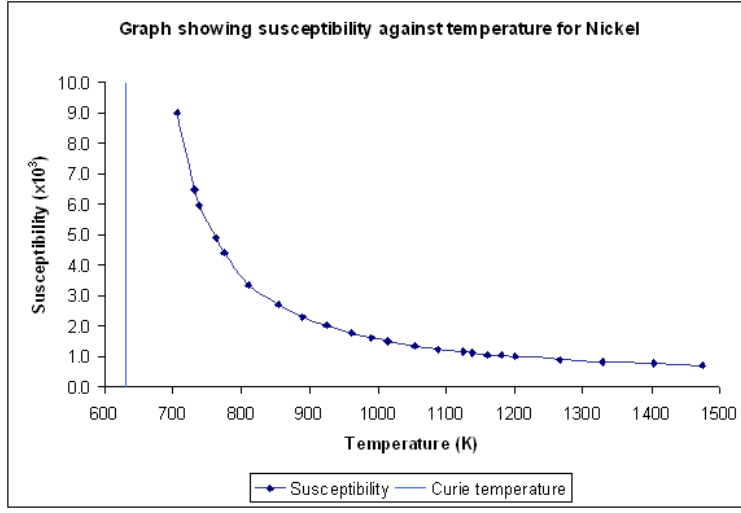


Figure 5: A plot of the magnetic susceptibility of nickel, as a function of temperature, above the Curie temperature which is at 627K. The rapid increase of susceptibility as the temperature approaches the Curie temperature is clear.

$$= \frac{1}{kT} \langle S^2 \rangle - \langle S \rangle \frac{1}{Z} \left(\frac{\partial Z}{\partial h} \right)_T, \quad (18)$$

where we used the definitions of $\langle S \rangle$ and $\langle S^2 \rangle$. But

$$\frac{1}{Z} \left(\frac{\partial Z}{\partial h} \right)_T = \frac{1}{Z} \frac{\partial}{\partial h} \sum_{\text{all states}} \exp(-\epsilon/kT + hS/kT) = \frac{1}{Z} \sum_{\text{all states}} \frac{S}{kT} \exp(-\epsilon/kT + hS/kT) = \frac{\langle S \rangle}{kT}, \quad (19)$$

and so

$$\left(\frac{\partial \langle S \rangle}{\partial h} \right)_T = \frac{\langle S^2 \rangle}{kT} - \frac{\langle S \rangle^2}{kT} = \sigma^2/kT. \quad (20)$$

where σ is the standard deviation of the fluctuations in the total spin S , defined as the mean of the square minus the square of the mean

$$\sigma^2 = \langle S^2 \rangle - \langle S \rangle^2. \quad (21)$$

Now, the derivative of $\langle S \rangle$ with respect to h , and per spin, is called the *susceptibility* which is a type of function called a *response function*. It is given the symbol χ , so

$$\chi = \frac{1}{N} \left(\frac{\partial \langle S \rangle}{\partial h} \right)_T. \quad (22)$$

When the response function is large, then the spin $\langle S \rangle$ changes rapidly as the magnetic field is varied: the response of the total spin to the magnetic field is strong, whereas if the response function is small, $\langle S \rangle$ changes only by a small amount if the magnetic field is varied. Another example of a response function, is the heat capacity C_v . It measures the response of the energy to changes in temperature.

Now, we can combine the definition of χ , Eq. (22) with Eq. (20) to get

$$kTN\chi = \langle S^2 \rangle - \langle S \rangle^2 = \sigma^2. \quad (23)$$

This is an important result: the fluctuations in the spin S are equal to the response function, $N\chi$, times the thermal energy kT . It shows that if $\langle S \rangle$ is found to vary rapidly with field h , then the fluctuations in $\langle S \rangle$ *must* be large. Conversely, if the fluctuations in $\langle S \rangle$ of a magnet are found to be large, then we know that $\langle S \rangle$ will change greatly if we increase or decrease the magnetic field h . Also, of course if $\langle S \rangle$ varies only by a small amount as the field is varied, then its fluctuations are small.

Finally, let us go back to our mean-field theory. In Eq. (7) the argument of the tanh function was minus the energy of a spin due to interactions with 4 other spins, assumed to have values of the spin equal to the mean, $\langle s \rangle$, divided by

kT . In the presence of a magnetic field h , the energy just has an additional term due to the interaction between the spin and the field, thus Eq. (7) becomes

$$\langle s \rangle = \tanh(4\langle s \rangle J/kT + h/kT). \quad (24)$$

We will not study this equation in detail, but above the Curie temperature $T_c = 4J/k$, we know $\langle s \rangle = 0$, when the field $h = 0$. So above T_c and for small h , we know that both terms in the tanh function are small so we linearise it to get

$$\langle s \rangle \approx \frac{4\langle s \rangle J}{kT} + \frac{h}{kT} = \frac{T_c}{T} \langle s \rangle + \frac{h}{kT} \quad T > T_c, \quad h/kT \ll 1, \quad (25)$$

where we have used our expression for the Curie temperature T_c . We can find the susceptibility χ by taking the derivative with respect to h of both sides of this equation. As $\langle s \rangle$ is the mean value of a single spin $\langle s \rangle = \langle S \rangle/N$ and so from Eq. (22), $\chi = (\partial \langle s \rangle / \partial h)$. So, taking the h derivative, we have

$$\frac{\partial \langle s \rangle}{\partial h} = \frac{T_c}{T} \frac{\partial \langle s \rangle}{\partial h} + \frac{1}{kT}. \quad (26)$$

Rearranging

$$\chi = \frac{\partial \langle s \rangle}{\partial h} = \frac{1/kT}{1 - T_c/T} \quad T > T_c, \quad h/kT \ll 1. \quad (27)$$

The interesting point about χ at small fields, $h/kT \ll 1$, above the Curie temperature T_c , is that it diverges, tends to infinity, as the Curie temperature is approached. This is seen in the measurements of the susceptibility of nickel just above the Curie temperature plotted in Fig. 5. The closer the temperature T gets to T_c , the larger is the response of the total spin to the magnetic field, and so the larger are the fluctuations in the total spin $\langle S \rangle$. Above T_c , the mean value of the total spin $\langle S \rangle$ is zero but as T_c is approached the fluctuations in $\langle S \rangle$ become larger and larger. These rather strange infinite fluctuations can only occur near phase transitions.