Introduction

The study of magnetic materials is an area of academic and industrial interest **(Annon, dd/mm/yyyy)**. For example, magnetic technologies are important in the ongoing development of quantum computers, superconducting circuits and other examples in electronics **(Annon, dd/mm/yyyy)**. At a fundamental level magnetisation is a well understood phenomenon, yet it is difficult to theoretically model. One simple model of magnetic materials is the Ising model.

The Ising model is the simplest model of a ferromagnet **(Annon, dd/mm/yyyy)**. Despite the simplicity of the Ising model it displays rich physical behaviour and has analytic solutions in one and two dimensions **(Annon, dd/mm/yyyy)**. The Ising model is the simplest model to account for inter-molecular interactions and contain a phase transition. This makes it an excellent medium for studying magnetic phenomenon **(Annon, dd/mm/yyyy)**.

By modifying the basic Ising model we can simulate many phenomenon including glasses **(Annon, dd/mm/yyyy)**. The Ising model has broader significance and can be used to construct very simple neural networks called Boltzmann machines **(Annon, dd/mm/yyyy)**. We tested one and two dimension Ising models and confirmed that they matched theoretical predictions.

Theory

Materials have internal interactions. As physicists we like to ignore these where possible but often these approximations limit the accuracies of our models **(Annon, dd/mm/yyyy)**. Magnetic phenomenon are no different. To understand how spins interact in a magnet it helps to first construct the simplest possible model without interactions; a para-magnet.

Consider our magnet as a one-dimensional chain of atomic spins. For the moment ignore any external magnetic field and just consider the spins in isolation. Now lets limit the spins to be fixed up or down along one axis. If there are no interactions between the spins the energy is fixed. If we add an external magnetic field then we would expect the ensemble to develop a net magnetisation.

If the system has thermal energy we would expect some of the spins to align themselves anti-parallel to the magnetic field. We can see this affect by considering the partition function for a single spin in the ensemble. If the spin is aligned with the magnetic field then the energy is $-sB$, where s is the unit of magnetisation carried by the single spin and B is the strength of the external magnetic field. If the spin is anti-aligned with the field then the energy is sB.

This is a simple two level system and the partition function is given by,

$$\begin{aligned} Z &= \sum_{s=\pm 1} \exp\left(-\frac{sB}{\tau}\right) \\ &= \exp\left(-\frac{sB}{\tau}\right) + \exp\left(\frac{sB}{\tau}\right) \\ &= 2\cosh\left(\frac{sB}{\tau}\right), \end{aligned} \tag{1}$$

where, $\tau = kT$ is the temperature in units of energy. The probability of the spins being anti-aligned with the field is therefore,

$$P = \frac{\exp\left(-\frac{sB}{\tau}\right)}{2\cosh\left(\frac{sB}{\tau}\right)}. \tag{2}$$

Hence, as the temperature increase we expect the number of anti-aligned spins to increase and as we increase the magnetic field we expect the number of anti-aligned spins to decrease.

Since each of the spins in a para-magnetic system is independent the partition function of an ensemble of N spins is just the product of N partition functions for the single spin case. However, since the spins are indistinguishable we must also divide by a Gibbs correction factor of $N!$. The probability of finding a particular state however, is a case that is worth studying, since it indicates a diveregence between the Ising model of a ferromagnet and a para-magnet in a magnetic field. First we need to define our state.

The energy of the system, and any other physical parameters, only depend on the number of spins that are aligned with the magnetic field and not specifically which spins are aligned with the field. Naively we might expect that the probability of having $N_\uparrow$ spins aligned with the field would be,

$$P(N_\uparrow) = \frac{\exp\left(-\frac{sN_\uparrow B}{\tau}\right)\exp\left(\frac{s(N-N_\uparrow)B}{\tau}\right)}{\cosh\left(\frac{sB}{\tau}\right)^N}. \tag{3}$$

However, equation 3 has failed to account for the multiple micro-states that occupy this macro-state. We can account for this by multiplying by the multiplicity, which can be found using the chose function,

$$P(N_\uparrow) = \frac{N!}{N_\uparrow!(N-N_\uparrow)!}\frac{\exp\left(-\frac{sN_\uparrow B}{\tau}\right)\exp\left(\frac{s(N-N_\uparrow)B}{\tau}\right)}{\cosh\left(\frac{sB}{\tau}\right)^N}. \tag{4}$$

Equation 4 is the correct expression for the probability.

We can also determine the energy of the system and the entropy. Using the free energy we can also find the equilibrium state and hence determine the equilibrium properties of the system as a function of the temperature.

Para-magnets are a useful toy model but from our experience with natural and manufactured magnets we know that it is possibe to construct systems that are magnetic without external fields. The one-dimensional Ising model is a simple model of such systems. The Ising model is a natural extension of the paramagnetic model that we discussed, and operates on the same spin lattice.

The Ising model differs because it adds very simple interactions between neighbouring spins. This interaction favours pairs that are aligned by reducing the energy of this scenario. Representing up spins as $+1$ and down spins as -1 we can represent this mutal interaction as $\Delta\epsilon = \varepsilon s_i s_{i+1}$, where $\Delta\epsilon$ is the energy contribution of the interaction, ε is a scaling factor that represents the strength of the interaction and s_i is the i^{th} spin in the chain.

An obvious way that this differs from the para-magnetic model is that each spin can be independently resolved, and hence the Gibbs correction function is no longer needed. Let's isolate the case we are considering from a magnetic field as this simplifies the calculations. Again we start be considering the partition function of an individual pair. Similarly to the para-magnetic case this is a two level system; either the pair are aligned or they are anti-aligned with the corresponding energies.

$$\begin{aligned} Z_i &= \sum_{s_i=\pm 1} \exp\left(-\frac{\varepsilon s_i s_{i+1}}{\tau}\right) \\ &= \exp\left(-\frac{\varepsilon}{\tau}\right) + \exp\left(\frac{\varepsilon}{\tau}\right) \\ &= 2\cosh\left(\frac{\varepsilon}{\tau}\right). \qquad (5) \end{aligned}$$

It is worth noting the strong similarity between equations 5 and 1.

Similarly to the para-magnetic case we can multiply the system partition functions of single constituents together to get the partition function of the entire system. However, the condition to do this was that the constiutuents were independent, but the Ising model contains interactions. In the case of the Ising model the constituents that are independent are the pairs, not the individual spins. You may think think then that we only consider $N/2$ unique pairs but this is not the case. In a chain each spin is counted in two pairs so the power is still N.

A small detail that I skipped was what happens at the boundary. The two spins on the end of the chains are not (neccessarily) counted twice. In the limit of a very large chain of spins we can see that the boundary affect will not matter however, we got about this nuance in a much more interesting way by considering cyclic boundary conditions. That is to say that the spin on the far end of the chain is a neighbour to the spin at the start of the chain and vice versa.

Given the partition function $Z = (2\cosh(\varepsilon/\tau))^N$, we calculated the internal energy using,

$$\begin{aligned} U &= \tau^2 \partial_\tau \ln(Z) \qquad (6) \\ &= \tau^2 \partial_\tau \ln\left(2\cosh\left(\frac{\varepsilon}{\tau}\right)^N\right) \\ &= N\tau^2 \partial_\tau \ln\left(2\cosh\left(\frac{\varepsilon}{\tau}\right)\right) \\ &= N\tau^2 \partial_\tau \left(2\cosh\left(\frac{\varepsilon}{\tau}\right)\right) \frac{1}{2\cosh\left(\frac{\varepsilon}{\tau}\right)} \\ &= N\tau^2 \partial_\tau \left(\frac{\varepsilon}{\tau}\right) \frac{\sinh\left(\frac{\varepsilon}{\tau}\right)}{\cosh\left(\frac{\varepsilon}{\tau}\right)} \\ &= -\varepsilon N \tanh\left(\frac{\varepsilon}{\tau}\right). \qquad (7) \end{aligned}$$

We calculated the free energy of the system using,

$$\begin{aligned} F &= -\tau \ln Z \qquad (8) \\ &= -\tau \ln\left(\left(2\cosh\left(\frac{\varepsilon}{\tau}\right)\right)^N\right) \\ &= -N\tau \ln\left(2\cosh\left(\frac{\varepsilon}{\tau}\right)\right) \\ &= -N\tau \ln\left(\exp\left(\frac{\varepsilon}{\tau}\right) + \exp\left(-\frac{\varepsilon}{\tau}\right)\right) \\ &= -N\tau \ln\left(\exp\left(\frac{\varepsilon}{\tau}\right)\left(1 + \exp\left(-2\frac{\varepsilon}{\tau}\right)\right)\right) \\ &= -N\tau \ln\left(\exp\left(\frac{\varepsilon}{\tau}\right)\right) - N\tau \ln\left(1 + \exp\left(-2\frac{\varepsilon}{\tau}\right)\right) \\ &= -N\varepsilon - N\tau \ln\left(1 + \exp\left(-2\frac{\varepsilon}{\tau}\right)\right). \qquad (9) \end{aligned}$$

The entropy followed from the combination of Equation 9 and Equation 7 using Equation 10,

$$\begin{aligned} \tau\sigma &= F - U \qquad (10) \\ &= -N\varepsilon \tanh\left(\frac{\varepsilon}{\tau}\right) + N\varepsilon + N\tau \ln\left(1 + \exp\left(-2\frac{\varepsilon}{\tau}\right)\right) \\ \sigma &= \frac{\varepsilon}{\tau}\left(1 - \tanh\left(\frac{\varepsilon}{\tau}\right)\right) + \ln\left(1 + \exp\left(-2\frac{\varepsilon}{\tau}\right)\right). \qquad (11) \end{aligned}$$

Finally, we determined the specific heat using Equation 12 and Equation 7,

$$\begin{aligned} C &= \partial_\tau U \qquad (12) \\ &= \partial_\tau \left(-N\varepsilon \tanh\left(\frac{\varepsilon}{\tau}\right)\right) \\ &= -N\varepsilon \partial_\tau \left(\frac{\varepsilon}{\tau}\right) \frac{1}{\cosh^2\left(\frac{\varepsilon}{\tau}\right)} \\ &= \frac{N\varepsilon^2}{\tau^2 \cosh^2\left(\frac{\varepsilon}{\tau}\right)}. \qquad (13) \end{aligned}$$