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.

It is informative to calculate the internal energy and free energy of the system. Starting with the internal energy,

$$\begin{aligned} U &= \tau^2 \partial_\tau \ln Z \\ &= \tau^2 \partial_\tau \ln\left(2^N \cosh^N\left(\frac{sB}{\tau}\right)\right) \\ &= -NsB\tanh\left(\frac{sB}{\tau}\right). \end{aligned} \tag{5}$$

We can also calculate the free energy, but further calculations result in tedious analytical expressions so we have omitted them.

$$\begin{aligned} F &= -\tau \ln Z \\ &= -\tau \ln\left(2^N \cosh^N\left(\frac{sB}{\tau}\right)\right) \\ &= -NsB - N\tau\ln\left(1+\exp\left(-\frac{2sB}{\tau}\right)\right). \end{aligned} \tag{6}$$

As we will see when we analyse the Ising model without an external field these results are general of any two level system. Using equation 5 we can calculate the magnetisation as a function of the magnetic field and temperature,

$$\begin{aligned} U = mB &= -NsB\tanh\left(\frac{sB}{\tau}\right) \\ m &= -Ns\tanh\left(\frac{sB}{\tau}\right). \end{aligned} \tag{7}$$

Therefore, the net magnetisation system will decrease with temperature and increase with the magnetic field, much as we would expect.

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.

$$\begin{aligned} Z_i &= \sum_{s_i=\pm1} \exp\left(-\frac{\varepsilon s_i s_{i+1}}{\tau}\right) \\ &= \exp\left(-\frac{\varepsilon}{\tau}\right) + \exp\left(\frac{\varepsilon}{\tau}\right) \\ &= 2\cosh\left(\frac{\varepsilon}{\tau}\right). \end{aligned} \tag{8}$$

It is worth noting the strong similarity between equations 8 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,

$$\begin{aligned} U &= \tau^2\partial_\tau \ln(Z) \qquad (9)\\ &= \tau^2\partial_\tau \ln\left(2\cosh\left(\frac{\varepsilon}{\tau}\right)^N\right)\\ &= N\tau^2\partial_\tau \ln\left(2\cosh\left(\frac{\varepsilon}{\tau}\right)\right)\\ &= N\tau^2\partial_\tau\left(2\cosh\left(\frac{\varepsilon}{\tau}\right)\right)\frac{1}{2\cosh\left(\frac{\varepsilon}{\tau}\right)}\\ &= N\tau^2\partial_\tau\left(\frac{\varepsilon}{\tau}\right)\frac{\sinh\left(\frac{\varepsilon}{\tau}\right)}{\cosh\left(\frac{\varepsilon}{\tau}\right)}\\ &= -\varepsilon N\tanh\left(\frac{\varepsilon}{\tau}\right). \qquad (10)\end{aligned}$$

We calculated the free energy of the system using,

$$\begin{aligned} F &= -\tau\ln Z \qquad (11)\\ &= -\tau\ln\left(\left(2\cosh\left(\frac{\varepsilon}{\tau}\right)\right)^N\right)\\ &= -N\tau\ln\left(2\cosh\left(\frac{\varepsilon}{\tau}\right)\right)\\ &= -N\tau\ln\left(\exp\left(\frac{\varepsilon}{\tau}\right)+\exp\left(-\frac{\varepsilon}{\tau}\right)\right)\\ &= -N\tau\ln\left(\exp\left(\frac{\varepsilon}{\tau}\right)\left(1+\exp\left(-2\frac{\varepsilon}{\tau}\right)\right)\right)\\ &= -N\tau\ln\left(\exp\left(\frac{\varepsilon}{\tau}\right)\right)-N\tau\ln\left(1+\exp\left(-2\frac{\varepsilon}{\tau}\right)\right)\\ &= -N\varepsilon-N\tau\ln\left(1+\exp\left(-2\frac{\varepsilon}{\tau}\right)\right). \qquad (12)\end{aligned}$$

The entropy followed from the combination of Equation 12 and Equation 10 using Equation 14,

$$\begin{aligned} \tau\sigma &= F-U \qquad (13)\\ &= -N\varepsilon\tanh\left(\frac{\varepsilon}{\tau}\right)+N\varepsilon+N\tau\ln\left(1+\exp\left(-2\frac{\varepsilon}{\tau}\right)\right)\\ \sigma &= \frac{\varepsilon}{\tau}\left(1-\tanh\left(\frac{\varepsilon}{\tau}\right)\right)+\ln\left(1+\exp\left(-2\frac{\varepsilon}{\tau}\right)\right). \qquad (14)\end{aligned}$$

Finally, we determined the specific heat using Equation 16 and Equation 10,

$$\begin{aligned} C &= \partial_\tau U \qquad (15)\\ &= \partial_\tau\left(-N\varepsilon\tanh\left(\frac{\varepsilon}{\tau}\right)\right)\\ &= -N\varepsilon\partial_\tau\left(\frac{\varepsilon}{\tau}\right)\frac{1}{\cosh^2\left(\frac{\varepsilon}{\tau}\right)}\\ &= \frac{N\varepsilon^2}{\tau^2\cosh^2\left(\frac{\varepsilon}{\tau}\right)}. \qquad (16)\end{aligned}$$

You will immediately notice that in the absence of an external magnetic field the Ising model reduces to the model of the para-magnet.

What happens if we place the Ising model into an external magnetic field. Again we can break it down by considering a single pair in the chain as our constituent object. There are three energies that it is possible for this pair to have; parallel and aligned with the magnetic field, parallel and anti-aligned with the magnetic field and anti-parallel. However, the final state has a multiplicity of two since either of the spins could be aligned with the field.

It is possible to compute the partition function for this the single pair and hence also the entrie system.

$$\begin{aligned} Z_1 &= \sum_s \exp\left(-\frac{\epsilon_s}{\tau}\right)\\ &= \exp\left(\frac{-\epsilon-2B}{\tau}\right)+2\exp\left(\frac{\epsilon}{\tau}\right)+\exp\left(\frac{-\epsilon+2B}{\tau}\right)\\ &= 2\exp\left(\frac{-\epsilon}{\tau}\right)\cosh\left(\frac{2B}{\tau}\right)+2\exp\left(\frac{\epsilon}{\tau}\right). \qquad (17)\end{aligned}$$

From here we can compute all the physical properties of the system. Since each pair is independent the partition function is simply the product of N partition function by the same reasoning as in the case above when there was no magnetic field. We have not shown the calculation of the energy ect., because the expressions are complex and uninformative.

Another interesting effect that can be explored using the Ising model is anti-ferro-magnetism. This phenomenon was only recently discovered in nature **(Annon, dd/mm/yyyy)**and refers to and interaction between neighbouring spins that causes them to have lower energy when they are aligned anti-parallel rather than parallel. We do not need to cover any new equations in this case as an anti-ferro-magnet can be explored by letting ϵ become negative.

We have spent a lot of time discussing the one-dimensional scenario but real systems are typically higher dimensional. There is a an analytical solution to the two-dimensional ising model **(Annon, dd/mm/yyyy)**. This solution is a tour de force and has comparatively little practical use due to its complexity. Multiple approximation methods have been developed for dealing with the two-dimensional case, most notably the mean field approximation.

The mean field approximation treats a group of neighbours as an a single spin, parametrised by the mean. In this way we recover the two level system and arrive at a two level system that is very similar to what we have already covered for the para-magnet and the Ising model when there is no external magnetic field. Ultimately the mean field approximation is an approximation and its predictions are not always correct.

Another aspect of higher dimensions that it is worth discussing is what counts as a neighbour. For example, in two-dimensions we could connet the spins together so that each spins is equally far from six other spins. This triangular Ising model will have markedly different behaviour than a square grid of spins **(Annon, dd/mm/yyyy)**. For our analysis we have considered a square grid of spins since it is simpler to simulate.

Without going into the complex analytical solutions we can still make useful qualitative guesses about the behaviour of the Ising model in higher dimensions based on its behaviour in lower dimensions. For example, we expect the spins will tend to align at lower temperatures and tend to disorder at higher temperatures. For the anti-ferro-magnetic case we expect the spins to become anti-aligned at low temperatures and tend to disorder at higher temperatures.

It is worth noting that in the presence of a magnetic field the qualitative behaviour of the anti-ferro-magnetic and ferro-magnetic Ising models becomes markedly different. The ferro-magnetic model results in a positive feedback loop as the magnetic field coerces spins to align with the field they also want to align with each other. On the other hand the anti-ferro-magnet exerts a dampening effect for the opposite reason.

Method

We started by simulating a one dimensional Ising model with no external magnetic field, which we compared to the analytic expressions derived in the theory. As we described in theory we used periodic boundary conditions and chose to implement our models using a lattice size of one-hundred spins for the most part. We chose to use one-hundred spins because it evaluated fast on our device and was large enough to be interesting.

The Ising algorithm scales very non-linearly with the size of the lattice. This is because when taking a sample you want to run the system for enough iterations so that every spin has a chance to be visited many times and then average the result. In addition, operations such as finding the energy, require that you visit every spin and hence have linear time complexity independently. Starting with our one dimensional model we equilibrated the system for multiple different temperatures and settled on using $1000N$ as the length of the loop. This was likely too many but we found that for low temperatures when the probability of a flip becomes small, a larger number of steps was required. For each temperature we started the chain of spins at a random temperature.

Once we had determined the numberic details of our simulations we proceeded to measure the physical properties of the system. To calculate the energy of the one dimensional case we employed the following algorithm:

```
function calc_energy
    energy = 0
    for spin in 0:length
        energy += ensemble[spin] * ensemble[spin + 1]
    return energy
```

Similarly for the entropy we counted all of the aligned pairs. This works because as discussed in the theory the "base unit" of the Ising model is a pair of spins not an individual spin. As noted in the Theory there are N pairs of spins. Moreover, we ued Stirling's approximation in the logarithmic form, because we found that the program could not calculate numbers of the size 100!. This will have had negligible affects at higher temperatures where the system tends torward disorder, but at lower temperatures the approximation becomes less accurate. We were not too concerned with the loss of accuracy since the entropy tends to zero at low temperatures.

```
function calc_entropy
    up = 0
    for spin in 0:length
        up += ensemble[spin] == ensemble[spin + 1]
    down = length - up
    entropy = length * log(length) - up * log(up) - down *
    return entropy
```

The free energy was calculated using its definition, $F = U - \tau\sigma$, where $\tau = kT$ and σ is the entropy. The heat capacity was calculated using the thermodynamic identity,

$$C_V = \frac{\mathrm{var(U)}\tau^2}{.} \tag{18}$$

A large part of the computational expense came from estimating the uncertainty in the physical parameters. It did not make sense to initialise the system randomly at every temperature and then wait for it to equilibrate before taking measurements. Instead we initialised the system at a high temperature where the random configuration is a good approximation to the equilibrium configuration and equilibrated it.

From this higher temperature we allowed the system to evolve for $1000N$ steps measuring the physical properties at every step. We then cooled the system by a small incremement and without re-equilibrating the system evolved it for $1000N$ steps taking measurements every step. In this way we halved the amount of CPU time required by each run but introduced a small error by starting the system at a slightly out of equilibrium state. Given the large number of runs we believe that this error is negligible, although it is visible at lower temperatures as the heat capacity becomes over-estiamted.

Another flaw of running the simulation this way was that it serialised the loops (i.e. made the next iteration depend on the state of the previous one). This prevented us from making efficient parallelisation of the inner loop, however, the outer loop was not serial and could be efficiently paralellised. After each run of $1000N$ the average was taken for each physical parameter.

Please note that we did not use the standard error of the $1000N$ trials as the error. It does not make sense to do so because each state is deterministically dependent on the previous one and the sample gridding is much too fine. Instead we repeated the entire process a fixed number of times 100 for the one-dimensional case and used the standard error of the means from these 100 trials as the estimate of our uncertainty. Note that we defined the standard error as $\sqrt{\mathrm{Var} N}$.

We noticed that the infinite one-dimensional Ising model is predicted to have no net magnetisation at $0K$. To test this hypothesis, we created histograms of the magnetisation at $\tau = 0.5J, 1.0J$ and $2.0J$ for $N = 100$ and $N = 500$. We expected the histograms to be narrower as the number of spins in the system was increased.

Once we were satisfied with the one-dimensional ising model we repeated a similar analysis for the two-dimensional model. First we tested the time required for equilibration by initialising the model and running it for $1000N^2$ where N is the width of the grid.

Satisfied with the equilibration time we employed the same techniques described for the one-dimensional case to the two-dimensional case to measure the physical parameters. In short, we incrementally cooled the system measuring every iteration and recording the mean. We repeated this process a fixed number of times and used the standard error as our uncertainty estimate. The energy calculation is clearly modified, so we have included the relevant pseudocode below:

Results

We noticed that the net magnetisation set in at lower temperatures for the larger N. This tells us that there is no phase transition because a phase transition should occur at exactly the same temperature for all latice sizes. Moreover, it agrees with the theoretical prediction that the Ising model is not magnetised at $0K$ in the infinite case because it we increase the latticed temperature to infinity then the temperature of net magnetisation should decrease below $0K$.