Foreword

I used the c programming language to complete this task. I represented the system of spins as a `struct`, defined below in one dimension.

```
typedef struct ising_t
{
  float epsilon;
  float magnetic_field;
  float epsilon;
  int length;
  int *ensemble;
} ising_t;
```

Scaling this to two dimensions was more difficult because the `*ensemble` had to be transformed into `**ensemble`. It is possible to implement this in a single `struct` using `union ensemble {int *1d, int **2d};`, but in the code available on my `github` I have used two separate `structs` resulting in code duplication for many of the methods. I made this decision because I had not used `c` prior to this project and was unaware of the `union` keyword and its uses. I am describing this because you may notice discrepancies in the code snippets that I have include where `int *(*)ensemble = system -> ensemble;` is invoked to access the array of spins.

Question 1 a)

I selected three different temperatures, $1.0, 2.0$ and $3.0\epsilon/k$, and ran the metropolis algorithm for $1000N$ steps. At each of these temperatures the system was initialised in a random state and allowed to equilibrate.

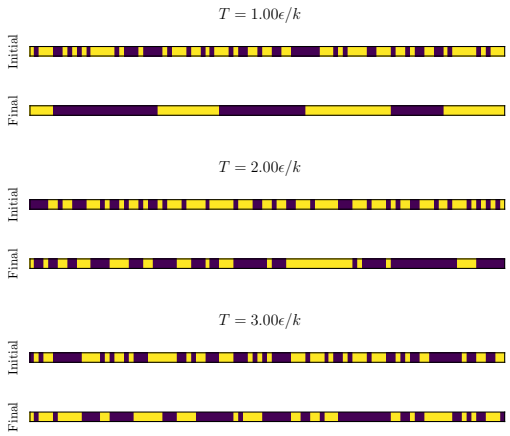

Figure 1: Each vertical pair of lines represents the spin state. The top one is the random initial state and the bottom one is the equilibrated final state.

We noticed that at lower temperatures the spin chunks were much larger than at higher temperatures. This is particularly pronounced between the $T = 3.0\epsilon/k$ and $T = 1.0\epsilon/k$ plots in figure 1. To evolve the system we used the version of the metropolis algorithm shown below,

```
/*
 * metropolis_step
 * -----------------------
 * Evolve the system by attempting to
 * flip a spin. The step is weighted
 * by the Boltzmann factor.
 *
 * parameters
 * ----------
 * ising_t *system: A struct
 *   enscapulating the information
 *   related to the system.
 */
void metropolis_step(ising_t *system)
{
  float temp = system -> temperature;
  int *ensemble = system -> ensemble;
  int length = system -> length;
  int spin = random_index(length);
  int change = 2*ensemble[spin]*(
    ensemble[modulo(spin+1,length)] +
    ensemble[modulo(spin-1,length)]);

  if ((change < 0)
    || (exp(-change/temp)>randn()))
  {
    ensemble[spin] *= -1;
  }
}
```

where, `rand` generates a random number in the range $[0, 1]$, and `modulo` is modified to produce positive input on negative numbers like the `python` implmentation. This is not the native `c` implementation. I used the `||` short circuit operator so that the second comparison was not evaluated on every call to the function.

Question 1 b)

I found that it was worth considering what the *basic unit* of the Ising model was. In the absence of an external magnetic field the energy is a function of the pairs. I start by considering the partition function of an individual pair. This is a two level system; either the pair are aligned or they are anti-aligned with the corresponding energies.

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

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,

$$\begin{aligned} U &= \tau^2 \partial_\tau \ln(Z) && (2)\\ &= \tau^2 \partial_\tau \ln\left(2\cosh\left(\frac{\varepsilon}{\tau}\right)^N\right)\\ &= N\tau^2 \partial_\tau \ln\left(2\cosh\left(\frac{\varepsilon}{\tau}\right)\right)\\ &= N\tau^2 \partial_\tau \left(2\cosh\left(\frac{\varepsilon}{\tau}\right)\right)\frac{1}{2\cosh\left(\frac{\varepsilon}{\tau}\right)}\\ &= N\tau^2 \partial_\tau \left(\frac{\varepsilon}{\tau}\right)\frac{\sinh\left(\frac{\varepsilon}{\tau}\right)}{\cosh\left(\frac{\varepsilon}{\tau}\right)}\\ &= -\varepsilon N \tanh\left(\frac{\varepsilon}{\tau}\right). && (3) \end{aligned}$$

We calculated the free energy of the system using,

$$\begin{aligned} F &= -\tau \ln Z && (4)\\ &= -\tau \ln\left(\left(2\cosh\left(\frac{\varepsilon}{\tau}\right)\right)^N\right)\\ &= -N\tau \ln\left(2\cosh\left(\frac{\varepsilon}{\tau}\right)\right)\\ &= -N\tau \ln\left(\exp\left(\frac{\varepsilon}{\tau}\right)+\exp\left(-\frac{\varepsilon}{\tau}\right)\right)\\ &= -N\tau \ln\left(\exp\left(\frac{\varepsilon}{\tau}\right)\left(1+\exp\left(-2\frac{\varepsilon}{\tau}\right)\right)\right)\\ &= -N\tau \ln\left(\exp\left(\frac{\varepsilon}{\tau}\right)\right) - N\tau \ln\left(1+\exp\left(-2\frac{\varepsilon}{\tau}\right)\right)\\ &= -N\varepsilon - N\tau \ln\left(1+\exp\left(-2\frac{\varepsilon}{\tau}\right)\right). && (5) \end{aligned}$$

The entropy followed from the combination of Equation 3 and Equation 1 using Equation 5,

$$\begin{aligned} \tau\sigma &= F - U && (6)\\ &= -N\varepsilon \tanh\left(\frac{\varepsilon}{\tau}\right) + N\varepsilon + N\tau \ln\left(1+\exp\left(-2\frac{\varepsilon}{\tau}\right)\right)\\ \sigma &= \frac{\varepsilon}{\tau}\left(1-\tanh\left(\frac{\varepsilon}{\tau}\right)\right) + \ln\left(1+\exp\left(-2\frac{\varepsilon}{\tau}\right)\right). && (7) \end{aligned}$$

Finally, we determined the specific heat using Equation 3 and Equation 5,

$$\begin{aligned} C &= \partial_\tau U && (8)\\ &= \partial_\tau\left(-N\varepsilon\tanh\left(\frac{\varepsilon}{\tau}\right)\right)\\ &= -N\varepsilon\partial_\tau\left(\frac{\varepsilon}{\tau}\right)\frac{1}{\cosh^2\left(\frac{\varepsilon}{\tau}\right)}\\ &= \frac{N\varepsilon^2}{\tau^2\cosh^2\left(\frac{\varepsilon}{\tau}\right)}. && (9) \end{aligned}$$

Question 1 c)

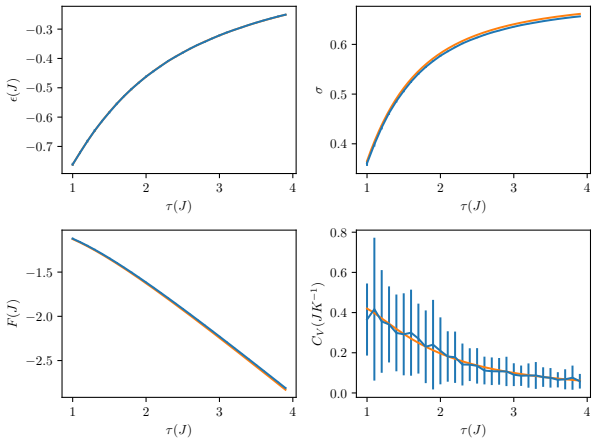

Figure 2: The top left is the energy and the top right is the entropy. The bottom left is the free energy and the bottom right is the heat capacity.

I started by simulating a one dimensional Ising model with no external magnetic field, which I compared to the analytic expressions derived above. I used periodic boundary conditions and chose to implement my models using a lattice size of one-hundred spins. I chose to use one-hundred spins because it evaluated fast on my device and was large enough to be interesting.

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 I found that for low temperatures when the probability of a flip becomes small, a larger number of steps was required.

I chose to sample the temperatures over the range $0.0 - 4.0\epsilon/k$ incrementing by $0.2\epsilon/k$. I initialised the system

only once at the highest temperature that we sampled, $3.8\epsilon/k$. I equilibrated the system at this temperature by evolving it for $1000N$ and then started to cool the system taking measurements at each new system.

The alternative model was to randomly initialise the system at every temperature. This would require approximately twice the number of steps since the system would have to be equilibrated at every temperature. I realize that the cooling method has a side affect of leading to "overflow". By "overflow" I mean that the first few measurements of each temperature are slightly out of equilibrium at the higher temperature.

The entire *measured* cooling process was performed by the program 1000 times. At each temperature in the *measured cooling* loop the energy and entropy were measured by taking the average of all $1000N$ iterations. The heat capacity was also measured by taking the variance of the energy and applying,

$$C_v = \frac{\mathrm{var}(\epsilon)}{\tau^2} \tag{10}$$

The energy and entropy were re-averaged over the outer *fixed size* loop. I chose to re-average then on the outer loop because I was certain that the trials were statistically independent. This does not matter so much for the mean value estimate since the $1000N$ inner loop allows the system to explore the equilibrium space but I think that it does matter for the error estimate.

I belive that it matters for the error estimate because the state of the system is highly correlated to the past state of the system within some *correlation length*. This *correlation length* is roughly the same amount of time that the system requires to explore the equilibrium state, or $1000N$.

By running multiple simulations for the *correlation length* and averaging these results I have guaranteed robust results. I estimated the error using the *standard error* of the independent *correlation length* simulations. This means that the error presented in figure 2 is given by equation 11.

$$\Delta\hat{\beta} = \sqrt{\frac{\mathrm{var}(\beta)}{N}}, \tag{11}$$

where, $\hat{\beta}$ is the parameter estimate, β is a vector of measurements and N is the number of measurements.

To calculate the energy of the system I used the following algorithm,

```
/*
 * energy_ising_t
 * --------------
 * Calculate the energy of the system.
 *
 * parameters
 * ----------
 * ising_t *system: A struct
 *   enscapulating the information
 *   related to the system.
 *
 * returns
 * -------
 * float energy: The energy of the
 *   system in Joules.
 */
float energy_ising_t(ising_t *system)
{
  int length = system->length;
  int *ensemble = system->ensemble;
  float energy = 0.;

  for(int spin=0; spin<length; spin++)
  {
    energy -= ensemble[spin] *
      ensemble[modulo(spin+1,length)];
  }

  return energy;
}
```

You may notice that I am only counting the righthand neighbour of each spin. I chose this method because it is more optimal. If I was to count each neighbour then every pair would be counted twice and we would have to divide the final result by `2.`. By only counting one of the neighbours I have halved the number of computations.

A pair of spins is the *base unit* of the ising model so to calculate the entropy I counted the number of aligned pairs and then used the *chose* function to calculate the multiplicity. However, it was not quite this simples since 100! is $\sim 10^{157}$, which overflows an integer in the programs memory.

To fix this problem I used the stirling approximation to compute the entropy directly. This implies that the entropy should be less accurate at lower temperatures where the entropy is low and the Stirling approximation diverges from the actual entropy. The code that I used to calculate the entropy was,

```
/*
 * entropy_ising_t
 * ---------------
 * Calculate the entropy of a
 * configuration.
 *
 * parameters
 * ----------
 * ising_t *system: A struct
 *   enscapulating the information
 *   related to the system.
 *
 * returns
 * -------
 * float entropy: The entropy of the
 *   system in natural units.
 */
float entropy_ising_t(ising_t *system)
```

```
{
  int length = system->length;
  int *ensemble = system->ensemble;
  int up = 0;

  for (int spin=0; spin<length; spin++)
  {
    up += ensemble[spin] ==
      ensemble[modulo(spin+1,length)];
  }

  int down = length - up;

  float entropy = length * log(length) -
    up * log(up) - down * log(down);

  return entropy;
}
```

Question 1 d)

Consider the energy depicted in figure 2. We see that the energy is a decreasing function of the temperature. This implies that the spins tend to align as the temperature decreases. This makes sense because the Boltzmann factor for the lower state becomes more favoured. Similarly the entropy is a increasing function of the temperature. As the spins tend to align at lower temperatures the number of ways to arrange the state becomes smaller, decreasing the entropy.

The heat capacity, also shown in figure 2 is interesting because it increases rapidly before asymptotically decreasing. If it was discontinuous then we would expect a phase transition however it is continuous. so we know that there is no phase transition. We know it is continuous because of equation 9.

Question 1 e)

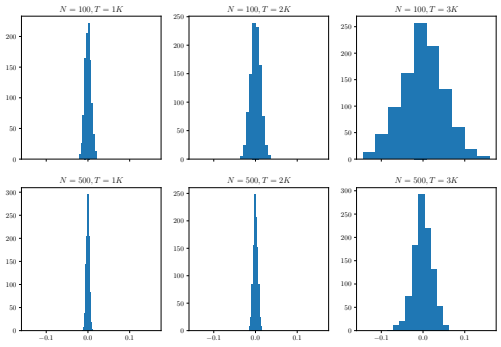

Figure 3: Histograms of the magnetisation for two ising systems of sizes $N = 100$ and $N = 500$. The temperatures are labelled in the titles and the y-axis is a unitless count.

Figure 3 showed me that the magnetisation was not zero as it was predicted to be at $0\epsilon/k$. I am not concerned because the distribution of samples, which roughly corresponds to a time average is symmetrically distributed around zero implying that the time average is identically zero. I would expect some variation of the results around zero as spins randomly flipped.

Since magnetisation sets in at a lower temperature for the larger sample I concluded that there was no phase transition. I decided this because the phase transition should occur at the same temperature for all lattice sizes. Taking the limit of a decreasing function presumably reduces to zero implying that there is no spontaneous magnetisation for the one-dimensional Ising model. This means that there is no phase transition.

Question 2 a)

For $\tau = 1.0\epsilon/k$ the random lattice very quickly relaxed into large *domains* of up and down spins. Over time the boundaries of the *domains* moved around the lattice coherently. I am/will using/use *coherent motion* to refer to a blob transporting across the network. For example, a group of down spins may start in the top right corner and remaining a single blob move to the middle of the system.

I noticed that given enough time the $\tau = 1.0\epsilon/k$ lattice relaxed until it was entirely one color. This is not shown in figure **??** simply because the lattice was not allowed to evolve for enough time. I used the same evolution time for the two dimensional Ising model that I used for the one dimensional Ising model, that is $1000N^2$ where I will use N to represent the side length of the system.

This is important because at lower temperatures the system took longer to equilibrate. As I saw for the one-dimensional case the *coherent domains* have a *meta-stable* lifetime before decaying. The shape of this domain influences the lifetime. The size seems to be a direct predictor of lifetime with the largest domain nearly always coming out on top. Another important feature that we noticed was that the coherent domains became particularly *meta-stable* if they formed rings.

The ring structures were *meta-stable* because of the cyclic boundary conditions. In a ring structure there are only two edges that are exposed to the other *meta-stable* state meaning that the anti-aligned interactions at the boundary are minimised. Additionally since the interaction depth of the Ising model is only nearest neighbour the *meta-stable* ring could exit in a band of just five spins. *The spins on the boundary have no idea how large their respective domains are.*

A final point to address for the $\tau = 1.0\epsilon/k$ model is the *time speckling*. As the system is allowed to evolve in equilibrium spins at random locations will randomly flip. This is a byproduct of the metropolis algorithm but it is important because the *speckles* almost always remain a single spin. You will see later that this changes as the tempera-

ture is increased.

Heating the lattice to $\tau = 2.0\epsilon/k$ we see mush of the same behaviour. $\tau = 2.0\epsilon/k$ is still less than the critical temperature, so all of the same evolutionary events occur. *Meta-stable* domains form, move and die. Even the more dangerous *meta-stable* rings can form at this temperature. I would like to say that the lifetime of the *domains* has declined but I have no evidence.

The key difference between the $\tau 2.0\epsilon/k$ and the $\tau = 1.0\epsilon/k$ models is the *speckling*. At the higher temperatures the speckles occur more often and can result in very local short lived domains. This is why I postulated that the *domains* are shorter lived. The system is more active meaning that the spins on the boundary flip more readily. Moreover, the rapid speckling assists in the destruction of the *domain* when it occurs on the boundary.

Something worthy of note before we move above the condensation temperature is that *domains* die at there corners. This is because the corners represent an interface where a spin has more neighbours of one color than the other. This is another factor that prolongs the life of the *meta-stable* states, since they have no corners and minimised contact.

The behaviour was markedly different for the $\tau = 3.0\epsilon\ k$ model, because it is above the critical temperature. For starters the activity of the system has increased significantly. This means, among other things that the relaxation into equilibrium is almost instantaneous compared with the lower temperature models. In addition *domains* do not form at this temperature.

I have been using *domain* to refer to a structure that is *macroscopic* and *semi-permanent*. *Zonation* does occur at $\tau = 3.0\epsilon/k$ bur it does not meet these criteria. By this I mean that the zones are small ~ 10 spins maximum and temporary. Rather than considering the rapid zonation to be the evolution of the *domain* behaviour I consider it the evolution of the *speckling* behaviour.

At $\tau = 3.0\epsilon/k$ we also loose the *coherent* end state. At both of the other temperatures the final state was a completely magnetised block or a *meta-stable* ring. However, at $\tau = 3.0\epsilon/k$ there is no such state and the *zonation* appears to randomly move about the grid. At higher temperatures still the *zonation* is completely destroyed and not even microscopic domains are able to form.

Question 2 b)

Smoothly varying the temperature using I found that the *speckling* and *zonation* seems to dominate above $\sim 2.3\epsilon/k$ while below this *domains* start to form and given enough time the entire crystal becomes magnetised. The transition is smooth with respect to the *speckles*, which at very low temperatures are very small and isolated with out a lifetime.

As I increased the temperature the *speckles* increases in size and in lifetime. A *speckle* is differentiated from a *zone* rather arbitrarily, the two main differences being transport and lifetime. The *zones* have a lifetime of long enough that they are able to *coherently move* across the crystal. On the other hand a *speckle* tends to die where it started and very quickly.

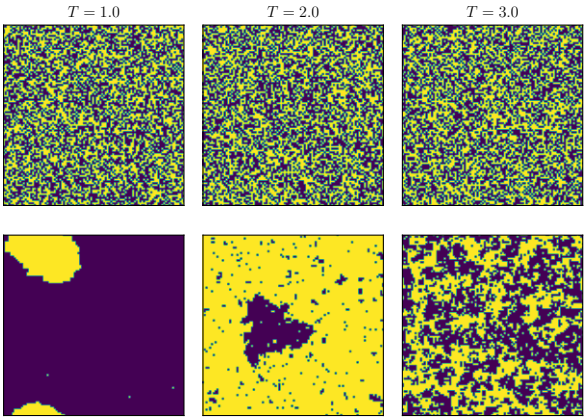

Figure 4: Snapshots of the Ising system at multiple temperatures given a random initial starting position (top). You will notice that $\tau = 1.0\epsilon/k$ and $\tau = 2.0\epsilon/2$ have similar net magnetisation, but that $\tau = 2.0\epsilon/k$ has stronger *speckling* than $\tau = 1.0\epsilon/k$. You will notice that there is not net magnetisation for $\tau = 3.0\epsilon/k$ and that the *zonation* I described above is occurring.

As we approach the critical temperature from below the *speckles* increase in size and disrupt the domains more quickly but, the system is still able to fully magnetise. At the critical temperature the *speckles* become so disruptive that the magnetisation cannot occur macroscopically but it still occurs locally in the form of the *zones* which outlive the now very active *speckles*.

Increasing the temperature further still the coherent *zones* disappear (visually) entirely and the speckles become the dominant behaviour. As a final note it is worth noting that these behaviours I have described were visible to me in part because of the settings of my simulation. I found it was best to run them with many steps per frame $5000 \sim 10000$ because it allows you to see the macroscopic behaviours.

I acknowledge that although I wanted to use the `qt` frame work to create my own `gui` I ran out of time. Instead I used the free online applet created by Daniel V. Schroeder for Weber state university to make the higher level observations. The code that I used to evolve the two dimensional system was,

```
/*
 * metropolis_step_ising_t
 * -----------------------
 * Evolve the system according to a
 * randomly weighted spin flip that
 * compares the probability of the
```

```
 * two states based on the Boltzmann
 * distribution of the two systems.
 *
 * parameters
 * ----------
 * ising_t *system: The system to
 *   evolve.
 */
void metropolis_step(ising_t *system)
{
  int length = system->length;
  int **ensemble = system->ensemble;
  float epsilon = system->epsilon;
  float temp = system->temperature;
  float field = system->magnetic_field;

  int row = random_index(length);
  int col = random_index(length);

  int spin = ensemble[row][col];
  int neighbours =
    ensemble[modulo(row+1,length)][col] +
    ensemble[modulo(row-1,length)][col] +
    ensemble[row][modulo(col+1,length)] +
    ensemble[row][modulo(col-1,length)];

  float magnetic_change=-2*spin*field;
  float interaction_change=2*epsilon*
    neighbours*spin;
  float change=magnetic_change+
    interaction_change;

  if ((energy_change < 0) ||
    (exp(-change/temperature) > randn())))
  {
    ensemble[row][col] *= -1;
  }
}
```

Note: The `magnetic_field` was set to zero in the provided simulation and discussion, while the `epsilon` was set to one.

Question 2 c)

I noticed that the heat capacity *spike* increased in height as I increased the size of the crystal. This suggests that the infinite Ising model will have an infinitely tall heat capacity *spike* at the critical temperature. I also noticed that at the critical temperature all of the physical parameters changed the fastest.

This makes sense because a phase transition is loosely defined as a sudden discontinuity in the bulk properties of the sample. Although the entropy and energy are not discontinuous over the the critical temperature they do change very suddenly. The discontinuity is in the heat capacity which is the derivative of the energy with respect to temperature. Because a derivative is the discontinuous quantity it implies that the phase transition is second order.

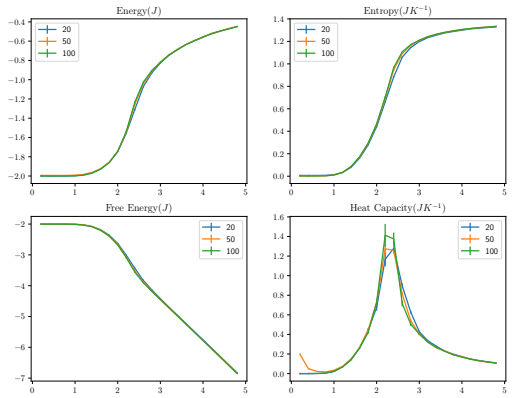

Figure 5:

To measure the energy of the two dimensional Ising system I used a very similar piece of code to the one dimensional scenario.

```
/*
 * energy_ising_t
 * --------------
 * Calculate the energy of the
 * Ising system.
 *
 * parameters
 * ----------
 * ising_t *system: The system to
 *   measure.
 */
float energy(ising_t *system)
{
  int length = system->length;
  int **ensemble = system->ensemble;
  float epsilon = system->epsilon;
  float field = system->magnetic_field;
  float magnetic = 0.0;
  float interactions = 0.0;

  for (int row=0; row<length; row++)
  {
    for (int col=0; col<length; col++)
    {
      float neighbours =
        ensemble[modulo(row+1,length)][col] +
        ensemble[modulo(row-1,length)][col] +
        ensemble[row][modulo(col+1,length)] +
        ensemble[row][modulo(col-1,length)];

      magnetic -= ensemble[row][col] *
        field;
      interactions -= neighbours *
        epsilon * ensemble[row][col];
    }
```

```
  }

  return interactions / 2. + magnetic;
}
```

For the entropy the calculation was also very similar.

```
/*
 * entropy_ising_t
 * ---------------
 * Calculate the entropy of the Ising
 * system.
 *
 * parameters
 * ----------
 * ising_t *system: The system to
 *   measure.
 */
float entropy_ising_t(ising_t *system)
{
  int len = system->length;
  int **ensemble = system->ensemble;
  int up = 0;

  for (int row=0; row<len; row++)
  {
    for (int col=0; col<len; col++)
    {
      up += ensemble[row][col] ==
        ensemble[modulo(row+1,len)][col];
      up += ensemble[row][col] ==
        ensemble[row][modulo(col+1,len)];
    }
  }

  int total = 2 * len * len;
  int down = total - up;

  return total * log(total) -
    up * log(up) - down * log(down);
}
```

Question 2 d)

I noticed that the magnetisation began to diverge at the same temperature irrespective of the size of the system. This is what I would expect from a phase transition because it should not depend on the size of the sample. To give a real world example iron melts at the same temperature regardless of the size of the block. We might more quickly melt a smaller block but that is just because there is less of it and less self insulation.

As N increases the critical temperature will stay the same, but the steepness of the transition appears to radically increase. I was surprised to see this relationship and I believe it may be because we are at the very low number end of the spectrum. In this regime if one or two spins flip it becomes visible on the graph. What I expect to see is

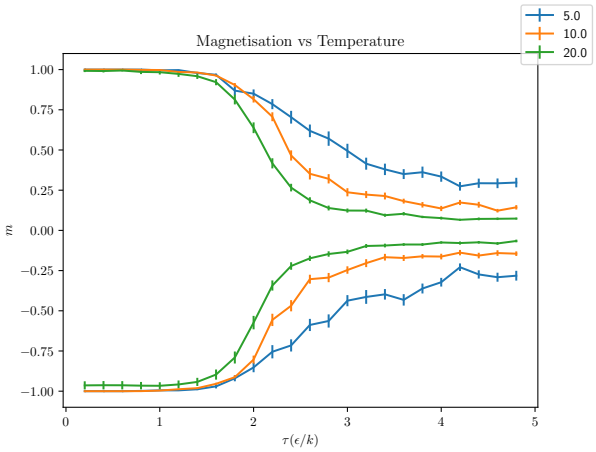

Figure 6: The magnetisation of the Ising model as the temperature and number of spins is varied.

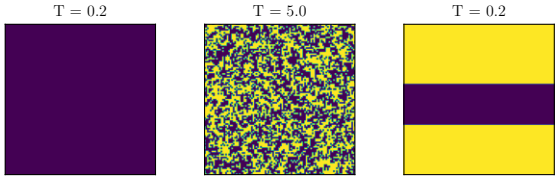

Figure 7: Heating and cooling an Ising system to change the magnetisation. The leftmost figure is the initial state at the lowest temperature, the middle figure is the highest temperature state and the rightmost figure is the final final state after the system has again been cooled.

that the lines smoothly converge down to a step function at the critical temperature.

Question 2 e)

I initialised the system randomly. This corresponds to the equilibrium of a system that is at a high temperature. Therefore, I first cooled the system to reach an equilibrium that I would expect for a low temperature state. This was done slowly letting the system equilibrate at each new temperature. This technique avoids the *meta-stable* rings from forming.

The cooled system represents the leftmost figure in 9. We can see that the magnetisation is complete and in this case there are not even any speckles. This is suspiciously good but I cannot find the error in my code so I will run with it. At the highest temperature we see that the state

appears to be almost entirely random. Cooling it back down I managed to get a *meta-stable* ring state.

In all the heating and cooling operations I raised the temperature slowly and re-equilibrated the system at each new temperature. I am annoyed by the ring state because this gradual cooling is supposed to prevent such states for the most part. Again this state is markedly non-speckled and I think this is because the temperature is very close to $0.0\epsilon/k$. We also see that the edges of the ring are pixel flat.

I justify this because the corners are where the *domains* die as I discussed above. Hence any incursion that yellow makes into the purple band is unstable because the incurring yellow are more likely to have purple neighbours than yellow neighbours. The same can be said for the purple incursions into yellow territory. Therefore, by far the most stable configuration is the flat edged band which we observe.

The final thing I want to discuss is the change in the magnetisation of the system between the first cool state and the final cool state. We can see that the injection of thermal energy into the system has changed the magnetisation from purple to predominantly yellow ignoring the *meta-stable* ring.

The Currie temperature is defined as the temperature at which the magnetic properties of a metal change dramatically. Since this is the behaviour that we are observing at the critical temperature it makes sense that the critical temperature is analogous to the Curie temperature. In the briefing we were given that the critical temperature for the two dimensional Ising model was $T_c \approx 2.27\epsilon/k$. The Curie temperature of iron is $T_c = 1043K$, hence $\epsilon = 1043K * k/2.27 = 0.0396eV$.

Introduction

The study of magnetic materials is an area of academic and industrial interest [**?**]. For example, magnetic technologies are important in the ongoing development of quantum computers, superconducting circuits and other examples in electronics. 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 a simple model of a ferro-magnet [**?**]. Despite the simplicity of the Ising model it displays rich physical behaviour and has analytic solutions in one and two dimensions [**?**, **?**]. 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 [**?**].

By modifying the basic Ising model we can simulate many phenomenon including glasses [**?**]. The Ising model has broader significance and can be used to construct very simple neural networks called Boltzmann machines [**?**]. We used the Ising model to compare ferro-magnetic, para-magnetic and anti-ferro-magnetic materials. Iron is a good example of a material that is ferro-magnetic, whereas gold is para-magnetic and chromium is anti-para-magnetic.

Theory

Materials have internal interactions. As physicists we like to ignore these where possible but often these approximations limit the accuracies of our models [**?**, **?**]. 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,

$$\begin{aligned} Z &= \sum_{s=\pm 1} \exp\left(-\frac{sB}{\tau}\right) \\ &= \exp\left(-\frac{sB}{\tau}\right) + \exp\left(\frac{sB}{\tau}\right) \\ &= 2\cosh\left(\frac{sB}{\tau}\right), \end{aligned} \tag{12}$$

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

$$P = \frac{\exp\left(-\frac{sB}{\tau}\right)}{2\cosh\left(\frac{sB}{\tau}\right)}. \tag{13}$$

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 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.

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

$$\begin{aligned} U &= \tau^2 \partial_\tau \ln Z \\ &= \tau^2 \partial_\tau \ln\left(2^N \cosh^N\left(\frac{sB}{\tau}\right)\right) \\ &= -NsB\tanh\left(\frac{sB}{\tau}\right). \end{aligned} \tag{14}$$

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

$$\begin{aligned} F &= -\tau \ln Z \\ &= -\tau \ln\left(2^N \cosh^N\left(\frac{sB}{\tau}\right)\right) \\ &= -NsB - N\tau \ln\left(1 + \exp\left(-\frac{2sB}{\tau}\right)\right). \end{aligned} \tag{15}$$

Curiously this matches with the results we found for the Ising model when there was no magnetic field. Using equation 9 we can calculate the magnetisation as a function of the magnetic field and temperature,

$$\begin{aligned} U = mB &= -NsB\tanh\left(\frac{sB}{\tau}\right) \\ m &= -Ns\tanh\left(\frac{sB}{\tau}\right). \end{aligned} \tag{16}$$

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

Using equations 16 and 15 we can calculate the energy. Since the math is essentially the same as in the derivation of equation 11 I have omitted some steps.

$$\begin{aligned}\tau\sigma &= F - U \\ &= -Ns\left(B + \tanh\left(\frac{sB}{\tau}\right)\right) - \\ &\quad N\tau \ln\left(1 + \exp\left(-\frac{2sB}{\tau}\right)\right) \end{aligned} \tag{17}$$

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 mutual interaction as $\Delta U = \epsilon s_i s_{i+1}$, where ΔU 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.

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.

Based on our analysis of the paramagnetic system we would expect that the magnetic field would coerce spins into alignment by decreasing there energy. This produces a positive reinforcement loop because now the energy of the neighbouring spin is not only decreased by sB when it aligns with the field but is also decreased by $\epsilon s_i s_{i+1}$. We predict that adding the external field will raise the critical temperature of the system.

We expect the type of phase transition to change. In general the spins will be flipping much less rapidly and as a result the humpy in the heat capacity will be smoothed out because the variance in the temperature will not peak as largely. Since, we expect that the heat capacity will be continuous this implies that the type of phase transition is now first order, where the energy is getting provided by the magnetic field.

Moreover, we expect that many of the rich behaviours we observed in the absence of an external magnetic field will vanish. For example, below the critical temperature we expect the lifetime of *domains* to be significantly shorter as the entire crystal quickly condenses into the ground state. In addition, we expect *speckling* to be even rarer and slower because the flip now has a weight lower be a factor of $\exp(-sB)$.

Another interesting effect that can be explored using the Ising model is anti-ferro-magnetism. This phenomenon was only recently discovered in nature 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.

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.

Hypothesis

We predicted that the anti-ferro-magnetic material would have a phase transition at the same temperature as the ferro-magnetic material in the absence of an external magnetic field. We came to this conclusion because the type of interaction is the same and all that has changed is the sign. The presence of an external field was expected to change this phase transition, which we expected to be second order based on the ferro-magnetic Ising model, to a first order phase transition.

We also predicted that the phase transition of the ferro-magnetic Ising model would change from a second order phase transition to a first order phase transition in the presence of an external magnetic field. This prediction was based on the unequal weighting of the orientations reducing the variability of the energy and hence smoothing out the peak in the heat capacity. A corollary of this second hypothesis was that the magnetic field would increase the critical temperature of the model.

Finally we presented a number of equations predicting how the para-magnetic material would evolve as the magnetic field was varied.

Method

We tested our the anti-ferro-magnetic phase transition hypothesis by measuring the physical parameters at a number of different temperatures and plotting the results. This allowed us to search for a suspected discontinuity in the heat capacity which would indicate a second order phase transition akin to the phase transition of the ferro-

magnetic substance. We repeated the same thing at three different strengths of magnetic field noting how the peak in the heat capacity qualitatively changed. As a result we were able to estimate the Neel temperature of the lattice based on the location of the $B = 0$ peak.

We used the same method to test how the ferro-magnetic phase transition was changed by the external magnetic field. However, we also tested increasing the strength of the magnetic field once the system was equilibrated below above and at the critical temperature. This gave us the ability to look for a similar, but not the same phase transition which we expected to be first order.

To test our predictions for the paramagnetic substance we simulated it over a fine grid of temperatures and the same three magnetic fields as the other simulations. We quantitatively assessed our models by calculating the χ^2 statistics for each fit and the associated p-value.

My original code could not be used to test these predictions so I modified it to accommodate the flexible ϵ and B into the sub-routines. Below I have included snapshots for the energy subroutine, entropy subroutine and the monte-carlo step subroutine.

```
/*
 * metropolis_step_ising_t
 * -----------------------
 * Evolve the system according to a
 * randomly weighted spin flip that
 * compares the probability of the
 * two states based on the Boltzmann
 * distribution of the two systems.
 *
 * parameters
 * ----------
 * ising_t *system: The system to
 *   evolve.
 */
void metropolis_step(ising_t *system)
{
  int length=system->length;
  int **ensemble=system->ensemble;
  float epsilon=system->epsilon;
  float temp=system->temperature;
  float field=system->magnetic_field;

  int row = random_index(length);
  int col = random_index(length);

  int spin = ensemble[row][col];
  int neighbours =
    ensemble[modulo(row+1,length)][col]+
    ensemble[modulo(row-1,length)][col]+
    ensemble[row][modulo(col+1,length)]+
    ensemble[row][modulo(col-1,length)];

  float magnetic=-2*spin*field;
  float interaction=2*epsilon*
    neighbours*spin;
  float change=magnetic+interaction;

  if ((change<0) ||
    (exp(-change/temp)>randn()))
  {
    ensemble[row][col]*=-1;
  }
}


/*
 * energy_ising_t
 * --------------
 * Calculate the energy of the Ising
 * system.
 *
 * parameters
 * ----------
 * ising_t *system: The system to measure.
 */
float energy_ising_t(ising_t *system)
{
  int len=system->length;
  int **ensemble=system->ensemble;
  float epsilon=system->epsilon;
  float field=system->magnetic_field;
  float magnetic=0.0;
  float interactions=0.0;

  for(int row=0;row<len;row++)
  {
    for(int col=0;col<len;col++)
    {
      float neighbours = 0.0;
      neighbours+=
        ensemble[modulo(row+1,len)][col]+
        ensemble[modulo(row-1,len)][col]+
        ensemble[row][modulo(col+1,len)]+
        ensemble[row][modulo(col-1,len)];

      magnetic+=ensemble[row][col]*field;
      interactions-=neighbours*epsilon*
        ensemble[row][col];
    }
  }

  return interactions / 2. + magnetic;
}

/*
 * entropy_ising_t
 * ---------------
 * Calculate the entropy of the Ising
 * system.
 *
 * parameters
 * ----------
 * ising_t *system: The system to
 *   measure.
 */
```

```
float entropy_ising_t(ising_t *system)
{
  int len=system->length;
  int **ensemble=system->ensemble;
  int up=0;

  for(int row=0;row<len;row++)
  {
    for(int col=0;col<len;col++)
    {
      up +=
        ensemble[row][col]==
        ensemble[modulo(row+1,len)][col]+
        ensemble[row][col]==
        ensemble[row][modulo(col+1,len)];
    }
  }

  int total=2*len*len;
  int down=total-up;

  return total*log(total)-up*log(up)-
    down*log(down);
}
```

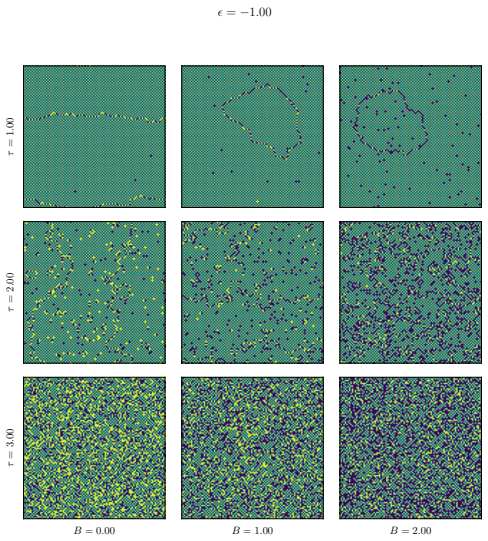

Figure 8: Snapshots of the evolution of the anti-ferro-magnetic material at three different temperatures and three different strengths of magnetic field.

However, the entropy subroutine that I have provided above does not work for the case $\epsilon = 0$. This is because the base unit for the paramagnet is not a pair but a single spin. In this case we need to change how we count the number of up pairs/spins to actually count the number of up spins. I achieved this by changing the contents of the nested `for` loop to `up += ensemble[row][col] > 0`. The two different entropy calculations added the minor detail that the program had to chose/know which version of the function to apply. I will not bore you with the details, but I used function pointers to perform this task.

Results

It is informative to make some qualitative notes on the behaviour of the anti-ferro-magnetic material. I noticed that most of the behaviours we observed in the ferro-magnetic material could also be observed in the anti-ferro-magnetic material. One of my favourites was the *domains* that formed. A small one is visible near the top left edge of the bottom left plot in figure 8. These are characterised by two (or more) regions of chest-board spins separated by a line of aligned spins.

A key difference between the anti-ferro-magnetic material and the ferro-magnetic material is that the former has only one possible species. This may call into question my discussion of the *domains* however, these are formed where the chest-board patterns are anti-aligned within two neighbouring regions (see figure 8). This also calls into question what actually happens at the phase transition, since the net magnetisation is practically always zero.

Varying the temperature we noticed that the size of the *domains* reduced as we increased the temperature and there seemed to be a temperature around $2.0\epsilon/k$ where the size of a *zone* was became comparable to the neighbourhood of a single spin. Hence we postulated that the phase transition was from anti-ferro-magnetism to para-magnetism. Our logic was that once the *zones* were this small the net impact on any one spin essentially cancelled.

Adding the magnetic field had all of the impacts that we might have expected from the ferro-magnetic material. The size of the *zones* around the critical temperature reduced and *speckling* became much faster for spins aligned with the magnetic field, but slower for spins anti-aligned with the magnetic field. If purple represents the aligned spins then purple speckles would rapidly appear in the crystal before been overcome, while yellow speckles were almost never observed. We can very clearly see this affect on figure 8 along the top row.

Interestingly, even at the greatest magnetic field we tests $B = 3.0T$ we the size of the *domains* in the low temperature state remained approximately the same. This makes sense as the states on either side of the domain wall remain equally favoured. Examining figure 8 we can see that there is an analouge to the *meta-stable* states we encountered in the ferr-magnetic case. That is a ring that has formed. For the anti-ferromagnetic case all *domains* appeared to be *meta-stable* in our simulations.

The para-magnetic material goes out of its way to be boring. There is only one behaviour and that is *speckling*. The temperature tunes the rate that the *speckling* occurs while magnetic field causes the one color to dominate the sample in a very linear fashion. At the strongest magnetic field the number of spins anti-aligned was almost none one the temperature was below $2.0\epsilon/k$ as shown in figure 9.

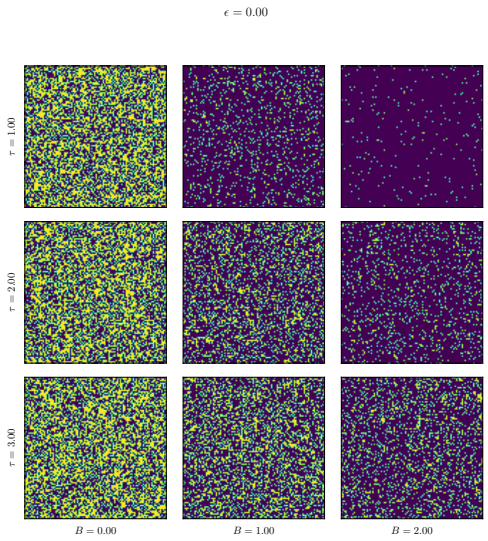

Figure 9: Snapshots of the paramagnetic material equilibrated at a variety of temperatures and magentic fields.

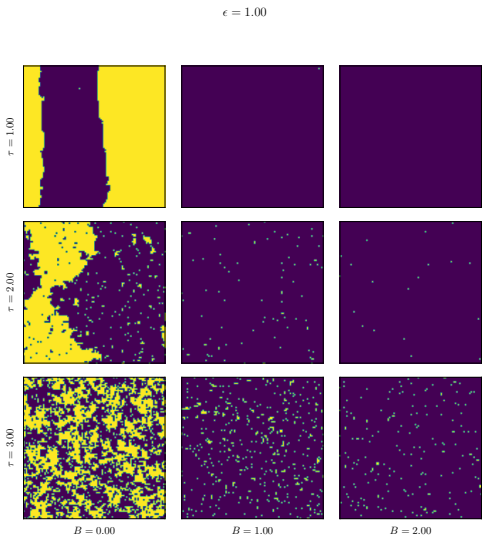

Figure 10: Snapshots of a ferro-magnetic material for multiple different magnetic field strengths and temperatures. For a discussion of the behaviours I invite you to review my earlier work.

Figure 11 is a very important figure so I will discuss it in a lot of detail. This figure evidences a lot of the qualitative discussion that I have undergone so far. Let's start by analysing the leftmost column which represents the anti-ferro-magnetic simulations. The most important result, which I will discuss first is the discontinuity in the heat capacity that occurs at approximately $2.10\epsilon/k$. This tells us that there is a second order phase transition.

Moreover, comparing the plots for the entropy, energy, free energy and magnetisation to those in the middle column we can see that the anti-ferro-magnet begins to behave like the para-magnet. This confirms the prediction that the phase transition was from anti-ferro-magnetic to para-magnetic. Curiously both the energy and the entropy rise in the wrong order by magnetic field. The stronger magnetic field resulting in an earlier rise than the weaker. This does not match the para-magnetic behaviour although the asymptotes seem to be the same.

We observe, once again as predicted, that the peak in the heat capacity shifts to lower temperatures as we increase the magnetic field. That said the effect is not noticeable for the first increase in the magnetic field strength which fails to noticeably shift the peak to the left. I also observed that the heat capacity seems to converge to a constant value on the hotter side of the peak. This matches the behaviour of the para-magnetic heat capacity.

Now let's consider the middle column which represents the para-magnetic material. The most interesting thing about the para-magnetic material is that the high temperature behaviour matches the high temperature anti-ferro-magnetic behaviour. We observe that the heat capacity without an external magnetic field drops to zero. This makes sense as according to equation **??** the energy will be constant.

In particular the energy will be constant on average for an infinite lattice. There are clearly energy changes occurring all the time as spins flip agnostically up and down. However, the spins are exactly as likely to flip up as they are to flip down so the result is that the average works out to zero. The derivative of a constant is then of course zero. By the same reasoning the magnetisation and the energy are both zero.

Adding the magnetic field causes the energy and the entropy to vary smoothly as a function of temperature. Examining equations 16 and 17 we see that the temperature dependence of the system is related to the quantity B/τ. Heuristically, this leads to the conclusion that the magnetic field and the temperature have complementary effects. That is if we increase the magnetic field strength we have to increase the temperature to maintain the same value of B/τ.

I have already given a large amount of discussion to the behaviour of the ferro-magnetic Ising model so I will keep the analysis of the rightmost column brief. The interesting behaviour is invoked by the presence of the external magnetic field. In particular we see as predicted that the heat capacity peak is smoothed out and shifted to higher temperatures implying that the phase transition is now first order. This matches our predictions and confirms the presence of a positive feedback relation as opposed to an anti-ferro-magnetic material.

Using equations **??**, **??**, **??**, **??** and 12 we computed χ^2 statistics for the fitted model. To do this we used Poisson

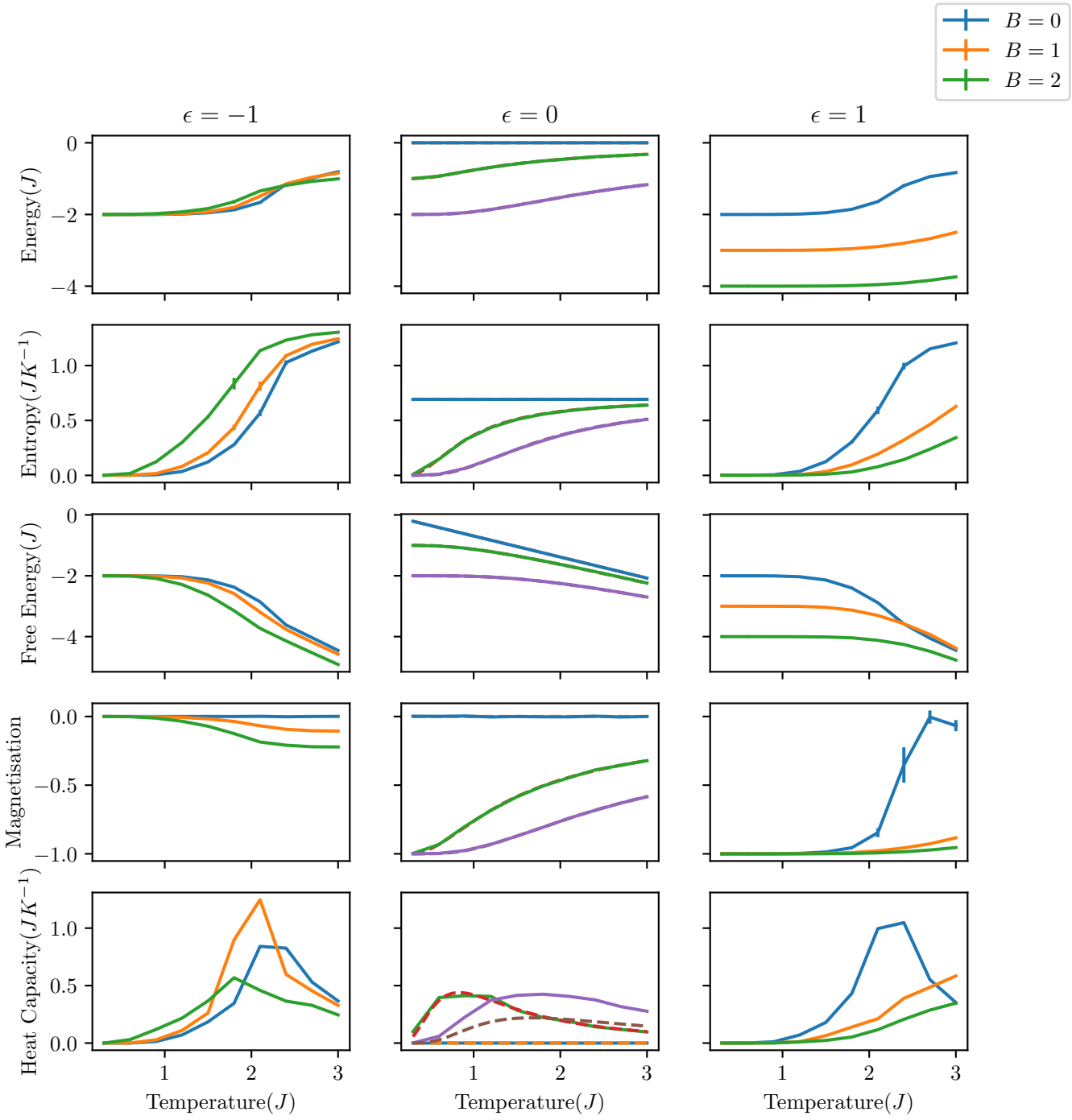

Figure 11: The physical properties of the anti-ferro-magnetic, para-magnetic and ferro-magnetic systems as a function of the temperature and for multiple magnetic field strengths. The anti-ferro-magnetic material properties are plotted on the leftmost graph. The para-magnetic material properties are plotted in the center and the ferro-magnetic are on the right.

	$B(T)$	χ^2	p
U	0	NAN	NAN
σ	0	3.17×10^{-5}	NAN
F	0	3.17×10^{-5}	NAN
C_V	0	NAN	NAN
$\|m\|$	0	NAN	NAN
U	1	5.34×10^{-4}	$<< 0.05$
σ	1	2.36×10^{-3}	$<< 0.05$
F	1	1.99×10^{-5}	$<< 0.05$
C_V	1	4.44×10^{-1}	$<< 0.05$
$\|m\|$	1	5.34×10^{-4}	$<< 0.05$
U	2	4.95×10^{-5}	$<< 0.05$
σ	2	1.77	0.00540
F	2	9.84×10^{-5}	$<< 0.05$
C_V	2	80.2	~ 1
$\|m\|$	2	4.95×10^{-5}	$<< 0.05$

Table 1: χ analysis of goodness of fit. I have included three significant figures when quoting the χ^2 statistic but it was used to maximum precision in calculations.

counting,

$$\chi^2 = \sum_i \left(\frac{o_i - e_i}{e_i} \right)^2 , \tag{18}$$

where o_i is the observed data point in the i^{th} value and e_i is the expected value. This revealed what we would have expected based on the visual appearance of the data. The results of this analysis are included in table 1.

Table 1 shows some very interesting trends. Firstly, we see that our model matches, to within a very good approximation, what we predicted in equations **??**, **??**, **??** and **??**. You may be suspicious of the NAN, χ^2 values that I am reporting. You may notice that in these cases the predicted and model values are constant at zero in appropriate units. This resulted in divide by zero errors when I applied equation 18.

The next interesting element of table 1 is that the heat capacity performs much worse than the other physical parameters in terms of goodness of fit measured using the χ^2 analysis. I believe that this is because of how the heat capacity is measured, which from equation 14 we can see uses the variance. For each parameter we run $1000N^2$ trials with measurement and then average the result giving us extremely high accuracy. The heat capacity is the variance of these measurements and has consistently shown to converge slower than the mean (see 2 and 4).

Although hard to see figure 11 contains error bars on all of the parameters except the heat capacity. We calculated the error in the heat capacity in the same way as other parameters using equation 15, but it was very large compared to the data and obscured the results on figure 11. We proposed that better estimates for the heat capacity could be obtained by increasing the size of the lattice. We proposed this because it results in more runs and single flips cause smaller percentage changes in the energy.

To generate figure 11 we recorded data at ten evenly space points between zero and three ϵ/k incremented by $0.3\epsilon/k$. As a result we used nine degrees of freedom to compute the p-values displayed in table 1. The remaining unexplained aspects of the method were explain in the discussion of Question 1 b) and Question 2 b) respectively. The same method was applied here extended to account for the additional parameters.

I did not use figure 11 to estimate the Neel temperature because the samples were taken to broadly. Instead I wrote another program to measure the heat capacity over a much finer grid for a 20×20 lattice. This program sampled temperatures from $2.5\epsilon/k$ to $2.0\epsilon/k$ in increments of $0.025\epsilon/k$. At each temperature the program ran for only $100N^2$. I believe that lower number of steps maintains accuracy because the cooling is much slower.

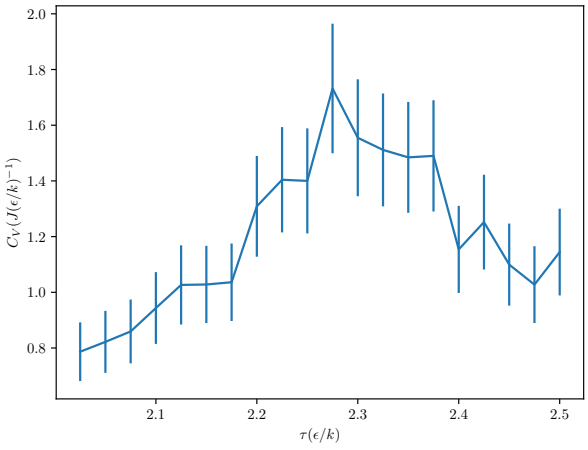

Figure 12: A finely gridded heat capacity measurement on a 20×20 lattice.

Figure 12 allows use to estimate the Neel temperature, but before we do it is worth discussing some of its features. Unlike figure 11 the heat capacity is included with error. This is because I ran more independent simulations, eight instead of five. Apparently even this small increase dramatically reduced the spread. Additionally, we observe that the curve, appears bumpy, when we know that minus the peak, the curve should be smooth.

To estimate the Neel temperature I took the temperature corresponding to the greatest heat capacity, in this case $T = 2.28 \pm 0.01$. The uncertainty that I have quoted for the Neel temperature is half the the temperature increment rounded to one significant figure. Remarkably the Neel temperature is very similar to the Currie temperature. I believe that in our scenario this makes sense since the interactions strengths are the same and all that has changed is the sign.