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 descision 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.

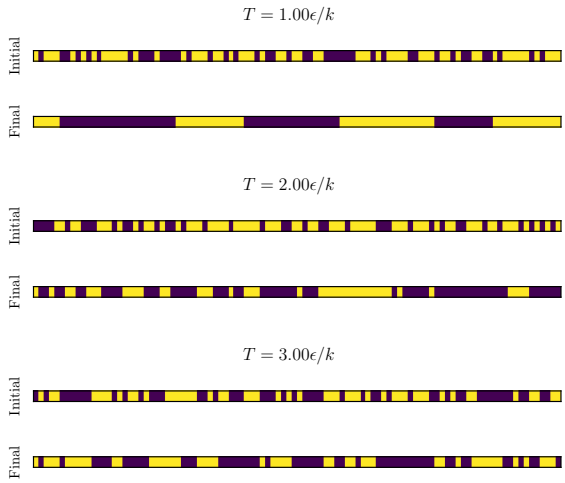


Figure 1: Each vertical pair of lines represents the spin state. The top one is the random initial state and the bottom one is the equilibrated final state.

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,

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

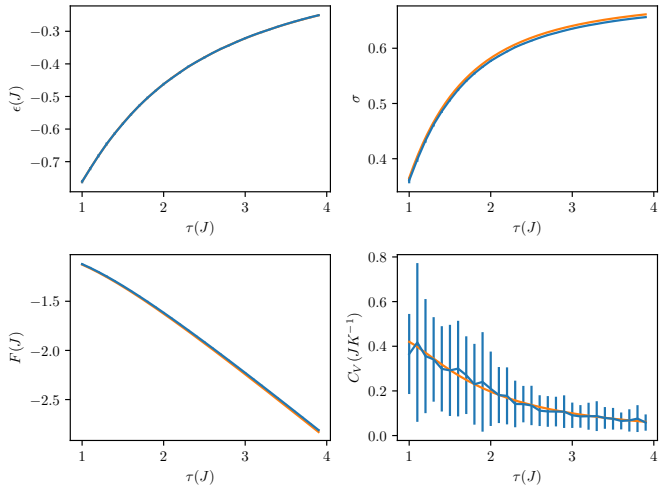
The entropy followed from the combination of Equation 3 and Equation 1 using Equation 5,

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

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)



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.

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

```
/*
 * energy
 * ------
 * Calculate the energy of the system.
 *
 * parameters
 * ----------
 * ising_t *system: A struct
 *   enscapulating the information
 *   related to the system.
 */
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.
 *
 *
 *
 *
 *
 */
```

Question 1 d)

Question 1 e)