

# PHYS3020 Computational Project Report

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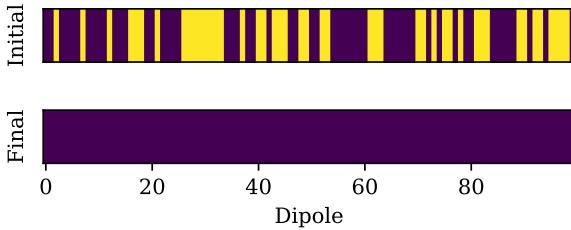
Semester 2, 2022

The programming language Python was used for this project, with the packages `numpy` and `matplotlib` used to perform analysis and generate plots.

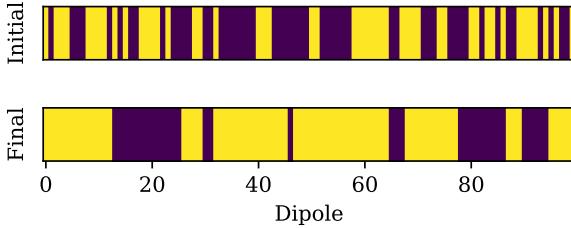
## 1 Question 1

### 1.1 1D Ising Model

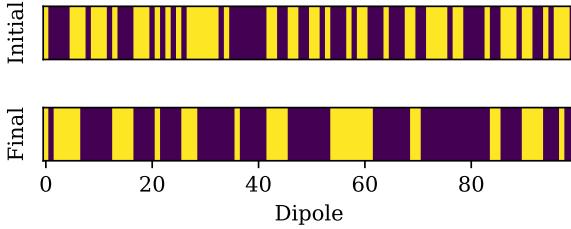
Beginning from an initial (approximately) random state with periodic boundaries, the system was subject to  $10^5$  time steps, so that each one of the 100 dipoles could have, in principle,  $10^3$  chances to flip their alignment. The results are shown, for 4 different temperatures, in Figure 1.



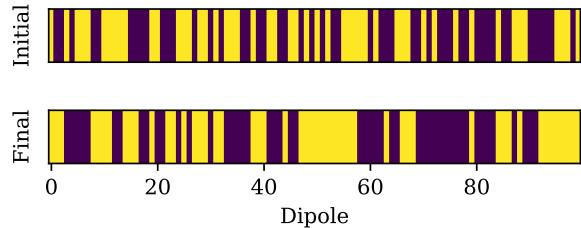
(a) Initial and final states with  $T = 0.5\epsilon/k$ .



(b) Initial and final states with  $T = 1\epsilon/k$ .



(c) Initial and final states with  $T = 2\epsilon/k$ .



(d) Initial and final states with  $T = 5\epsilon/k$ .

**Figure 1** The initial and final states of a 1D Ising Model with  $N = 100$  dipoles, joined on the horizontal axis. Yellow bars represent a spin-up state, while purple bars represent a spin-down state.

As the temperature gets lower, it appears that the size of spin-parallel chunks increases. We'd expect that as  $T \rightarrow 0$ , all of the spins would be aligned in parallel, while as  $T \rightarrow \infty$ , each dipole would be aligned antiparallel to its neighbours.

The Python code that was used to generate both the initial state (given by the function `gen_init_Ising()`) and the metropolis algorithm (in 1D given by `metropolis()`) is shown in the following code block.

```
1 def gen_init_Ising(N):
2     initState = np.random.uniform(0, 1, N)
3     s = [1 if initState[i] >= 0.5 else -1 for i
4         in range(N)]
5     return s
6
7 def metropolis(states, iters, temperature):
8     beta = 1 / temperature
9     RVs = np.random.uniform(0, len(states) - 1,
10                           iters)
11    RVs = [int(x) for x in RVs]
12    for i in range(iters):
13        if RVs[i] == len(states) - 1:
14            Ldipole = states[RVs[i] - 1]
15            Rdipole = states[0]
16        elif RVs[i] == 0:
17            Ldipole = states[len(states) - 1]
18            Rdipole = states[1]
19        else:
20            Ldipole = states[RVs[i] - 1]
21            Rdipole = states[RVs[i] + 1]
22            energy = lambda D : -1 * ((Ldipole * D)
23                                         + (Rdipole * D))
24            dipole = states[RVs[i]]
25            initEnergy = energy(dipole)
```

```

23     flipEnergy = energy(-1 * dipole)
24     deltaEnergy = flipEnergy - initEnergy
25     if deltaEnergy <= 0:
26         dipole *= -1
27     else:
28         flipProb = np.exp(-beta *
29             deltaEnergy)
30         evaluation = np.random.uniform(0, 1)
31         if evaluation <= flipProb:
32             dipole *= -1
33     states[RVs[i]] = dipole
34
35 return states

```

## 1.2 Ising Thermodynamic Parameters

We're given that the partition function of the system of  $N$  dipoles is

$$Z = (2 \cosh(\beta\epsilon))^N \quad (1)$$

The average internal energy of the system is then

$$\begin{aligned} U = \langle E \rangle &= -\frac{\partial}{\partial \beta} \ln Z \\ &= -\frac{\partial}{\partial \beta} N \ln (2 \cosh(\beta\epsilon)) \\ &= -\frac{\partial}{\partial \beta} N \ln (e^{\beta\epsilon} + e^{-\beta\epsilon}) \\ &= -N \cdot \frac{1}{e^{\beta\epsilon} + e^{-\beta\epsilon}} \cdot (\epsilon e^{\beta\epsilon} + -\epsilon e^{-\beta\epsilon}) \\ &= -N\epsilon \left( \frac{e^{\beta\epsilon} - e^{-\beta\epsilon}}{e^{\beta\epsilon} + e^{-\beta\epsilon}} \right) \\ &= -N\epsilon \tanh(\beta\epsilon) \end{aligned}$$

And since the internal energy per dipole is  $u = U/N$ , we get that

$$u = -\epsilon \tanh(\beta\epsilon) \quad (2)$$

Next, the free energy is given by  $F = -kT \ln Z$ , and so

$$\begin{aligned} F &= -kT \ln Z \\ &= -kT \cdot N \ln (2 \cosh(\beta\epsilon)) \\ &= -kTN \ln (e^{\beta\epsilon} + e^{-\beta\epsilon}) \\ &= -kTN \ln \left( \frac{1 + e^{-2\beta\epsilon}}{e^{-\beta\epsilon}} \right) \\ &= -kTN [\ln(1 + e^{-2\beta\epsilon}) - \ln(e^{-\beta\epsilon})] \\ &= -kTN [\ln(1 + e^{-2\beta\epsilon}) + \beta\epsilon] \\ &= N (-\epsilon - kT \ln(1 + e^{-2\beta\epsilon})) \end{aligned}$$

And since the free energy per dipole is given by  $f = F/N$ ,

$$f = -\epsilon - kT \ln(1 + e^{-2\beta\epsilon}) \quad (3)$$

The entropy can be obtained by  $S = -\partial F/\partial T$ , and so the entropy per dipole can be obtained by

$$\begin{aligned} S &= S/N = -\frac{\partial f}{\partial T} \\ &= -\frac{\partial}{\partial T} (-\epsilon - kT \ln(1 + e^{-2\beta\epsilon})) \end{aligned}$$

$$\begin{aligned} &= k \ln(1 + e^{-2\beta\epsilon}) + \left( \frac{kT}{1 + e^{-2\beta\epsilon}} \right) \\ &\quad \cdot -\frac{2\epsilon}{kT^2} e^{-2\beta\epsilon} \cdot -1 \\ &= \frac{2\epsilon}{T} \frac{e^{-\beta\epsilon}}{e^{\beta\epsilon} + e^{-\beta\epsilon}} + k \ln(1 + e^{-2\beta\epsilon}) \\ &= \frac{2\epsilon}{T} \frac{e^{-\beta\epsilon} + e^{\beta\epsilon} - e^{\beta\epsilon}}{e^{\beta\epsilon} + e^{-\beta\epsilon}} + k \ln(1 + e^{-2\beta\epsilon}) \\ &= \frac{2\epsilon}{T} \left( \frac{e^{-\beta\epsilon}}{e^{\beta\epsilon} + e^{-\beta\epsilon}} - \tanh(\beta\epsilon) \right) + k \ln(1 + e^{-2\beta\epsilon}) \end{aligned}$$

But  $e^{\beta\epsilon}/(e^{\beta\epsilon} + e^{-\beta\epsilon}) = \frac{1}{2}(\tanh(\beta\epsilon) + 1)$ , so

$$\begin{aligned} S &= \frac{2\epsilon}{T} \left( \frac{1}{2} [\tanh(\beta\epsilon) + 1] - \tanh(\beta\epsilon) \right) + k \ln(1 + e^{-2\beta\epsilon}) \\ &= \frac{\epsilon}{T} (1 - \tanh(\beta\epsilon)) + k \ln(1 + e^{-2\beta\epsilon}) \end{aligned} \quad (4)$$

Finally, the specific heat capacity is given by

$$\begin{aligned} c &= \frac{C_V}{N} = \frac{1}{N} \frac{\partial U}{\partial T} = \frac{\partial u}{\partial T} \\ &= \frac{\partial}{\partial T} (-\epsilon \tanh(\beta\epsilon)) \\ &= -\epsilon \left( \frac{1}{\cosh^2(\epsilon/kT)} \cdot -\frac{\epsilon}{kT^2} \right) \\ &= \frac{\epsilon^2 \beta}{T \cosh^2(\beta\epsilon)} \end{aligned} \quad (5)$$

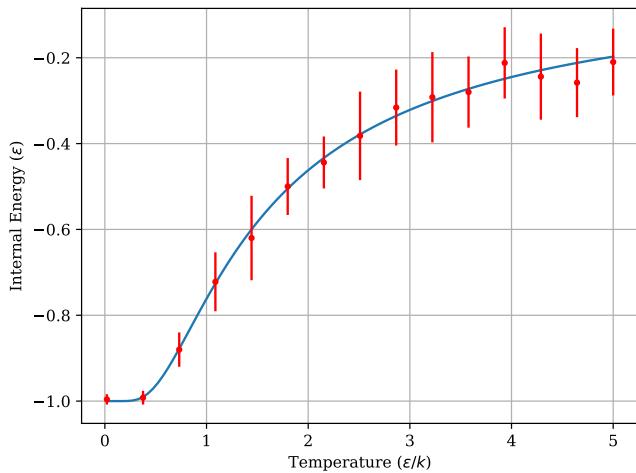
## 1.3 Plots of Thermodynamic Properties

For a range of different values of temperature, the internal energy, free energy, entropy, heat capacity and reduced magnetisation (all with respect to each dipole) was calculated at an approximate equilibrium value.

Beginning with internal energy per dipole, the experimental value for each system state was calculated by

$$u = \frac{1}{N} \left( -\epsilon \sum_{i,j} s_i s_j \right) \quad (6)$$

These values, contrasted by the theoretical value shown in equation (2), are shown in Figure 2

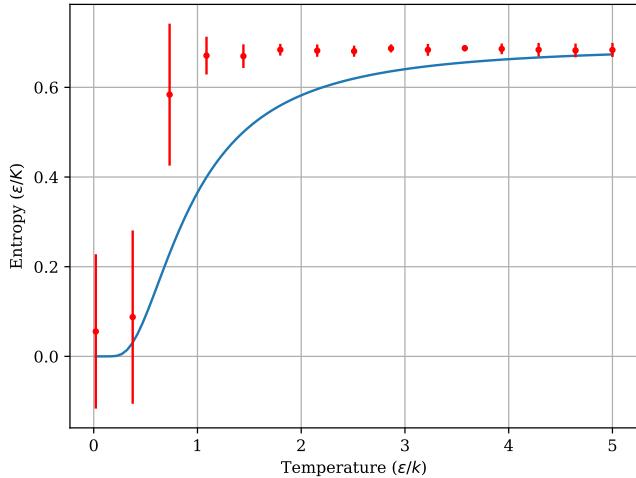


**Figure. 2** Average internal energy per dipole for 15 temperatures, compared with theoretical value. The theoretical relationship is shown by the blue curve, while the data points are given in red. The data points are the average across 20 trials, with the errorbars representing the standard deviation of the values across those trials.

Since all possible combinations for a system of 100 dipoles is a large number, I invoked Sterling's approximation to calculate the entropy of any state. The total number of dipoles  $N$  was used with the number of observed spin-up dipoles  $N_\uparrow$  to calculate entropy by

$$S \approx \frac{1}{N} (N \log N - N_\uparrow \log N_\uparrow - (N - N_\uparrow) \log(N - N_\uparrow)) \quad (7)$$

With this as the basis of the experimental approximations for entropy, the calculated values are contrasted against the theoretical relationship (equation (4)) in Figure 3

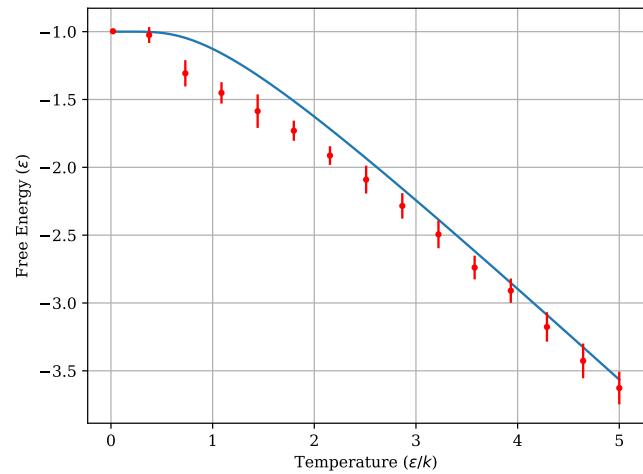


**Figure. 3** Average energy per dipole across 15 temperatures. As before, the blue curve is the theoretical relationship, and the red points the data averaged across 20 trials.

With the internal energy and entropy known per dipole, the free energy could be computed by

$$f = u + TS \quad (8)$$

The computed values together with the theoretical model (equation 3) are shown in Figure 4.

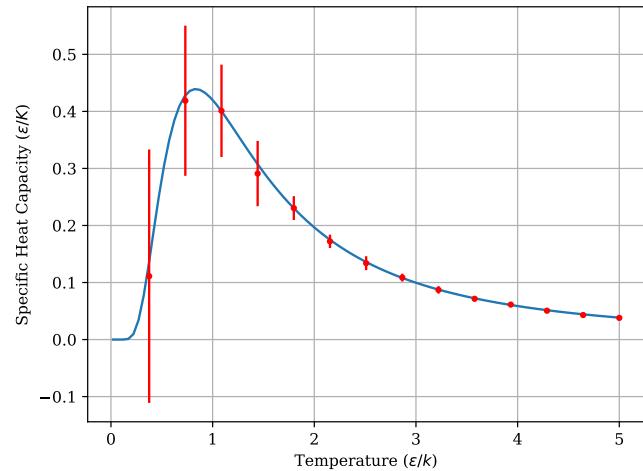


**Figure. 4** Average free energy per dipole across 15 temperature values and 20 trials.

The specific heat capacity of the model can be computed by

$$c = \frac{\langle U^2 \rangle - \langle U \rangle^2}{kT^2 N} \quad (9)$$

Once again, the computed values and the theoretical model (equation (5)) are contrasted in Figure 5.

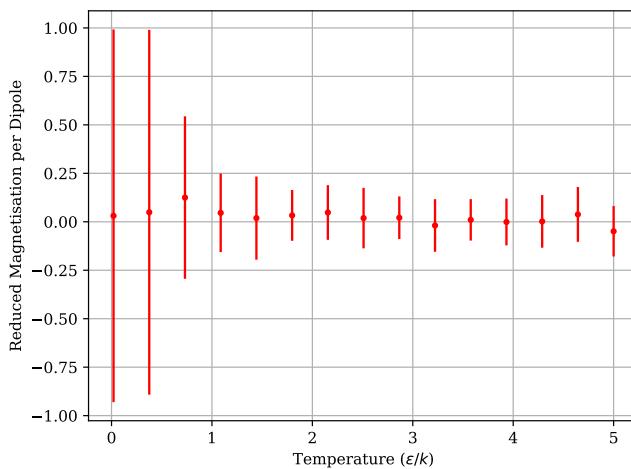


**Figure. 5** Specific heat capacity for a system at 15 temperatures, averaged across 20 trials.

Finally, the reduced magnetisation per dipole is given by the average spin value across the lattice. That is,

$$m = \bar{s} \quad (10)$$

No theoretical relation exists for this in terms of temperature, only in terms of the limit of temperature. The experimental observations of the net magnetisation per dipole is shown in Figure 6.



**Figure 6** Reduced magnetisation per dipole for 15 temperatures, averaged across 20 independent trials.

## 1.4 Plot Discussion

It's clear from looking at Figure 1 that increasingly large chunks of like-spin states emerge at lower temperatures for the 1D Ising model with periodic boundaries. We see that at sufficiently low temperature, the entire lattice transitions to the same spin state, while at high temperatures, the 'chunks' of spin states tend to size one.

Using the equation for internal energy per dipole to calculate  $u$  for some system state, the data aligns perfectly to the theoretical model (within uncertainty) as shown in Figure 2. This shows that, as the temperature increases, the internal energy of the system goes to 0 due to the dipoles being aligned antiparallel with respect to their neighbours.

Approximating an infinite 1-dimensional lattice by a "large" 1D lattice is most likely the underlying cause of the discrepancy between the observed and theoretical entropy values. We'd expect that a finite lattice would have a critical temperature at which a net magnetisation would occur, and that the sudden discontinuity in the data in Figure 3 is a result of this. We expect that a larger lattice would yield results that closer fits to the theoretical curve.

Given that the free energy per dipole is calculated according to the internal energy and the entropy, we would expect some deviation from the model since the entropy deviates from the model. That is exactly what we see in Figure 4, where the data is slightly more

negative than the model on account of the entropy being too large with respect to its own model. As the free energy has the entropy as a negative term, this yields the lower value which is seen. Apart from this, the overall trend of the data aligns well with the model.

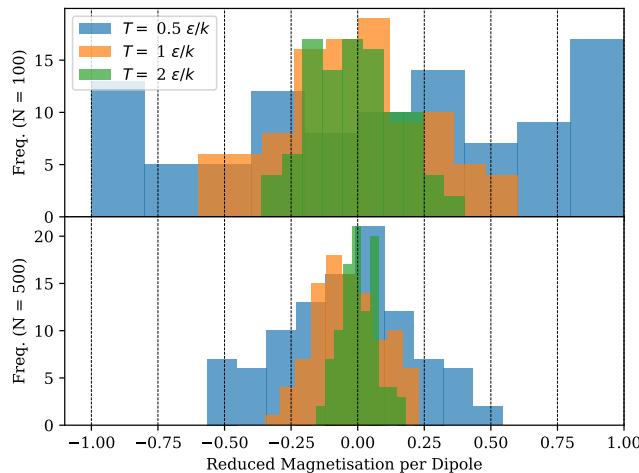
The data for heat capacity was incredibly sensitive to the equilibrium of the system, and we had to leave the system for many more spin-flip opportunities than the other thermodynamic property examinations to get data that aligned to the model. We observed deviation from the model only at low temperatures (which is evident by the significantly larger error bars in low temperature data points), and excellent, consistent agreement with the model at larger temperatures as seen in Figure 5. Curiously, we observe that the system is least willing to change its temperature when at  $T \sim 1\epsilon/k$ .

Finally, we observe the average magnetisation per dipole in Figure 6, where no exact solution exists. Clearly, lower temperatures correlate with larger standard deviations for the average magnetisation of a 1D Ising model. We postulate that this is due to low temperature systems aligning almost totally parallel in *either* spin-up or spin-down states (hence the large scatter), and high temperature systems being consistently aligned antiparallel (and so have a rough average of 0 with minimal scatter). This is supported by the instantaneous system states shown in Figure 1.

## 1.5 Net Magnetisation at Different Temperatures

Figure 7 shows the average magnetisation of a system for 3 different temperatures, and two different system sizes across 100 trials. We see immediately that for a lower number of dipoles, the system becomes more magnetised on average (by inferring the absolute value of the magnetisation,  $|m|$ ) for all temperatures.

Even though the average magnetisation for each temperature (across all trials) is about 0, the standard deviation is vastly bigger for lower temperatures and number of dipoles. As such, we'd expect that as  $N \rightarrow \infty$  that both  $\bar{m} = 0$  and  $s.d.(m) \rightarrow 0$ , essentially saying that an infinite 1D Ising model should have a time-average magnetisation of 0.



**Figure. 7** Final state reduced magnetisation per dipole for different temperatures and number of dipoles, across 100 trials. The top histogram represents trials with 100 dipoles, and the bottom 500 dipoles.

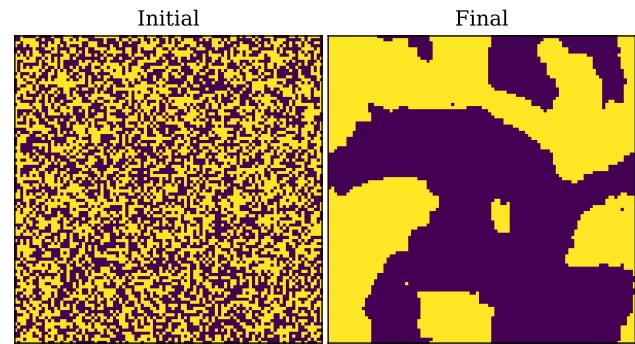
Because of this, we'd expect that an infinite 1D Ising model will have no total phase transition as there will always be some infinite number of dipoles aligned anti-parallel (and so the net magnetisation will always be 0). For sufficiently low temperature *finite* systems, we already see some total phase transitions in the upper half of Figure 7 (with  $T = 0.5\epsilon/k$  and  $N = 100$ ).

Furthermore, we see in Figure 7 that the ‘phase transition temperature’ seems to reduce for a higher lattice size. We’d expect that in the limit of  $N \rightarrow \infty$  that the  $T_c \rightarrow 0$  and hence there would be no phase transition for a non-zero temperature. Finally, since the expected magnetisation is 0 for increasingly large lattices, any local net magnetisation in the infinite lattice would be thermodynamically unstable and so there would be no total phase transition at  $T = 0\epsilon/k$  either.

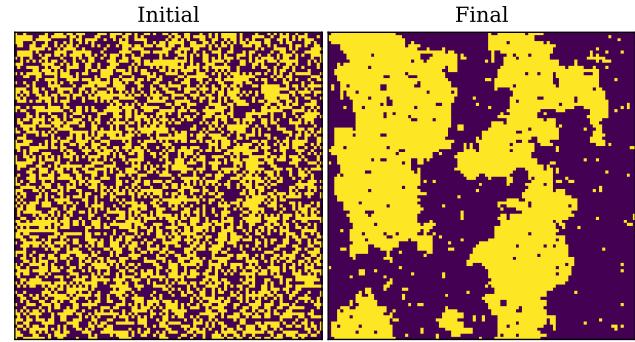
## 2 Question 2

### 2.1 2D Ising Model

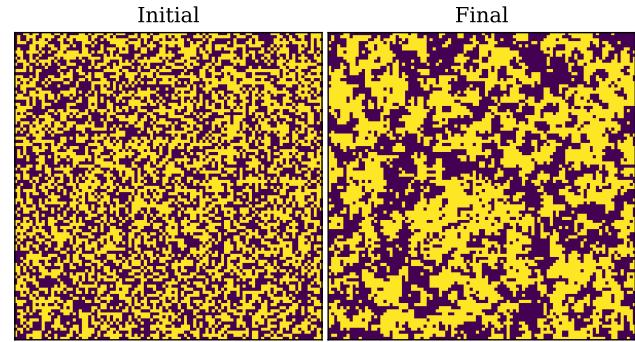
As in Question 1, a 2D lattice was initialised in a random state and left for  $10^6$  states to start to settle into an equilibrium position. In order to produce some interesting results, we did not want the lattice to be subject to a phase transition (for these plots). The results for this across 3 different temperatures are shown in Figure 8.



(a) Initial and final states with  $T = 1\epsilon/k$ .



(b) Initial and final states with  $T = 2\epsilon/k$ .



(c) Initial and final states with  $T = 3\epsilon/k$ .

**Figure. 8** The initial and final states of a 2D Ising Model with  $N = 100^2$  dipoles in a square lattice. Yellow squares represent a spin-up state, while purple squares represent a spin-down state.

As time progressed (i.e. as the state number increased) for the lower temperatures, regions of parallel-aligned spins arose and grew. Some of this behaviour was seen in the  $T = 3\epsilon/k$  state, but not to the same extent as the other two temperatures.

The code that generates these lattices is shown in the following code block.

```

1 def gen_init_Ising2d(N):
2     s = np.zeros((N, N))
3     for i in range(N):
4         initState = np.random.uniform(0, 1, N)
5         s[i, :] = [1 if initState[i] >= 0.5 else
6 -1 for i in range(N)]
7     return s
8
9 def DeltaU2d(LD, RD, UD, DD, D):
10    return -1 * ((LD * D) + (RD * D) + (UD * D)
11 + (DD * D))
12
13 def metropolis2d(states, iters, temperature):
14    """
15    Parameters
16    -----
17    states : np.array
18        and NxN array composed only of -1 and 1,
19        corresponding to the spin of each dipole
20    iters : int
21        The number of iterations (different
22    states) to simulate
23    temperature : float
24        The temperature (in units of epsilon / k
25    ) of the reservoir
26    """
27
28    beta = 1 / temperature
29    N = states.shape[0] # assume square lattice
30
31    RVhoriz = np.random.uniform(0, N, iters) # generate some random positions along
32    horizontal axis
33    RVvert = np.random.uniform(0, N, iters) # as
34    above but along vertical axis
35    RVhoriz = [int(x) for x in RVhoriz] # make
36    them correspond to an index
37    RVvert = [int(x) for x in RVvert]
38
39    evaluations = np.random.uniform(0, 1, iters)
40    for i in range(iters):
41
42        dipole = states[RVhoriz[i], RVvert[i]]
43        Ldipole = states[RVhoriz[i]-1, RVvert[i]
44        ] if RVhoriz[i] != 0 else states[N-1,
45        RVvert[i]] # value of the left dipole
46        Rdipole = states[RVhoriz[i]+1, RVvert[i]
47        ] if RVhoriz[i] != N-1 else states[0,
48        RVvert[i]] # right dipole
49        Udipole = states[RVhoriz[i], RVvert[i
50        ]-1] if RVvert[i] != 0 else states[RVhoriz[i
51        ], N-1] # upper dipole
52        Ddipole = states[RVhoriz[i], RVvert[i
53        ]+1] if RVvert[i] != N-1 else states[RVhoriz[i
54        ], 0] # lower dipole
55
56        initEnergy = DeltaU2d(Ldipole, Rdipole,
57        Udipole, Ddipole)
58        flipEnergy = DeltaU2d(Ldipole, Rdipole,
59        Udipole, Ddipole, -1*dipole)
60
61        deltaEnergy = flipEnergy - initEnergy
62        if deltaEnergy <= 0:
63            states[RVhoriz[i], RVvert[i]] *= -1
64        else:
65            flipProb = np.exp(-beta *
66            deltaEnergy)
67            if evaluations[i] <= flipProb:
68                states[RVhoriz[i], RVvert[i]] *=
69                -1
70    return states

```

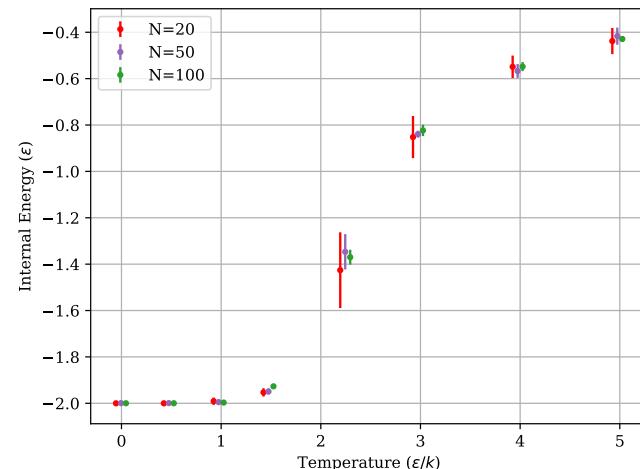
## 2.2 Crystal Size with Temperature

As was observed in the previous section, the size of the ‘crystals’ in the square lattice became larger as  $T$  decreased, and became larger faster at lower temperatures. It was observed that these parallel-aligned dipole crystals became significant for temperatures lower than  $T = 3\epsilon/k$ , and were a significant proportion of the total size of the lattice. This suggests that some critical temperature  $T_c$  exists between 2 and  $3\epsilon/k$ , that is,  $2\epsilon/k \leq T_c \leq 3\epsilon/k$ , where the entire system will become aligned parallel at some spin value.

## 2.3 Thermodynamic Properties of the 2D Ising Model

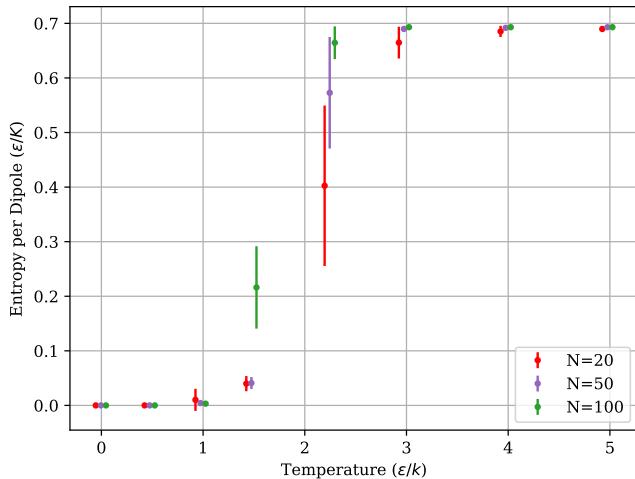
In each of the figures below, the  $N = 20^2$  population lattice was given  $5 \times 10^4$  flip chances to approximate equilibrium, the  $N = 50^2$  population  $5 \times 10^5$  chances, and the  $N = 100^2$  population  $5 \times 10^6$  chances.

To begin with, the internal energy per dipole for the 2D Ising model was computed in a very similar way to equation (6), where the only difference was that neighbours both horizontally and vertically were taken into account (rather than just horizontally as in the 1D model).



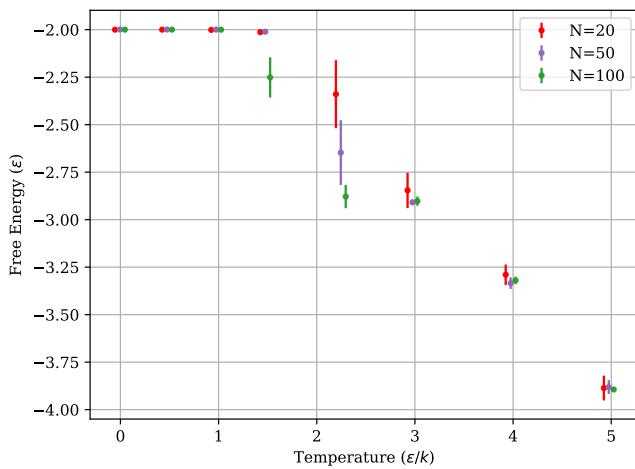
**Figure. 9** The average internal energy per dipole for a square lattice with various side lengths, against multiple temperatures and 10 trials. Since all 3 population lattices were tested at the same temperature, the data points were shifted about the temperature axis slightly so that each data point could be discerned from the others. The tested temperatures in this plot and all of the other plots in this subsection were  $T \in \{0.02, 0.5, 1, 1.5, 2.27, 3, 4, 5\} \epsilon/k$ .

The entropy per dipole of the lattice was computed in the same way as in equation (7), yielding the data in Figure 10.



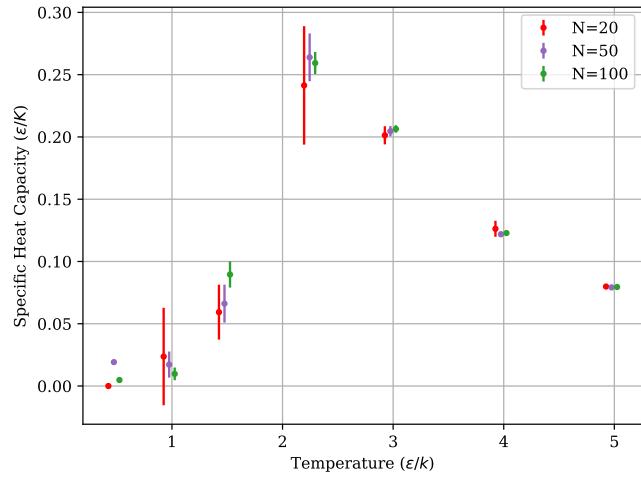
**Figure. 10** Entropy per dipole of the 2D Ising lattice, with varying temperature and dipole population across 10 trials. The temperatures tested are the same as in Figure 9, with the same data-point temperature jitter.

The free energy per dipole was calculated in the same way as in the 1D case.



**Figure. 11** Free energy per dipole of the 2D Ising lattice, with varying temperature and dipole population across 10 trials. The temperatures tested are the same as in Figure 9, with the same data-point temperature jitter.

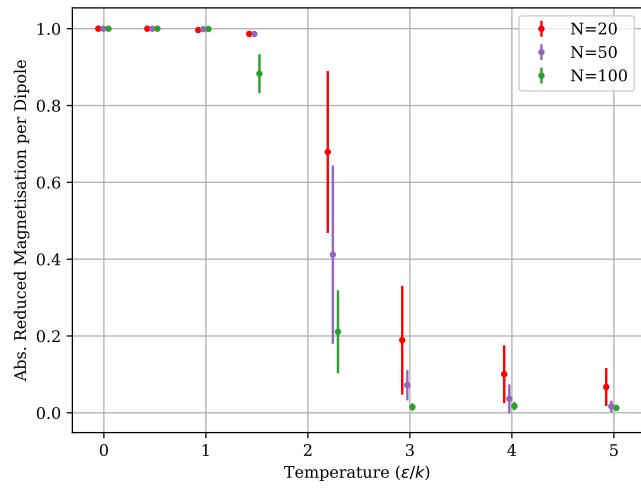
The specific heat capacity was computed in the same way as in the 1D Ising model case.



**Figure. 12** Specific heat capacity of the 2D Ising lattice, with varying temperature and dipole population across 10 trials. The temperatures tested are the same as in Figure 9 (bar the first temperature,  $T = 0.02\epsilon/k$ , as the variance was unreasonably large), with the same data-point temperature jitter.

We note here that the specific heat capacity appears to follow a similarly shaped curve as in the 1 dimensional case. At just over  $T = 2\epsilon/k$  (i.e. at the critical temperature  $T_c$ ), the heat capacity peaks for all of the lattice sizes (within error). As such, we'd expect that the specific heat capacity at  $T_c$  of an infinite 2D lattice would be this value too.

After this value of  $\sim T_c$ , we note that the specific heat capacity decreases consistently across population sizes.



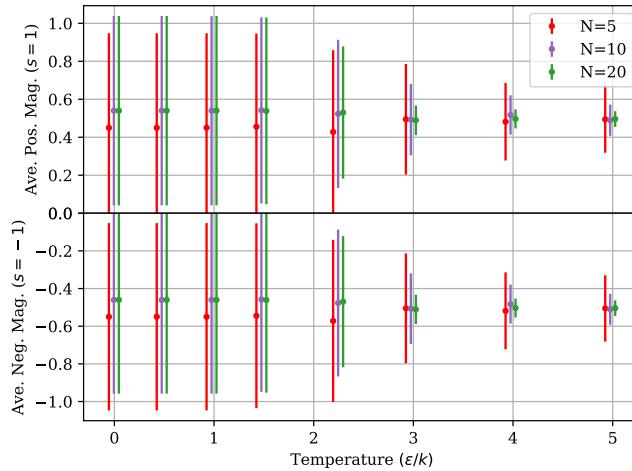
**Figure. 13** Absolute value reduced magnetisation per dipole of the 2D Ising lattice, with varying temperature and dipole population across 10 trials. The temperatures tested are the same as in Figure 9, with the same data-point temperature jitter.

As with the entropy, the values of the absolute reduced

magnetisation per dipole are not exactly what we expected for the high population lattices. In the entropy case, we expected the entropy per dipole to be lower across the low temperature and high population data points. In the magnetisation case, we expected the absolute reduced magnetisation per dipole to be much larger for high population lattices. We attribute these discrepancies to a low number of spin flip chances. With more time permitting, we would be able to run 10 to 100 times as many iterations which we expect would correct these observations. In both circumstances, the high temperature data points align with expectations, however.

## 2.4 Mean Magnetisation for Different Sized Lattices

The mean positive and negative magnetisation per dipole for a range of temperatures and 2D lattice sizes is shown in Figure 14.



**Figure. 14** Mean magnetisation per positive and negative dipole over a range of temperatures and population sizes. As in the previous subsection, the different population data points were scattered slightly about their true temperature value in order to discern the values and variance in the data points. The data points in the figure were averaged across 100 trials. The number of spin-flip chances given per system was dependent on population size, with  $N_{\text{flip}} = N^2 \times 5 \times 10^3$ .

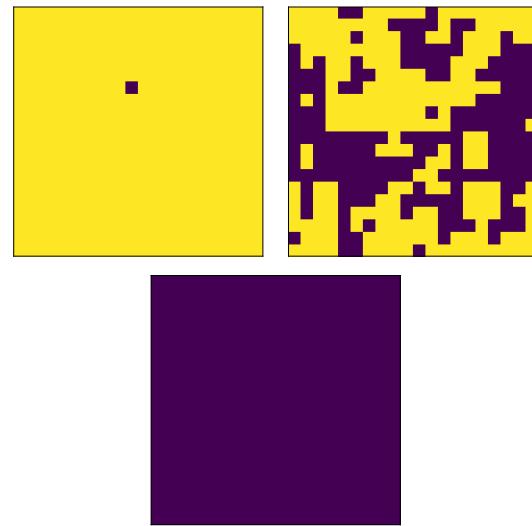
The variance of the data points (especially in the higher population lattices) begins to get smaller after  $T = 2\epsilon/k$ , which suggests that values are more consistently averaged at no net magnetisation for temperatures above about  $T = 2.5\epsilon/k$ . Furthermore, this suggests (along with previous tests on the model in the previous subsections) that the critical temperature lies between 2 and  $2.5\epsilon/k$ ; that is,  $2\epsilon/k \leq T_c \leq 2.5\epsilon/k$ .

Figure 14 shows that the average magnetisation is consistent against lattice populations, and so we claim that

$T_c$  is not dependent on population for the 2D Ising model (at least in the limit towards large numbers).

## 2.5 Heating and Cooling of a Lattice

To assess the behaviour of an Ising lattice over varying temperature, we initiated a  $20 \times 20$  lattice at a low temperature (below the critical temperature), heated it up and then cooled it again. The results of this are shown in Figure 15.



**Figure. 15** A  $20 \times 20$  Ising lattice over various temperatures. The temperature was varied over the range  $T \in [1, 3]\epsilon/k$ , and was incremented by  $\Delta T = 0.1\epsilon/k$  on each step. For each temperature increment, the system was iterated for  $2 \times 10^5$  steps in order to equilibrate between temperature variations. Top left: lattice at  $T = 1\epsilon/k$ . Top right: the same lattice after slowly being heated to  $T = 3\epsilon/k$ . Bottom: the same lattice once again cooled to  $T = 1\epsilon/k$ .

We note that, from an initial totally aligned state, a spontaneous magnetisation arose in the lattice after being heated above the critical temperature. In some cases, after cooling down again, the lattice would return to the original magnetisation state, and in others it would settle into the opposite state (as in the figure above). We rationalise that the final net magnetisation is independent of the initial magnetisation, and relies only on the  $T = 3\epsilon/k$  state at which it then begins to cool down (at least in the case of very slow cooling as was done here).

Since the lattice is totally aligned parallel after cooling below the critical temperature, we argue that the critical temperature  $T_c$  is analogous to the Curie temperature for ferromagnetic lattices. The critical

temperature can be found analytically as

$$T_{\text{critical}} = \frac{2\epsilon}{k \ln(1 + \sqrt{2})} \simeq 2.269\epsilon/k \quad (11)$$

Iron has a Curie temperature of approximately 1043K,<sup>35</sup> and so the value of  $\epsilon$  that would approximate an iron crystal by a 2D Ising model is found as<sup>36</sup>

$$T_{\text{curie}} = T_{\text{critical}} \quad (12)$$

$$1043\text{K} = 2.269\epsilon/k \quad (13)$$

$$\Rightarrow \epsilon = \frac{1043}{2.269} k \text{ K} \quad (14)$$

$$\simeq 6.343 \times 10^{-21} \text{ J} = 0.03959 \text{ eV} \quad (15)$$

### 3 Question 3

The logical next step in the progression of the report is to extend the Ising model to a third dimension. From our reliance on numpy `ndarrays`, this was a simple task to add an extra dimension to the existing two dimensional model. The foundational code to generate an initially noisy lattice, as well as the 3d metropolis algorithm is shown in the code block below.

```

1 def gen_init_Ising3d(N):
2     s = np.zeros((N, N, N))
3     for i in range(N):
4         for j in range(N):
5             initState = np.random.uniform(0, 1,
6                 N)
7                 s[i, j, :] = [1 if initState[i] >=
8 0.5 else -1 for k in range(N)]
9     return s
10 def DeltaU3d(LD, RD, UD, DD, FD, BD, D):
11     return -1 * ((LD * D) + (RD * D) + (UD * D)
12     + (DD * D) + (FD * D) + (BD * D))
13 def metropolis3d(states, iters, temperature):
14     """
15     Parameters
16     -----
17     states : np.array
18         and NxNxN array composed only of -1 and
19         1, corresponding to the spin of each dipole
20     iters : int
21         The number of iterations (different
22         states) to simulate
23     temperature : float
24         The temperature (in units of epsilon / k
25         ) of the reservoir
26     """
27     beta = 1 / temperature
28     N = states.shape[0] # assume square lattice
29
30     RVx = np.random.uniform(0, N, iters) #
31     generate some random positions along x axis
32     RVy = np.random.uniform(0, N, iters) # as
33     above but along y axis
34     RVz = np.random.uniform(0, N, iters)
35     RVx = [int(x) for x in RVx] # make them
36     correspond to an index
37     RVy = [int(x) for x in RVy]
38     RVz = [int(x) for x in RVz]
39
40     evaluations = np.random.uniform(0, 1, iters)

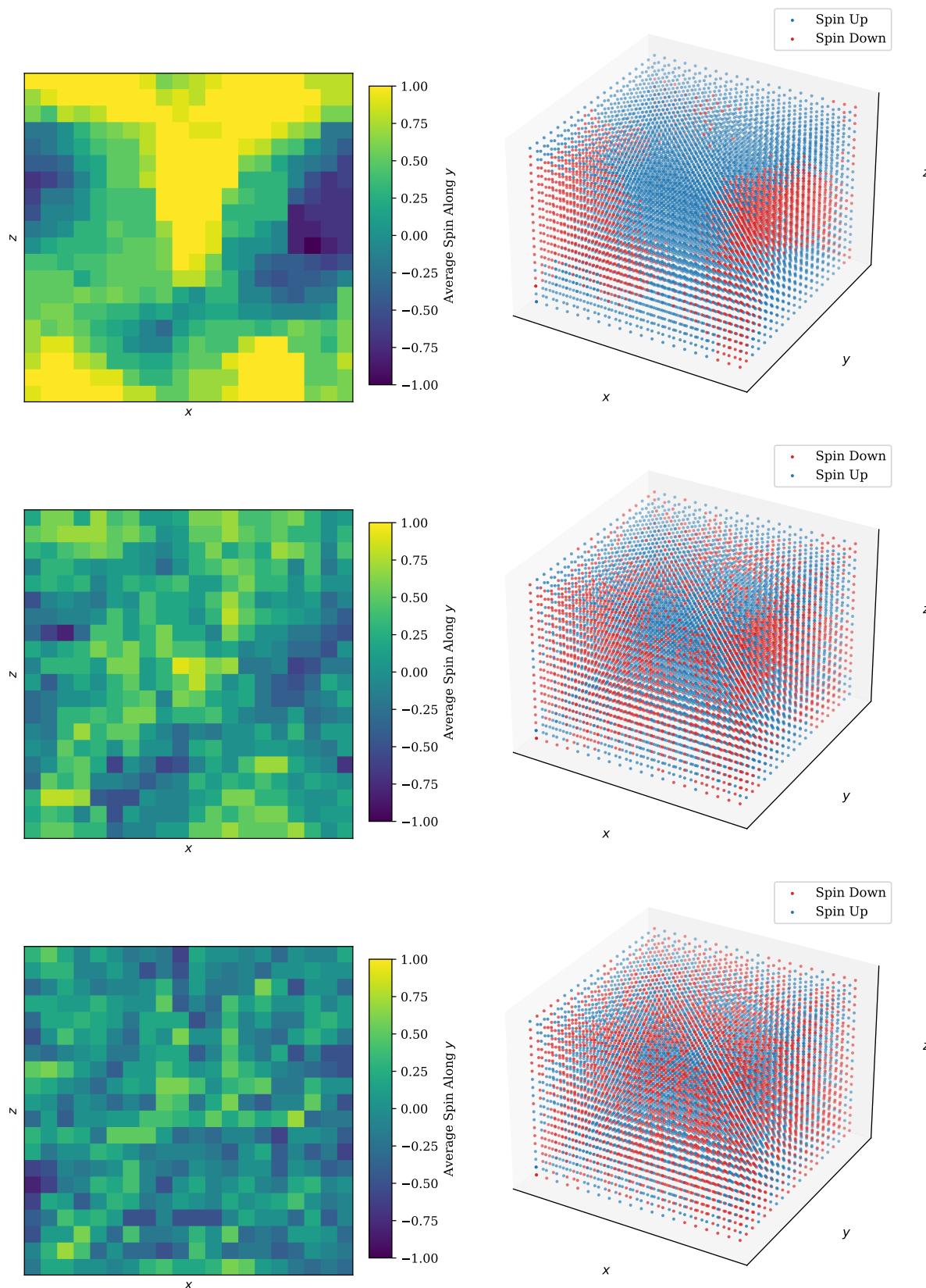
```

```

41
42     for i in range(iters):
43         dipole = states[RVx[i], RVy[i], RVz[i]]
44         Ldipole = states[RVx[i]-1, RVy[i], RVz[i]
45         ]] if RVx[i] != 0 else states[N-1, RVy[i],
46         RVz[i]] # value of the -x dipole
47         Rdipole = states[RVx[i]+1, RVy[i], RVz[i]
48         ]] if RVx[i] != N-1 else states[0, RVy[i],
49         RVz[i]] # +x dipole
50         Udipole = states[RVx[i], RVy[i]-1, RVz[i]
51         ]] if RVy[i] != 0 else states[RVx[i], N-1,
52         RVz[i]] # +y dipole
53         Ddipole = states[RVx[i], RVy[i]+1, RVz[i]
54         ]] if RVy[i] != N-1 else states[RVx[i], 0,
55         RVz[i]] # -y dipole
56         Fdipole = states[RVx[i], RVy[i], RVz[i]
57         ]-1] if RVz[i] != 0 else states[RVx[i], RVy[i],
58         N-1] # -z dipole
59         Bdipole = states[RVx[i], RVy[i], RVz[i]
60         ]+1] if RVz[i] != N-1 else states[RVx[i],
61         RVy[i], 0] # +z dipole
62
63     initEnergy = DeltaU3d(Ldipole, Rdipole,
64     Udipole, Ddipole, Fdipole, Bdipole, dipole)
65     flipEnergy = DeltaU3d(Ldipole, Rdipole,
66     Udipole, Ddipole, Fdipole, Bdipole, -1*
67     dipole)
68
69     deltaEnergy = flipEnergy - initEnergy
70     if deltaEnergy <= 0:
71         states[RVx[i], RVy[i], RVz[i]] *= -1
72     else:
73         flipProb = np.exp(-beta *
74         deltaEnergy)
75         if evaluations[i] <= flipProb:
76             states[RVx[i], RVy[i], RVz[i]] *= -1
77
78     return states

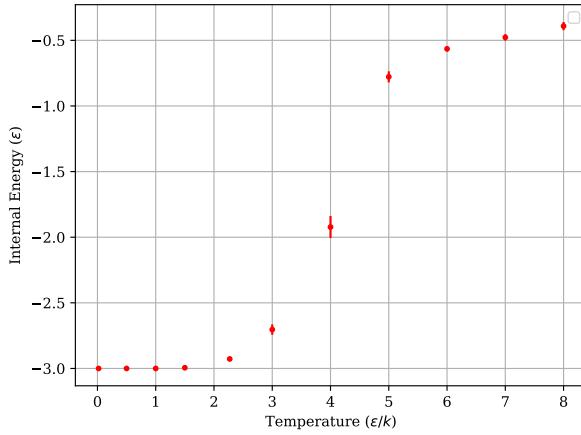
```

Due to the extra dimension, each dipole in the lattice has two more neighbours (corresponding to the forwards and backwards directions along a  $z$  axis). Because of this, we predict that dipoles will be even more susceptible to neighbour interactions, and so we'll see a phase transition at a higher temperature (where we wouldn't in a lower dimensional simulation due to fewer neighbour influences).



**Figure. 16** A cubic  $20^3$  3D Ising lattice after being left to equilibrate for  $10^5$  steps for 3 temperatures. The left column of figures shows the average magnetisation over the  $y$  axis for a given  $(x, z)$  coordinate, while the right column shows all of the dipoles in the lattice coloured by their respective spin. Top row:  $T = 2\epsilon/k$ ; middle row:  $T = 4\epsilon/k$ ; bottom row:  $T = 6\epsilon/k$ .

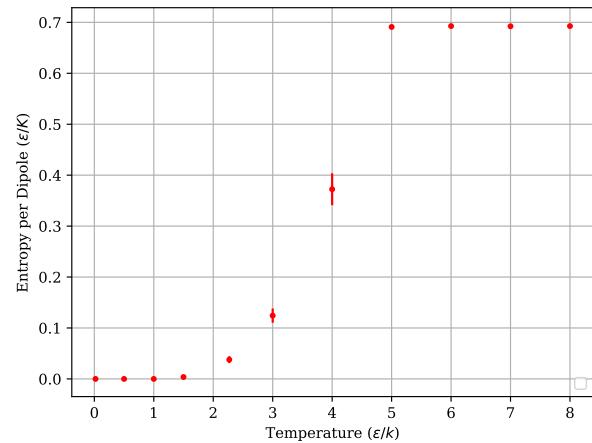
All of the tests carried out in the below figures were done with a  $N = 15^3$  cubic lattice with periodic boundaries. For each temperature,  $N \times 10^3$  steps were computed so that each dipole had roughly 1000 chances to change its spin orientation. Hotter temperature lattices were simulated first, and the next coolest temperature used the previous hotter state as an initial state prior to the metropolis stepping. All states from each of the 20 trials per temperature were stored, so that they might be used in the next temperature step. All of the states (as opposed to just one, for example) were stored so as to avoid repeating the same physical process on each trial. Overall, this method allowed for us to simulate far less steps while still generating useful results; physically this corresponded to slowly cooling each of the 20 lattices and performing tests on them at each temperature step towards 0.



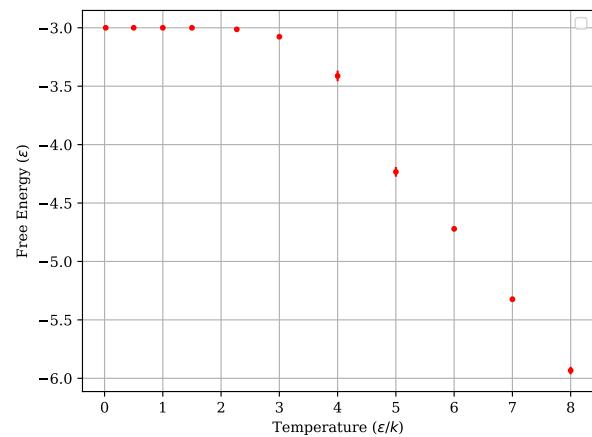
**Figure. 17** Internal energy per dipole for the  $15^3$  3D Ising lattice.

At this point, we note that the variance in observed values is significantly less than that in the 2D case, despite having a lattice with a comparable number of dipoles. We attribute this to the ‘slow cooling’ property of the testing in the 3D case, which allowed the system to equilibrate ‘quicker’ than previously seen.

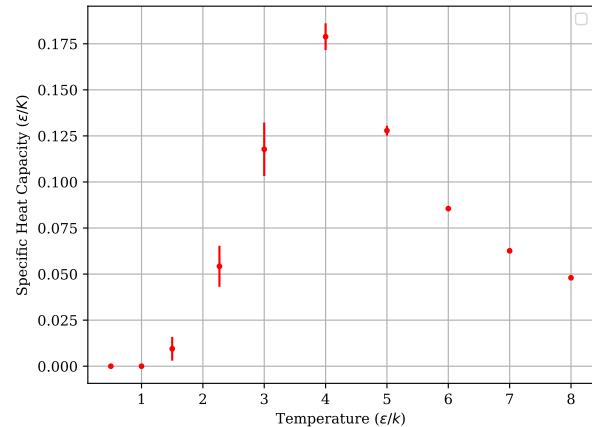
It’s easiest to visually identify the critical temperature from Figures 17, 18 and 20. With respect to the internal energy,  $T_c$  roughly corresponds to where the slope starts increasing at a decreasing rate. In terms of the entropy and the heat capacity, we’d expect that the slope would reach the maximum of about  $S \sim 0.7\epsilon/K$  and  $C \sim 0.2\epsilon/K$  respectively at  $T_c$ .



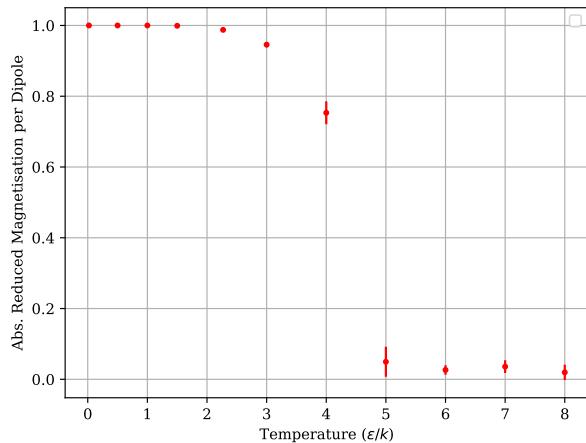
**Figure. 18** Entropy per dipole for the  $15^3$  3D Ising lattice.



**Figure. 19** Free energy per dipole for the  $15^3$  3D Ising lattice.



**Figure. 20** Specific heat capacity for the  $15^3$  3D Ising lattice.



**Figure. 21** Absolute value of the reduced magnetisation per dipole for the  $15^3$  3D Ising lattice.

Figure 21 also exactly resembles Figure 1 in [1], albeit with fewer data points. In the same paper, they conclude that the critical temperature for a 3D Ising model is approximately  $T_c \simeq 4.5\epsilon/k$ , which our data supports. In all of the above plots, we see a maximum/slope change between temperatures of 4 and  $5\epsilon/k$  as we'd expect from a phase transition in that domain. This critical temperature is also significantly larger than that of the two dimensional case, as expected. In future studies, we predict that the phase transition would be at a higher temperature still in higher dimensional lattices.

Interestingly, the behaviour of each thermodynamic parameter was consistent across dimensions and lattice sizes (only being shifted or stretched vertically/horizontally).

## References

- [1] A F Sonsin et al. “Computational Analysis of 3D Ising Model Using Metropolis Algorithms”. In: *Journal of Physics: Conference Series* 630 (July 2015), p. 012057. DOI: 10.1088/1742-6596/630/1/012057. URL: <https://doi.org/10.1088/1742-6596/630/1/012057>.