Figure 1: At low temperatures we observed smaller groups of aligned spins. We concluded that the influence of the heat (i.e. $\tau\sigma$) on the free energy was low and therefore, that the energy U was minmised.

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

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

We calculated the free energy of the system using,

$$\begin{aligned} F &= -\tau \ln Z \qquad (3) \\ &= -\tau \ln\left(\left(2\cosh\left(\frac{\epsilon}{\tau}\right)\right)^N\right) \\ &= -N\tau \ln\left(2\cosh\left(\frac{\epsilon}{\tau}\right)\right) \\ &= -N\tau \ln\left(\exp\left(\frac{\epsilon}{\tau}\right) + \exp\left(-\frac{\epsilon}{\tau}\right)\right) \\ &= -N\tau \ln\left(\exp\left(\frac{\epsilon}{\tau}\right)\left(1 + \exp\left(-2\frac{\epsilon}{\tau}\right)\right)\right) \\ &= -N\tau \ln\left(\exp\left(\frac{\epsilon}{\tau}\right)\right) - N\tau \ln\left(1 + \exp\left(-2\frac{\epsilon}{\tau}\right)\right) \\ &= -N\epsilon - N\tau \ln\left(1 + \exp\left(-2\frac{\epsilon}{\tau}\right)\right). \qquad (4) \end{aligned}$$

The entropy followed from the combination of Equation 4 and Equation 2 using Equation 5,

$$\begin{aligned} \tau\sigma &= F - U \qquad (5) \\ &= -N\epsilon \tanh\left(\frac{\epsilon}{\tau}\right) + N\epsilon + N\tau \ln\left(1 + \exp\left(-2\frac{\epsilon}{\tau}\right)\right) \\ \sigma &= \frac{\epsilon}{\tau}\left(1 - \tanh\left(\frac{\epsilon}{\tau}\right)\right) + \ln\left(1 + \exp\left(-2\frac{\epsilon}{\tau}\right)\right). \qquad (6) \end{aligned}$$

Finally, we determined the specific heat using Equation 7 and Equation 2,

$$\begin{aligned} C &= \partial_\tau U \qquad (7) \\ &= \partial_\tau \left(-N\epsilon \tanh\left(\frac{\epsilon}{\tau}\right)\right) \\ &= -N\epsilon \partial_\tau \left(\frac{\epsilon}{\tau}\right) \frac{1}{\cosh^2\left(\frac{\epsilon}{\tau}\right)} \\ &= \frac{N\epsilon^2}{\tau^2 \cosh^2\left(\frac{\epsilon}{\tau}\right)}. \qquad (8) \end{aligned}$$

Using our one-dimensional ising model we numerically validated these relationships, shown in Figure 2. Based on the energy and our knowledge of thermodynamics we concluded that all of the spins aligned at $\tau = 0$. This is evident because the magnitdue of the energy increases while the entropy approaches zero indicating a unique ground state. At high temperatures the heat capcity becomes very small indicating that the addition of more heat will not change the internal energy very much, and as predicted by the second law of thermodynamics it approaches zero at $\tau = 0$. We also tested the one-dimensional scenario for a phase shift, described in Figure **??** and found that the one-dimensional case did not have a phase shift.

To calculate the error bars shown in Figure 2 we used the variance of each parameter averaged over the runtime of the simulation following a burn-in period. This

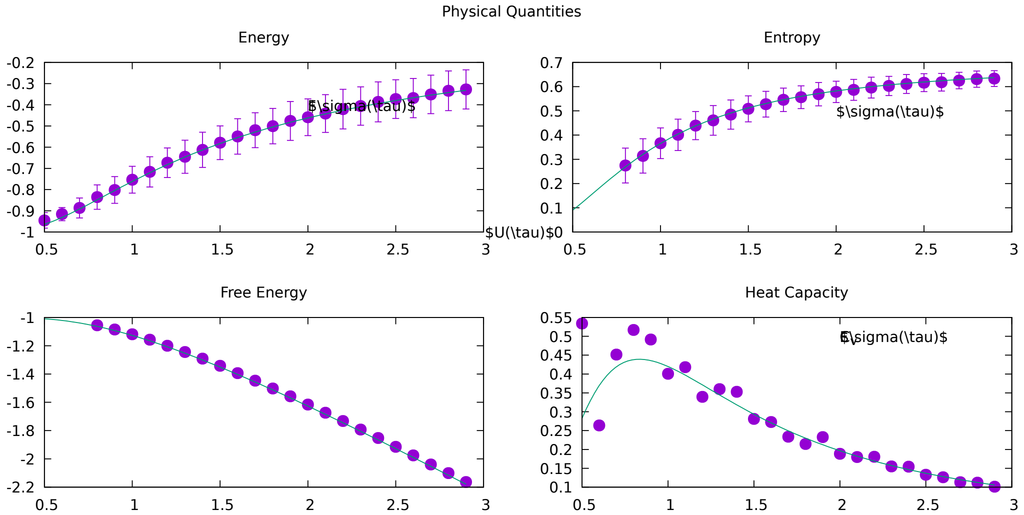

Figure 2: Physical properties of the one-dimensional ising simulation. These figures were generated with 100 repeats at each temperature where one repeat performed 100000 metropolis steps. We noticed the energy, entropy and free energy tended to converge faster than the heat capacity, shown by the relatively large noise. Because, the heat capcity is a function of the variance of the energy we were not able to calculate useful uncertainties in this set of simulations, but based on the larger convergence time we belive they would be large. As expected the variance in the energy was smaller at lower temperatures and increased with the temperature. This makes sense because at low temperature the energy is the factor towards minimising the free energy but at high temperature it is the entropy. Flipping a single spin has a larger affect on the entropy than on the energy explaining this trend in the variance, which remained roughly constant through the second half of the sampled temperatures.

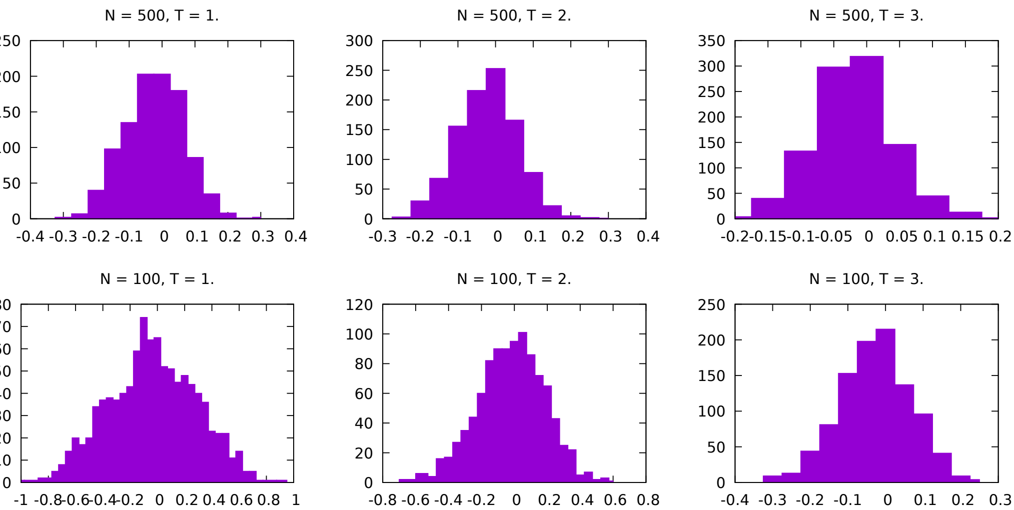

Figure 3: Histograms of the magnetisation per spin as a function of N and T. We noticed that the magnetisation remained symmetric around zero for all the temperatures and sizes that we sampled. This makes sense because in the abscence of an external magnetic field there should be no preference for the spins to align in either direction except for that imposed by the interactions between neighbours. We noticed that the distributions were approximately gaussian and that their standard deviations were a decresing function of the temperature. We also noticed that the standard deviation of the system was an increasing function of the number of spins. Because there was no shift of the magnetisation away from the zero value we concluded that the infinite ising model would become very flat at low temperatures but would not undergo a phase shift, i.e. spontaneous magnetisation.

??

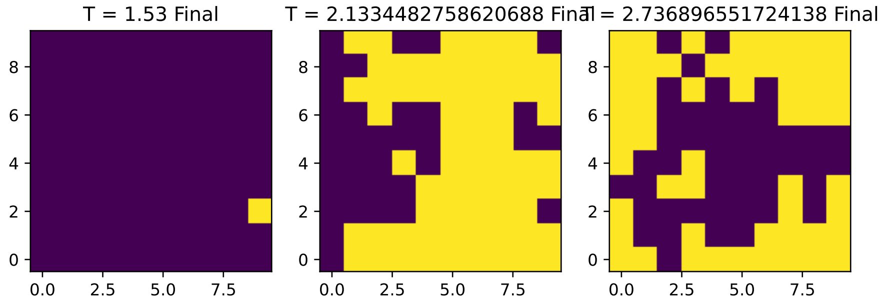

Figure 4: The initial and final states of our two-dimensional ising model simulations. We noticed that at lower temperatures the chunks of aligned spins increased in size. We concluded that the process behind this was a generalisation of the description we gave in the caption to Figure 1.

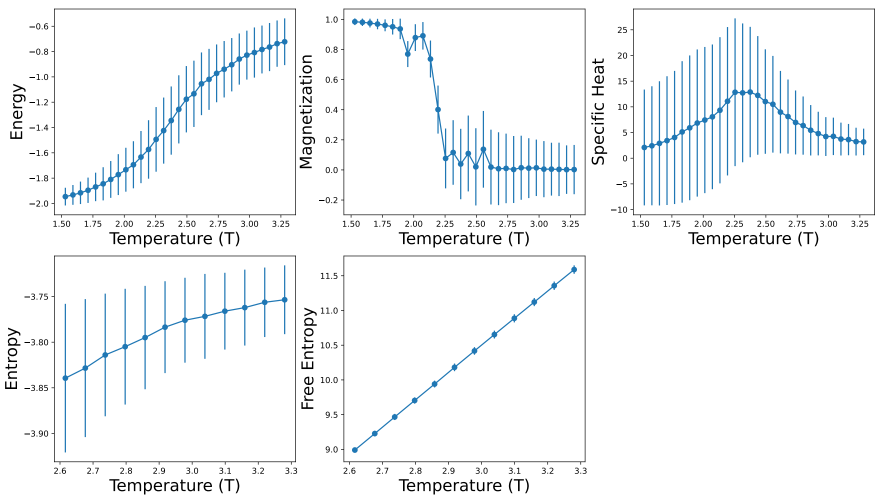

Figure 5: The physical properties of the two-dimensional ising model numerical simulations. We observed a sharp peak in the heat capcity at the phase transition, which we used to estimate the critical temperature of the simulation. From the heat capcity we determined that the critical temperature was $T_c = 2.25 \pm 0.02$ where our error corresponds to half the width of the apparent peak. We noticed that the error in the measurements was significant compared to their size particularly for the heat capcity. This was most likely a result of the lower number of that we used in the two-dimensional case. We were forced to use more trials because of the increased compuational complexity.

burn-in period was chosen to be 1000, since this provided enough time for each spin to be visited ten times without taking too long. To improve our investigation we could have produced plots of the parameters at each iteration and estimated the required burn-in time by identify on the graphs when equilibrium was reached.

We generalised this process to a two-dimensional ising simulation. As we decreased the temperature we found that there was a point where the net magnetisation shifted away from zero. This can somewhat be seen in Figure 4. By running many additional simulations we were able to visually estimate that the critical temperature for the spontaneous magnetisation was approximately T $2.25K$. We later confirmed this from the peak in the heat capacity as discussed in the caption to Figure 5. As in the one-dimensional simulations we estimated the error in the physical parameters from their variance over the duration of the simulation following a burn-in period.To estimate the error in the heat capacity we needed to take extra care and used,

$$\Delta c = \left(\mathrm{var}(\epsilon^2) + 2\mathrm{var}(\epsilon)\right)/N^2/\tau^2, \tag{9}$$

where we have attempted error propagation through the alternate formula for the variance, $\mathrm{var}(\epsilon) = \langle \epsilon^2 \rangle - \langle \epsilon \rangle^2$, using the variance itself as the error estimate for the means. This seems very meta and we are not confident that it is correct.