PHYS3020 – Computational Project Report – Rhys Tyne – s46481894

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Examples of the final state of 100 dipoles at 3 different temperatures, all runs were initialised with the same initial configuration. In the coldest run of the model the final state has all dipoles with the same spin state, the middle temperature run has clear “chunks” of up and down spin dipoles and the hottest run has an almost random configuration of spins. This follows the logic of the metropolis algorithm because as T increases, β approaches 0, which means exp(-β\*ΔU) approaches 1, resulting in it being more common for a switch which does not reduce U occurring. Similarly, as T approaches zero, β approaches ∞, which means exp(-β\*ΔU) approaches zero meaning if the dipole switch does not reduce U, then it will hardly occur.

Internal energy per dipole (*u*):

Free energy per dipole (*f*):

Using the identity:

Entropy per dipole (*S*):

From the derivation of I will use:

Since, N is held constant can be cancelled with the 1/N outside the derivative.

Solving and using the identity stated above we get:

Specific heat capacity per dipole (*c*):

For the following plots the error bars were calculated by running the 1D Ising model 10 times with 250 dipoles and calculating the average values. Then using these averages to solve uncertainty using the standard method , for each variable and temperature value (of which there were 15 evenly spaced between 0.1 and 3).

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The plot of internal energy per dipole (u) almost perfectly aligned with the exact solutions with very low uncertainty apart from a slight deviation at low temperatures. The free energy per dipole (f) was consistently lower than the value gained by the exact solution. Since the model calculates F = U – TS and entropy is over-estimated this explains the difference between model and exact solutions. The entropy per dipole (*S*) rose and plateaued earlier then the theory suggests it should. WHY?

The two specific heat capacity plots show different temperature ranges to better compare the simulated and exact values. At low temperature the model does not follow the exact solutions closely at all, but for T ⪆ 1.3 ε/k the model and exact solutions align. Similarly, as the temperature increases the uncertainty decreases. WHY? I think BUG

Schottky anomaly??

The reduced magnetism per dipole (m) behaved as expected. At low temperatures all the dipoles end up in the same state as seen earlier, however whether is state is up or down is dependent on the initial state of the dipoles and the randomness involved in the metropolis algorithm. Then as temperature increases and the dipoles become less organised *m* approaches zero. Hence, why S and |m| are somewhat inversely proportional. This makes intuitive sense as the multiplicity of a microstate with about half up and half down spins is much greater then when all spins are up/down.

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I did 100 runs of the model to make the histogram. In this case the two phases are when the dipoles are all aligned and when they are seemingly random (somewhat analogous to a solid and gas of a substance). Comparing at each temperature it is apparent the 500 dipole model undergoes this phase transition earlier then the 100 dipole model. This suggests that larger magnets do not require as high temperatures to be ferromagnetic. In the limit considering the infinite 1D model should approach m = 0 for any temperature value including T = 0, which is supported by the plots above.

**2D Ising Model**

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Very similar to the 1D model, as temperature increases the size of the crystals becomes less predictable. This happens for the same reason as described in the 1D case. From running my simulation many times, I estimate that at temperatures below T = \_\_\_\_, it is possible for all dipoles to have the same spin orientation, forming a crystal the size of the lattice.