Computational methods assignment 3
The Ising model

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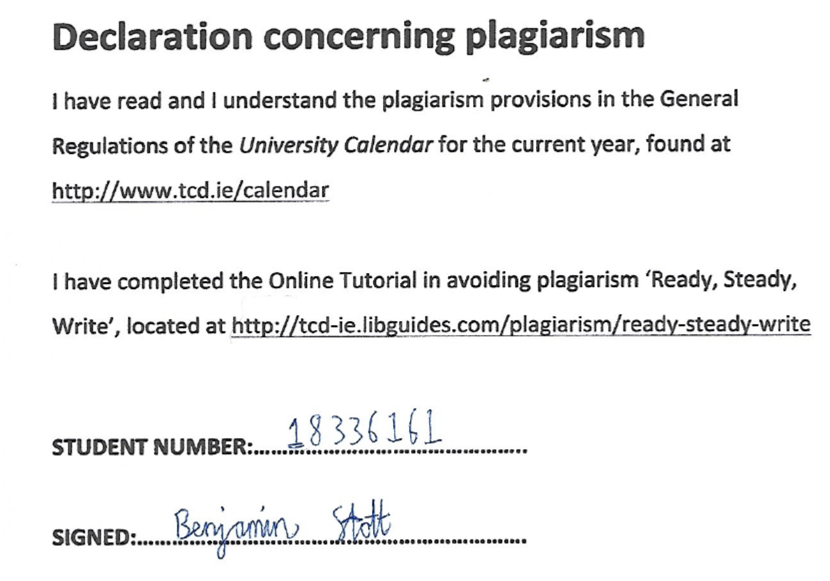
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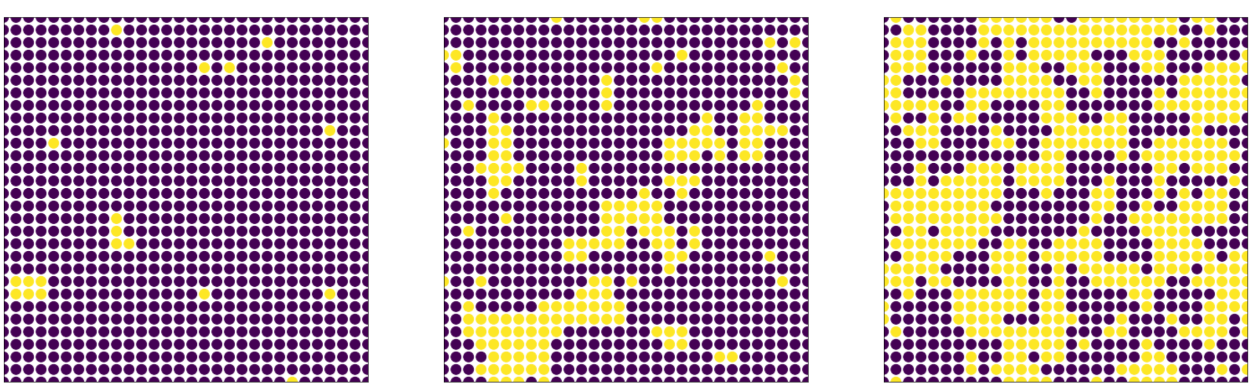
STUDENT NUMBER: 18336161

SIGNED: Benjamin Stott

1 3.1 - Phase transitions and thermodynamic variables:

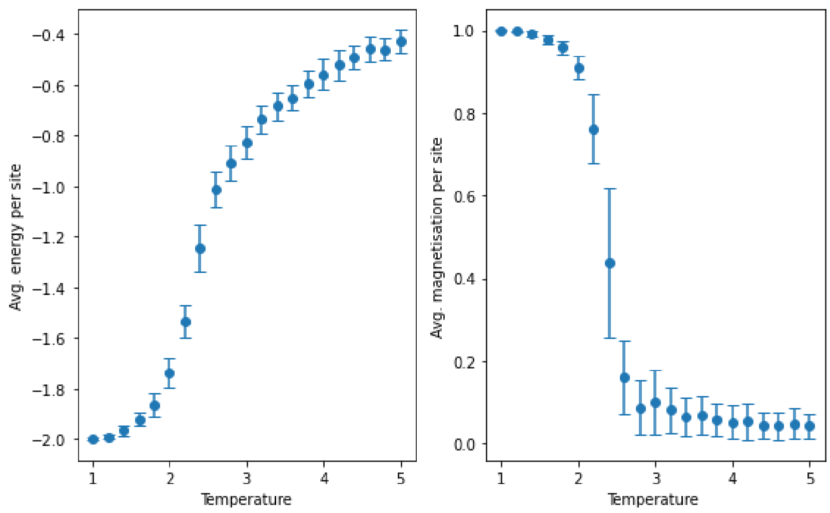
part a):
The first part of this assignment required investigating the behaviour of lattices at different values of temperature in an applied magnetic field of 0.



(a) lattice at 1.6 J/k_B(below critical temperature) (b) lattice at 2.27J/k_B(at critical temperature) (c) lattice at 3J/k_B(above critical temperature)

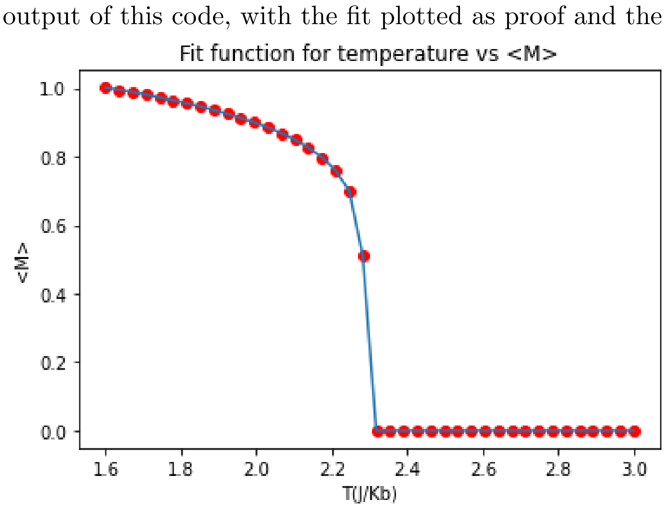
Figure 1: 2 Lattices for varying values of temperature

Below the critical temperature, spins are relatively uuniform and there is not much activity in the lattice. At the critical temperature, large clusters of opposite spins begin to form. Above the critical temperature, the system is disordered and oppositely aligned spins are scattered indiscriminately.
It was also asked to investigate the behaviour of $< E >$ and $< M >$ for different values of temperature, included on the following page.



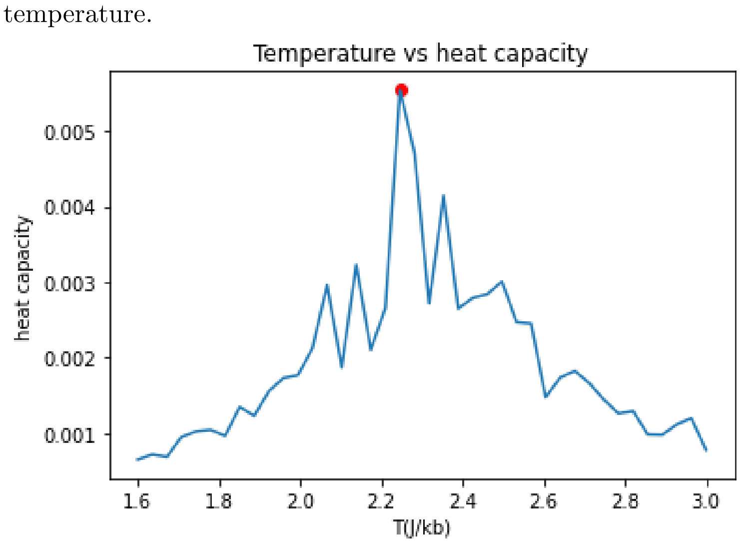
A range of $< E >$ and$< M >$ values were produced for varying values of lattice temperature. We observe a discontinuity in these graphs at the critical temperature(i.e where clusters of opposite spins suddenly form). It makes sense that the magnetisation decreases sharply here as the uniformity in the structure is gone. The energy increase at this value also makes sense since the temperature is increasing, therefore particles vibrate more and they are no longer bound in place by surrounding particles

part b): The second part of this experiment involved creating a fit curve using the piecewise analytic function defined in the lab manual to the obtained data for temperature vs $< M >$. In this manner we may obtain the fit parameters C and Tc. We should obviously expect Tc to reasonably agree with the analytic value. Below is the output of this code, with the fit plotted as proof and the parameters printed.



1.0505180659688873 is the estimated value of c
2.2851323901710976 J/Kb is the estimated value of Tc
These fit parameters were obtained by using scipy's optimization.fitcurve. This value of Tc is very close to the true value of 2.27. It is very close as I included 40 intervals of temperature instead of 21 used in the part a). As more intervals of temperature are used the fit becomes more accurate, however, there is also a cost in time for more steps so any increase beyond this would be impractical.

part c): Part c) required that I plot the heat capacity of the system as a function of temperature using the equation detailed in the manual. The only modification I made to the main code was to append values of E^2 to a list in order for them to compare with E. This plot is shown below with the peak of this being the critical temperature.



This peak is theoretically meant to appear at the critical temperature and indeed it comes very close to this, reaching a value of 2.24615385 J/Kb. This is less accurate than the fit to the analytical function and likely requires even smaller steps of temperature to reach the exact value. It would seem that fitting to the analytical value is a more expedient method of obtaining Tc.

2 3.2 - Hysteresis:

part a):

It was required that I modify the ising solver code to implement a hysteresis loop. The modified ising solver energy is given by the following equation:

$$H = -J\sum_{ij} S_i S_j - h\sum_i S_i$$

where h is an external magnetic field. Several slight modifications to the code need to be made to account for this.

We must define a variable referenced by h with self.h=h in the preamble of the code. This must be initialised as one of the factors in the ising solver as h=0 before any changes are made to it.

This value of h affects the probability and so we must change it accordingly

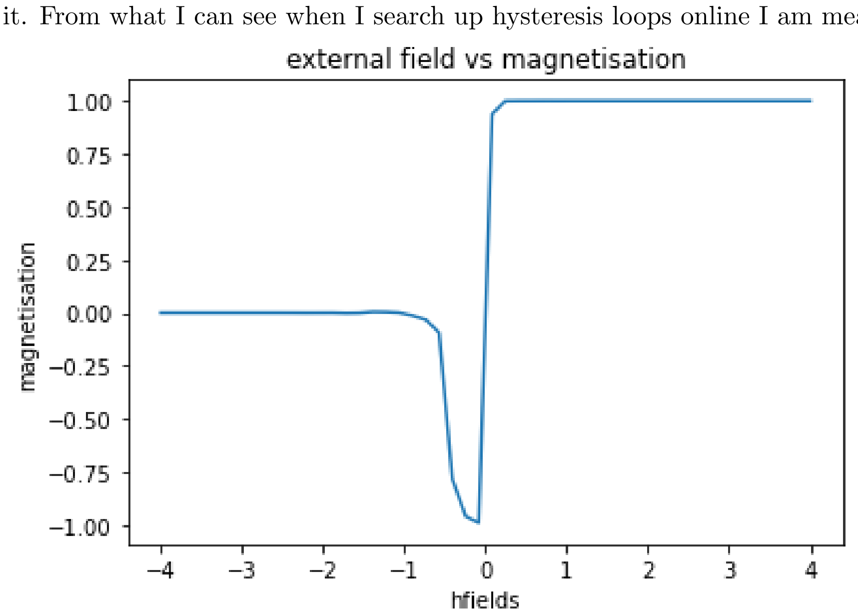
self.probs = np.exp(- 2 * (J[0]+self.h) *self.sums / (kB * self.temp)).

The energy value of the grid must also have self.h added to it.

The value of delta E will also change due to this. The value S_i is the sum of all the current moments of the lattice with S_j being neighbours. Keeping this in mind and acknowledging that an external magnetic field will produce a magnetic field opposed to it we obtain
deltaE = -2 *self.J[0] * neighsum + 2*self.h*(np.sum(self.current moments))

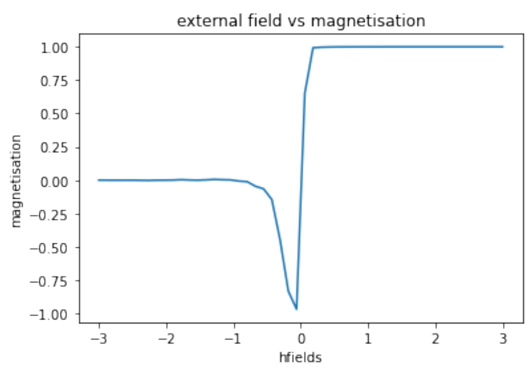
The final change that needs to be made to the code is to make sure it updates the lattice for each value of h as it does with temperature. For this we add to the run function the simple slice of code
if(h != 0):
self.h = h
if self.Jrule == 'nn':
self.probs = np.exp(- 2 * (self.J[0]+self.h) *self.sums / (kB * self.temp))

part b):
The second part of this experiment involved plotting the hysteresis loop for a temperature below Tc, for which I chose 1.3 J/Kb. I have included this graph below. I am somewhat confused by my results and why a canyon appears near hfield=0.It seems like my range for magnetic fields is too large but I do not see why that should affect it. From what I can see when I search up hysteresis loops online I am meant to be gaining a sort of step value.

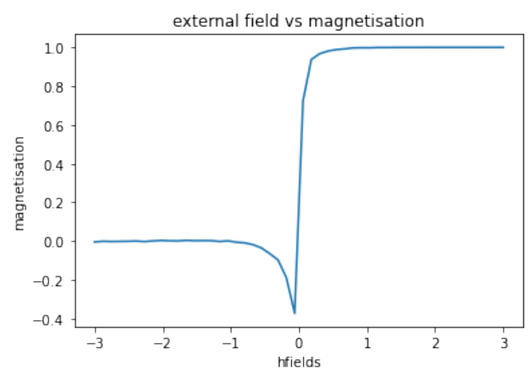


part c):

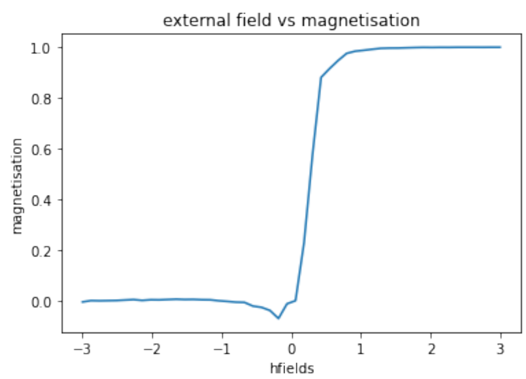
This part of the experiment involved running this modified code for a range of values of h and plotting hysteresis loops for h vs $< M >$ while varying temperature a few times to note its effect. This was done for external fields in the range -3,3.



(a) loop at 1.6 J/k_B(below critical temperature)



(b) loop at 2.27J/k_B(at critical temperature)



(c) loop at 3J/k_B(above critical temperature)

Figure 2: 3 loops for varying values of temperature

It was also required to calculate the coercivity from these graphs and plot it as a function of temperature. Unfortunately, while the shape of these graphs appears to be roughly correct, I believe the magnetisation values on the y axis are incorrect, or rather, I was expecting them to range from -1 to 1 and I'm not sure where I made my error.I think whatever error I made must be something small since my logic seems to agree with equations I see for this stuff. I will observe however, that as temperature increases, the ridge of the curve shifts to the right. I think this is meant to mean that the coercivity is decreasing.