Monte Carlo Simulation of the 2-D Ising Model

Abstract

This report will discuss the methods in which to carry out a Monte-Carlo simulation of the Ising model, which describes a lattice of spins which either point up or down. We will also discuss some of the properties which come from the calculations done on the simulation. The control variables are β which is proportional to inverse temperature, and $\underline{B}$, an external field. For low β the spins are randomly pointing up or down, and for high β the spins tend to align themselves in order to minimise free energy, and low β causes the spins to fluctuate at random due to thermal agitation. There is a phase transition between the two latter situations for which there is a critical temperature. Without any external magnetic field, the system has a more defined phase transition at a certain value of β, and it becomes shifted and spread in β as the external field increases. Increasing $\underline{B}$ also causes the energy to be translated down by an amount proportional to itself and the number of sites aligned to the magnetic field. For β fixed at a high value, varying the magnetic field incrementally and allowing the system to fall into equilibrium causes the spins to initially align, and then eventually oppose the external field. The reason is that once the spins are aligned they minimise free energy by staying the same direction, and low temperatures means that it is more improbable for the system to flip to fall into a different equilibrium.

I. Aims & Introduction

The Ising Model is a model describing a system of spins, arranged in a lattice, with energy:

$$E = -\frac{1}{2}\sum_{<i,j>} J_{ij}\underline{S}_i \cdot \underline{S}_j - \mu\underline{B}\cdot\sum_i \underline{S}_i$$

Where J_{ij} is the interaction energy, which is J for nearest neighbours, and 0 otherwise. The system is Boltzman distributed:

$$p_{\{s_i\}} = \frac{e^{-\beta E}}{Z}$$

where $p_{\{s_i\}}$ is the probability of a given microstate and where Z is the partition function

$$Z = \sum_{microstates} e^{-\beta E}$$

This report will look at how the following variables behave as the control variables β and B are varied:

- Energy as defined above.
- Magnetisation per spin:

$$\underline{m} = \frac{1}{N}\sum_i \underline{S}_i$$

  where N is the number of elements on the lattice.

- Magnetic susceptibility:

$$\chi = \frac{1}{N}\frac{J}{k_B T}\left(\langle \underline{S}^2\rangle - \langle \underline{S}\rangle^2\right)$$

- specific heat capacity:

$$c = \frac{1}{N}\frac{1}{k_B T^2}\left(\langle E^2\rangle - \langle E\rangle^2\right)$$

The last two values are always positive since they are of the form of variances, merely with an extra factor which is also positive.

II. Theory

I. Brief comments

One of the most fundamental predictors of how the Ising model will behave is the free energy:[Christensen, K. & Moloney, N. (2005)]

$$F = \langle E\rangle - TS$$

where $\langle E\rangle$ is:

$$\langle E\rangle = \sum_{\{s_i\}} p_{\{s_i\}} E_{\{s_i\}}$$

The system will in general evolve such that the free energy is minimised.

II. Predictions

At high temperatures there is a lot of thermal agitation, which causes the spins to flip almost at random, which means that regardless of any external field, the system's energy would fluctuate with it's mean near zero, as would the magnetisation per spin.

At lower temperatures, the spins tend to align with each other as this would lower the free energy. This causes the magnetisation per spin to increase as temperature increases.

With increasing magnetic field the magnetic susceptibility decreases because the magnetic field guides the system towards equilibrium.

Varying the magnetic field for low β will cause the system to equilibrate such that the magnetisation per spin is in the same direction as the magnetic field, the thermal agitation causes the system to fluctuate towards these equilibrium points. For low β the system aligns with the magnetic field initially, and when the field is varied past $\underline{B} = \underline{0}$ the system starts to oppose the external field, because he thermal fluctuations are too small to flip all the spins to minimise the $\underline{B}$ contribution to energy.

III. Methods

A system is set up with periodic boundary conditions, so that the spins on the top of the lattice are nearest neighbours with the spins at the bottom of the lattice, and the rightmost spins are nearest neighbours with the leftmost spins. The lattice is hence (topologically-speaking) on a surface of torus.

I. Metropolis Algorithm

The metropolis algorithm updates a randomly selected spin at a probability that is a function of the energy difference, given by:

$$p = \begin{cases} 1 & \Delta E \leq 0 \\ e^{-\Delta E \beta} & \Delta E > 0 \end{cases}$$

The step by step process is as follows:[Kingham, R. (2013)]

1. Choose a spin at random.
2. calculate ΔE due to flipping the spin.
3. If $\Delta E \leq 0$ then flip the spin, if $\Delta E > 0$ flip the spin with probability $e^{-\Delta E \beta}$.
4. Update all quantities of interest if the process successfully flips the spin, otherwise go back to step 1.

Proof of convergence to Boltzman Distribution 1. *[Christensen, K. & Moloney, N. (2005)] With a number of systems$N_{\{s_i\}}$ in microstate $\{s_i\}$ evolving into a number of systems with microstate $\{s_i'\}$, $N_{\{s_i'\}}$, the number of transitions is:*

$$N_{(\{s_i\}\to\{s_i'\})} \propto N_{\{s_i\}} e^{-\beta(E_{\{s_i\}} - E_{\{s_i'\}})}$$
$$N_{(\{s_i\}\to\{s_i'\})} \propto N_{\{s_i'\}}$$

The total number of transitions out of microstate $\{S_i\}$ is:

$$\begin{aligned} \Delta N_{(\{s_i\}\to\{s_i'\})} &= N_{(\{s_i\}\to\{s_i'\})} - N_{(\{s_i\}\to\{s_i'\})} \\ &\propto N_{\{s_i\}} e^{-\beta(E_{\{s_i\}} - E_{\{s_i'\}})} - N_{\{s_i'\}} \\ &\propto N_{\{s_i\}} \left(\frac{e^{-\beta(E_{\{s_i\}}}}{e^{-\beta E_{\{s_i'\}}}} - \frac{N_{\{s_i'\}}}{N_{\{s_i\}}} \right) \end{aligned}$$

Assuming that $\Delta N_{(\{s_i\}\to\{s_i'\})} > 0$, then $\frac{N_{\{s_i'\}}}{N_{\{s_i\}}}$ increases until $\Delta N_{(\{s_i\}\to\{s_i'\})} = 0$. If $\Delta N_{(\{s_i\}\to\{s_i'\})} < 0$, then $\frac{N_{\{s_i'\}}}{N_{\{s_i\}}}$ decreases until $\Delta N_{(\{s_i\}\to\{s_i'\})} = 0$, hence this algorithm reaches a steady state where the number of transitions between different macro states goes to zero. Hence:

$$\frac{N_{\{s_i'\}}}{N_{\{s_i\}}} = \frac{e^{-\beta(E_{\{s_i\}}}}{e^{-\beta E_{\{s_i'\}}}}$$

which corresponds to the ratio from the Boltzmann distribution. □

II. Wolff Cluster-Update Algorithm

The Wolff algorithm updates the system cluster by cluster. This method has a 100% probability of success for 0 magnetic field: the probabilistic nature comes from the fact that a particular neighbouring spin which is a member of a cluster being accepted into the cluster that is flipped is not unity. The step by step algorithm is as follows:[Wolff, U. (1989)]

1. Choose a spin i at random. At the start the cluster is empty $\mathcal{C} = \emptyset$
2. Add the spin to cluster $\mathcal{C} \cup \{i\}$, Add the spin to the boundary, $\mathcal{B}_{\text{old}} := \{i\}$
3. $\mathcal{B}_{\text{new}} := \emptyset$
4. $\forall i \in \mathcal{B}_{\text{old}}$ Do the following:
5. $\forall j_i$ where j_i is a neighbour of i, and such that $S_i = S_j$ and such that j is not already an element of the cluster, i.e. $j \notin \mathcal{C}$:
6. with the probability $p = 1 - e^{-2J\beta}$, union the boundary set with the element, and also the cluster set: $\mathcal{B}_{\text{new}} := \mathcal{B}_{\text{new}} \cup \{j\}$, $\mathcal{C} := \mathcal{C} \cup \{j\}$
7. redefine $\mathcal{B}_{\text{old}} := \mathcal{B}_{\text{new}}$, and go back to step 3, unless $\mathcal{B}_{\text{new}} = \emptyset$ in which case go to step 8.
8. With the probability

$$p = \begin{cases} 1 & \Delta E_B \leq 0 \\ 1 - e^{-\Delta E_B \beta} & \Delta E_B > 0 \end{cases}$$

flip all the spins in the selected cluster, $\forall i \in \mathcal{C}, S_i := -S_i$. (Where ΔE_B is the energy change contribution of the magnetic field due to flipping the cluster $\mathcal{C}$)

This algorithm is typically applied near critical temperatures, which can cause slowing down the evolution of the system.

III. Ascertaining equilibrium

The system goes into equilibrium faster when there is greater thermal agitation. This is because the fluctuations produced can move the energy into the correct state, and also because the failure rate of the metropolis algorithm is much lower. Although higher temperatures are slower at reaching equilibrium, they end up being more accurate in finding the correct microstates which correspond to a steady state.

The metropolis algorithm is typically used in this way to hopefully find a minimum point when there exists lots of local minima. The 'thermal agitation' is used to escape from local solutions to fall into better ones, and afterwards, temperature is gradually lowered to converge to a solution. This is why the method is sometimes known as 'simulated annealing'.

The method used to ascertain equilibrium here is using the running mean energy of a set of microstates that evolve via the metropolis algorithm. A state is initialised with randomised spins, it is evolved for a certain fixed magnetic field and temperature, a completely aligned state is initialised and also evolved, hence they both start with very different energy values. Once the running mean energy of both states intersect, the states are known to be in equilibrium.

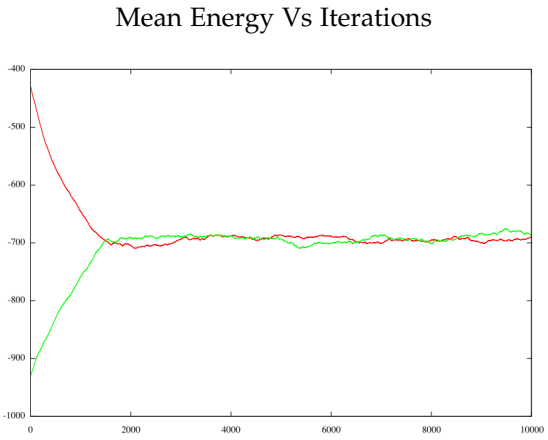

Figure 1: *Running mean energies (In units of interaction energy) of 2 states starting from different microstates, as a function of the number of iterations of the Wolff algorithm. Using the same control variables the metropolis algorithm fluctuates at around the same point, however has a higher amplitude in the fluctuations.*

In the case of starting from a completely aligned state, the reference state with which it intersects lags behind the original state, it only starts evolving after a certain number of iterations of the original state. when it starts evolving the original state reaches equilibrium first and eventually intersects with the reference state. Similarly one can also economise on the number of computations by using the

same state, and waiting for the state to intersect itself translated backwards in time, this should be equivalent because both the reference state and the original state starts from the same microstate.

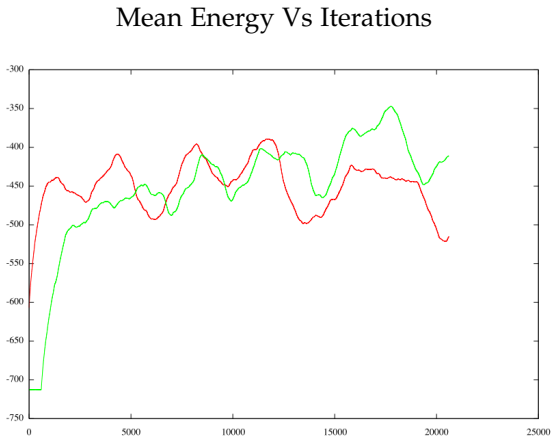

Figure 2: *Running mean energies (In units of interaction energy) of 2 states starting from the same microstates, but with a time lag, as a function of the number of iterations of the metropolis algorithm. on the bottom left of the graph, the system represented by the green line is not evolving, it can be seen that this prevents early-intersection of the running mean energies.*

It can be seen from the graphs that as soon as the system equilibrates itself, the method used to determine equilibrium triggers almost immediately. This is therefore a reasonably efficient method, taking around twice the number of operations required to evolve the system itself to equilibrium. This is also a method which successfully obtains the equilibrium states to a good accuracy. After averaging over a large number of seeds the equilibrium can be accurately obtained.

IV. Results

All of the following results were found using a 25 by 25 lattice of spins, this was a compromise between speed to reach equilibrium, reducing finite size effects and the system's resemblance to an infinite lattice. J is the *interaction energy* and does not stand for 'Joules' in all the following graphs.

I. Fixed Magnetic Field

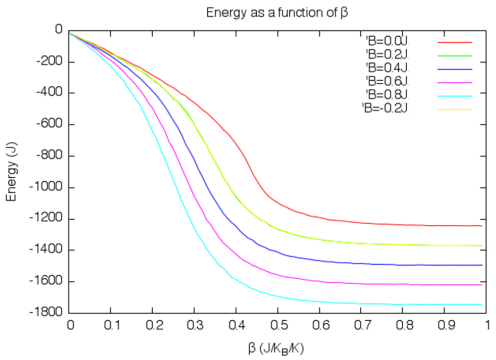

Figure 3: *Energy as a function of β for different external magnetic fields.*

As beta increases more spins become aligned and decreases the total energy. As predicted, higher magnetic fields decrease energy proportional to the number of aligned spins, and proportional to the magnetic field.

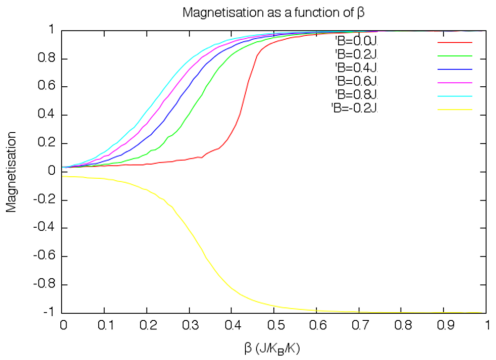

Figure 4: *Magnetisation as a function of β for different external magnetic fields*

Trivially, for negative values of the external field, the spins will align in the opposite direction. Also the Magnetic field shifts and spreads out the phase transition.

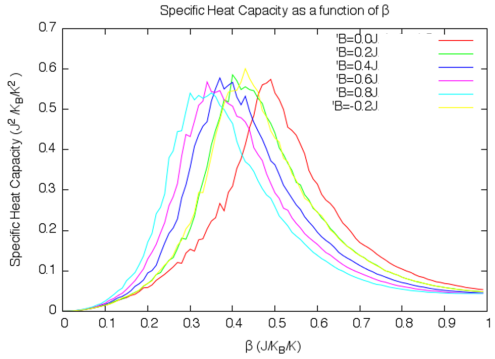

Figure 5: *Specific heat capacity as a function of β for different external magnetic fields*

Increasing the external field shifts the specific heat capacity back. This is expected because the profile of the energy is shifted back by the external field.

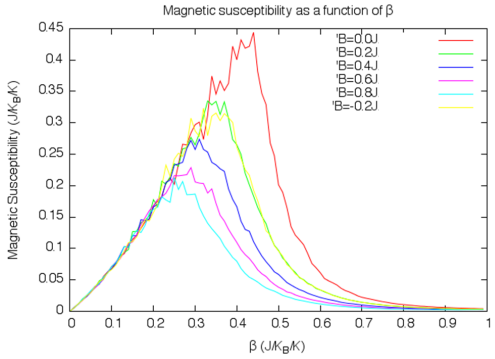

Figure 6: *Magnetic susceptibility as a function of β for different external magnetic fields*

Increasing the external field shifts the magnetic susceptibility in β because the external field also shifts the phase transition. The external field also causes the peak at which the phase transition occurs to be lower, this is due to the fact that the change in magnetisation is not as sharp, so it varies less with beta.

II. Fixed β

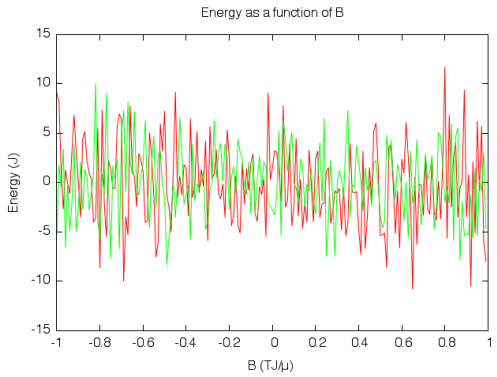

Figure 7: *Energy as a function of magnetic field for $\beta = 0$. Green line represents incrementing from -1 and the red line represents decrementing from 1.*

For $\beta = 0$, the external field has no effect because the thermal agitation is too high, the metropolis algorithm essentially flips any spin chosen at random.

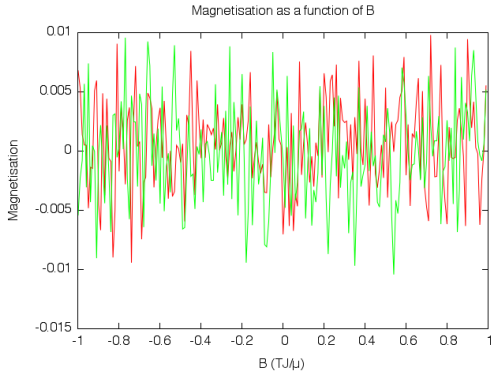

Figure 8: *Magnetisation per spin as a function of magnetic field for $\beta = 0.35$. Green line represents incrementing from -1 and the red line represents decrementing from 1.*

As before, the magnetisation also has no pattern to it since each spin is also being flipped at random.

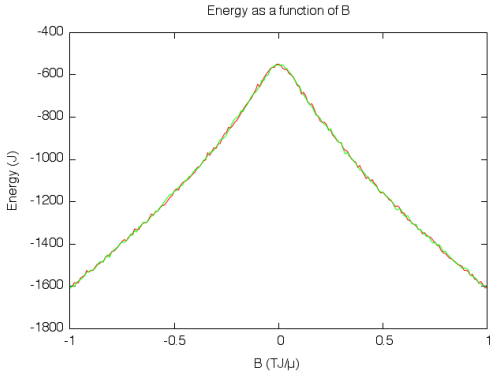

Figure 9: *Energy as a function of magnetic field for $\beta = 0.35$. Green line represents incrementing from -1 and the red line represents decrementing from 1.*

Since energy is proportional to magnetic field, it decreases when the magnitude of the magnetic field is increased.

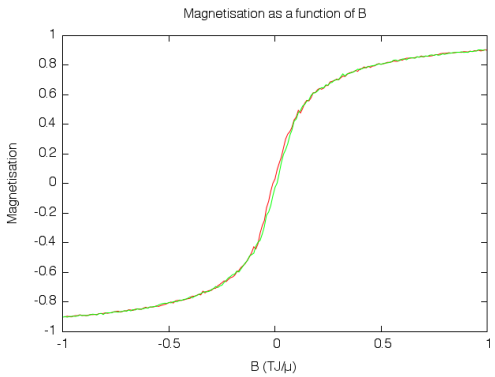

Figure 10: *Magnetisation per spin as a function of magnetic field for $\beta = 0.35$. Green line represents incrementing from -1 and the red line represents decrementing from 1.*

The magnetisation varies so that it is the same sign as the magnetic field. The greater the magnitude of the magnetic field the more spins align to it.

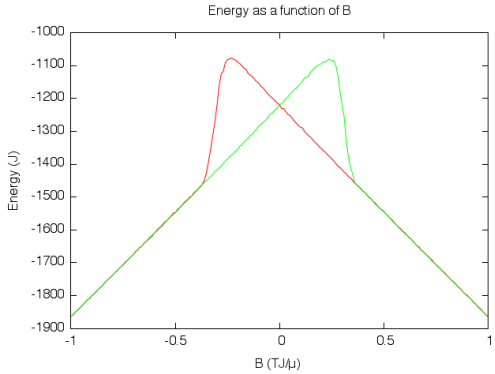

Figure 11: *Energy as a function of magnetic field for $\beta = 0.7$. Green line represents incrementing from -1 and the red line represents decrementing from 1.*

For $\beta = 0.7$ the magnetic field goes into different equilibria when the external field is incremented past 0. The reason for this is because the temperature is low so that the thermal fluctuations tend not to be enough to flip the system immediately as soon as the external field is incremented past $\underline{B} = \underline{0}$.

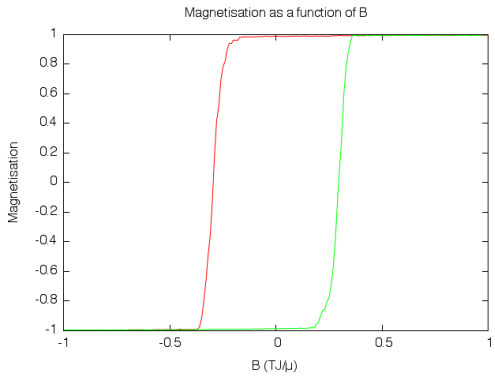

Figure 12: *Magnetisation per spin as a function of magnetic field for $\beta = 0.7$. Green line represents incrementing from -1 and the red line represents decrementing from 1.*

When the magnetic field is incremented enough to overcome the spin alignment the transition becomes much more immediate. Once enough spins have been flipped, the system will very quickly equilibrate to the correct value.

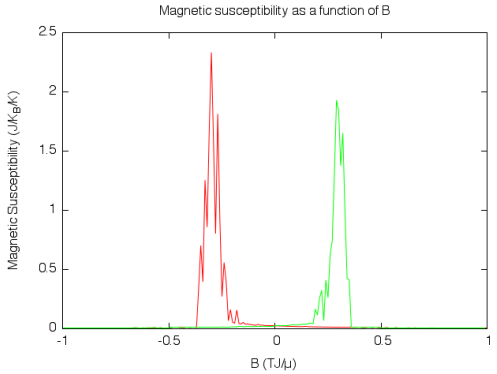

Figure 13: *Magnetic susceptibility as a function of magnetic field for $\beta = 0.7$. Green line represents incrementing from -1 and the red line represents decrementing from 1.*

The magnetic susceptibility becomes sharply peaked at the discontinuities, since at these points the magnetisation varies the most.

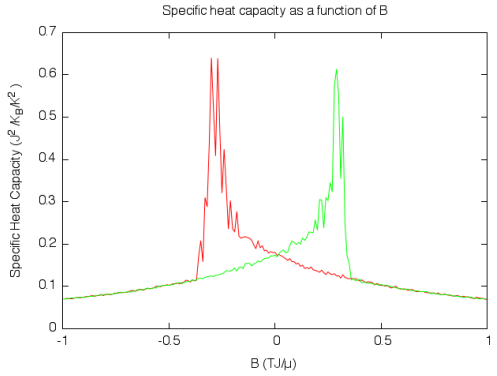

Figure 14: *Specific heat capacity as a function of magnetic field for $\beta = 0.7$. Green line represents incrementing from -1 and the red line represents decrementing from 1.*

The specific heat capacity also becomes sharply peaked at the discontinuities.

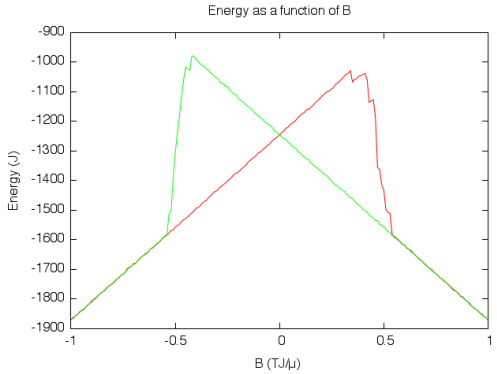

Figure 15: *Energy as a function of magnetic field for $\beta = 1$. red line represents incrementing from -1 and the green line represents decrementing from 1.*

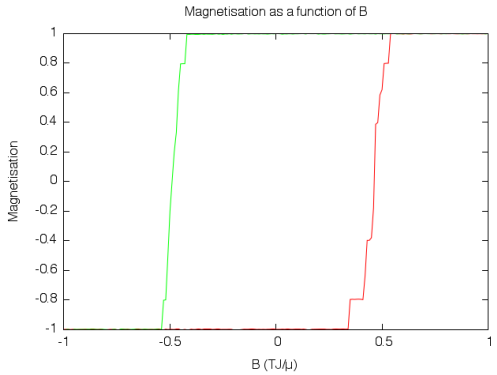

Figure 16: *Magnetisation per spin as a function of magnetic field for $\beta = 1$. red line represents incrementing from -1 and the green line represents decrementing from 1.*

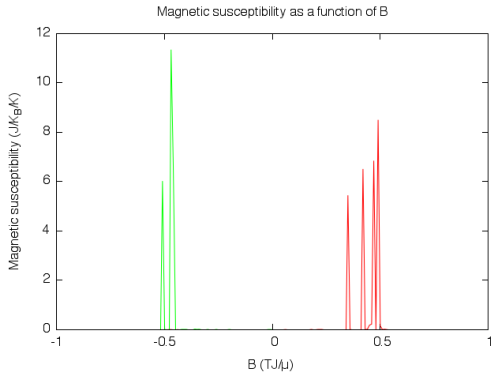

Figure 17: *Magnetic susceptibility as a function of magnetic field for $\beta = 1$. red line represents incrementing from -1 and the green line represents decrementing from 1.*

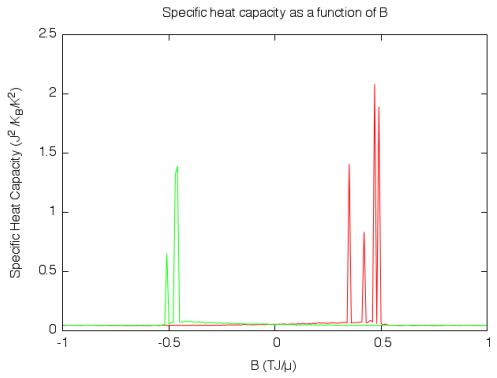

Figure 18: *Specific heat capacity as a function of magnetic field for $\beta = 1$. red line represents incrementing from -1 and the green line represents decrementing from 1.*

Varying the magnetic field exhibits all the same profiles as with $\beta = 0.7$ for the same reasons. The effect is greater and the specific heat capacity and magnetic susceptibility is even more sharply peaked indicating a greater change in Magnetisation and energy.

III. Clustering Behaviour

It was found that for high β,(close to 1) the entire lattice is all aligned, for low β all the spins are pointing in random directions, since the metropolis algorithm fails much less often, and tends towards flipping each spin at random for β approaching 0. For β close to the phase transitions, the system forms clusters of aligned spins.

V. Discussion

Although the Wolff algorithm was implemented in the code, it was never used to obtain the results in the previous section. The Wolff algorithm was seen to cause strange behaviour, for low temperatures it's likely that the entire system is flipped every iteration. However the energies did happen to converge to the same values as with the metropolis algorithm, after testing the code. In some cases the Wolff algorithm is slower, in others it is quicker: it is mostly useful for temperatures close to the critical temperature, near phase transitions, because the algorithm flips the system cluster by cluster, and in these microstates the system contains a clusters. What could be done would be to find β_{critical} as a function of the external field, and apply the Wolff algorithm near these regions.

None of the results behaved in a way that could not be reconciled with theory using knowledge of how the metropolis algorithm works and the minimisation of free energy.

VI. Conclusion

For low values of β the spins are randomly pointing up or down, and for high β the spins tend to align themselves, which is expected by using the minimisation of free energy to predict this behaviour.

With increasing magnetic field, the spins align themselves with the magnetic field, and the phase transitions occur at higher temperatures. This is expected because the added influence of the magnetic field guides the system towards being aligned with the magnetic field.

Varying the magnetic field behaves as expected for high temperature, as the temperature allows the system to fall into the correct equilibrium. For low temperatures the system aligns to the magnetic field, but as the field is varied past 0, the system refuses to flip to the lower energy because the thermal fluctuations are not high enough. Only when the field is varied past $0.5J$ for $\beta = 1$, the metropolis algorithm will manage to find the state which minimises the free energy.

References

[Kingham, R. (2013)] *Computational Physics Lecture notes.* Imperial College London.

[Wolff, U. (1989)] *Collective Monte Carlo Updating for Spin Systems.* Phys. Rev. Lett., 62:361.

[Christensen, K. & Moloney, N. (2005)] *Complexity and Criticality.* Imperial College Press