Physics 344 Assignment 6 Report

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Section 1: Introduction

This report discusses the effects of differing boundary conditions on the physical properties of the Ising Model. The behaviour of the Ising model is simulated in the C file titled "Assignment 6.c". Note that there is only one C file which can implement all the different boundary conditions by taking a parameter which specifies which boundary conditions must be simulated.

Each set of boundary conditions is described in more detail below. The relevant physical quantities being compared here are: the average magnetisation per spin, the magnetic susceptibility and the energy of the system. The presence or absence of a phase transition and the critical temperature will also be analysed. For the sake of comparison, each set of boundary conditions was implemented on a 200 x 200 square lattice for the same values of βJ in each case.

Periodic Boundary Conditions

The standard periodic boundary conditions were already implemented in Assignment 5 so the same implementation will be used here purely for comparative purposes.

"Polarised" Boundary Conditions

This boundary condition involves two of the opposite sides of a square lattice having exactly opposite spins. This means that, for example, the right edge of a square lattice will have all the spins in a spin-up state while the left edge has all its spins in a spin-down state.

Thus, there are two opposite "poles" of the system where all the spins are spin-up or spin-down. The usual periodic boundary conditions will still be applied to the other two edges of the square lattice.

Semi-polarised Boundary Conditions

This boundary condition is similar to the previous one, but only one edge will have all of its spins fixed in a spin-up or spin-down state. The other edges will have periodic boundary conditions implemented as usual.

Non-Interaction Boundary Conditions

In this case, all the spins on the outer edges of the lattice are fixed and in the same state (all spin-up or all spin-down). Thus, only the spins which are not on the edges of the square lattice will be changed during the course of the simulation.

Ferromagnetic and Anti-ferromagnetic Boundary Conditions

These boundary conditions involve the spins on the edges of the lattice interacting differently to the rest of the lattice. So, there are two cases. In the first case, the edge spins interact ferromagnetically while the rest of the lattice interacts anti-ferromagnetically. In the second case, the opposite is true: the edge spins interact anti-ferromagnetically and the rest of the lattice interacts ferromagnetically.

Section 2: Average Magnetisation, Magnetic Susceptibility and Specific Heat for each set of boundary conditions

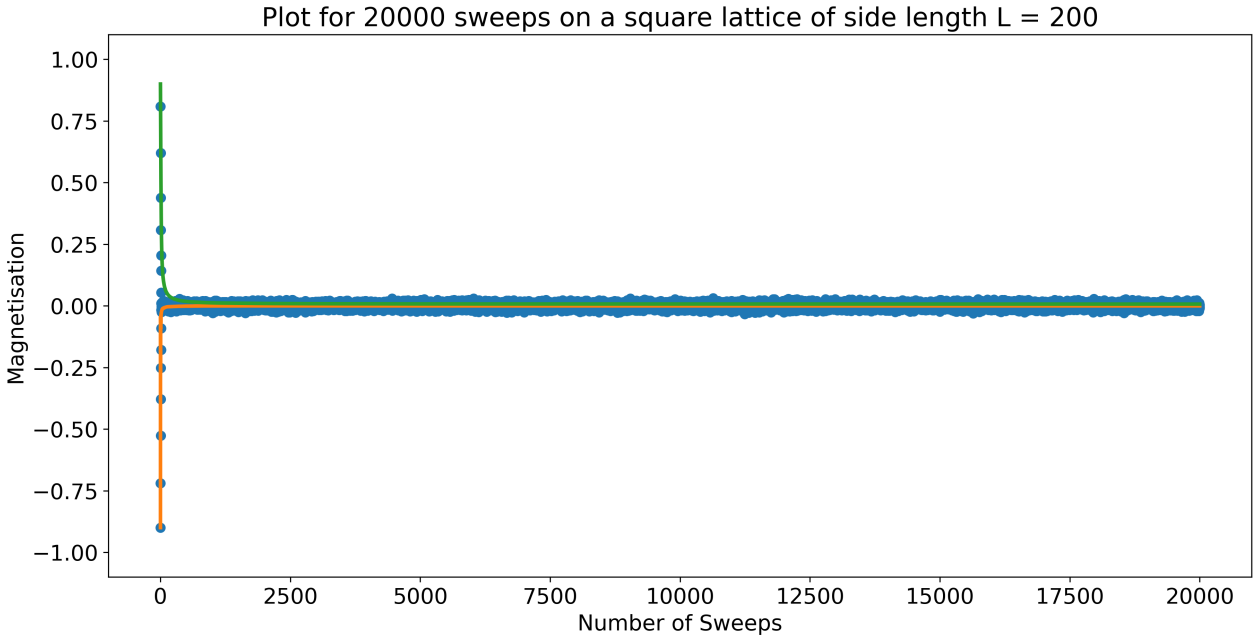
Each of the subsections below shows the graphs of the data obtained for each set of boundary conditions. The data is split into three further subsections: average magnetisation per spin, magnetic susceptibility and specific heat.

2.1 Periodic Boundary Conditions

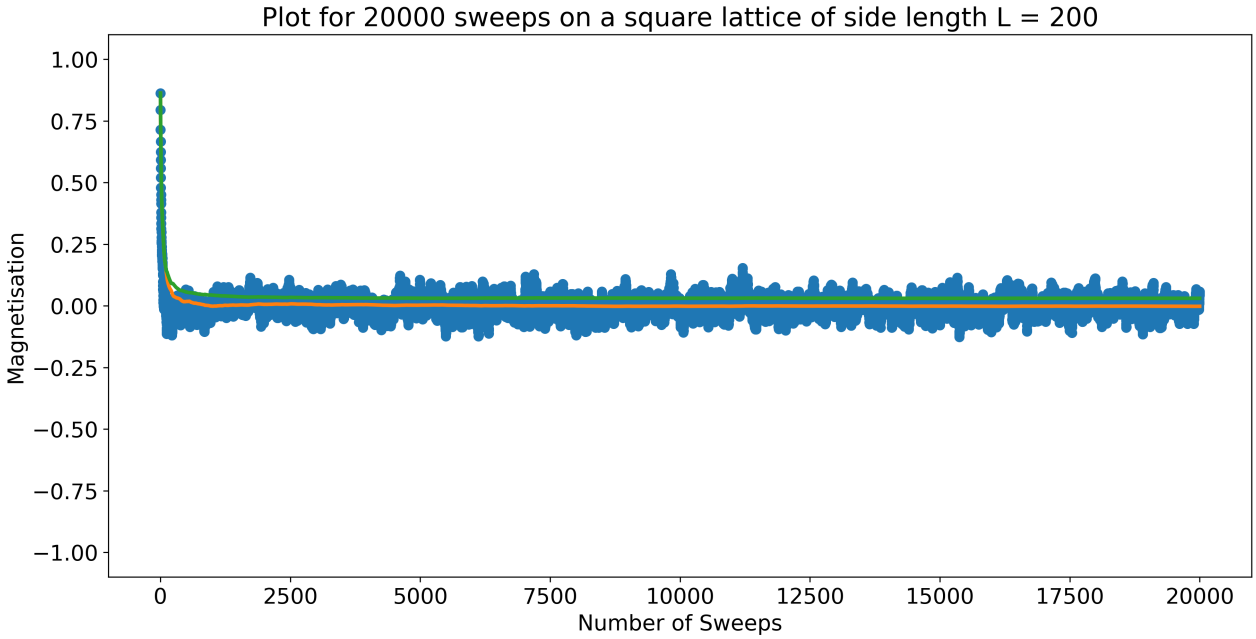
These boundary conditions were already analysed in Assignment 5, so the graphs are reproduced here only for comparative purposes. The important results are also restated at the end of this subsection.

2.1.1 Average Magnetisation

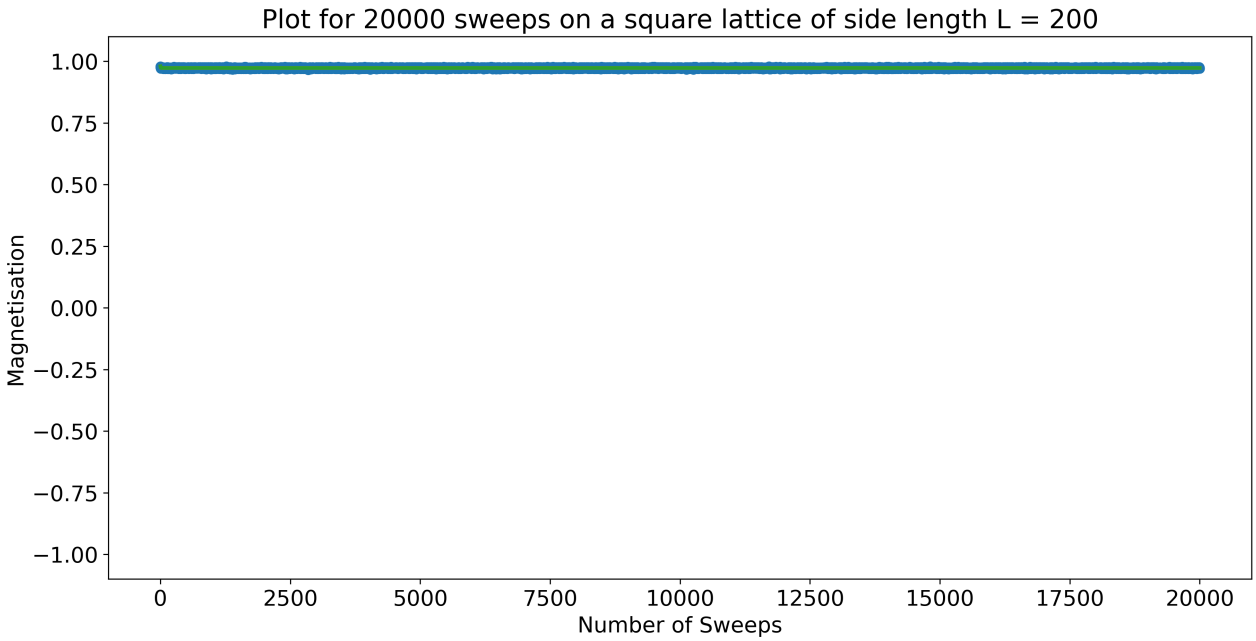
Case 1: βJ = 0.2



Case 2: βJ = 0.4



Case 3: βJ = 0.6

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At $\beta J$ = 0.2, the system is above the critical temperature and the magnetisation is 0 and does not change much. At
$\beta J$ = 0.4, the system is much nearer the crtical temperature (the critical temperature was found to correspond to
$\beta J$ = 0.42 in the previous assignment) and this is seen by the fact that the magnetisation is no longer constant but
it is frequently changing. At $\beta J$ = 0.6, the system is below the critical temperature and a clear phase transition
has taken place. All the spins are now aligned in the same direction (spin up) and the average magnetisation is 1.
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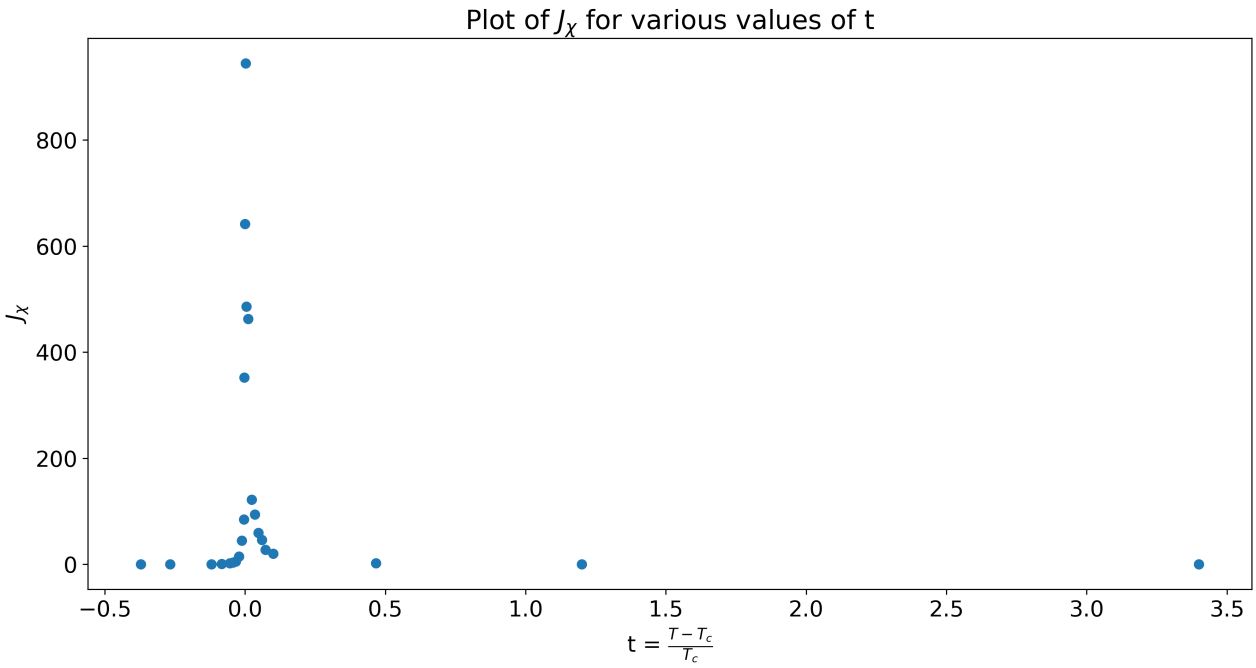
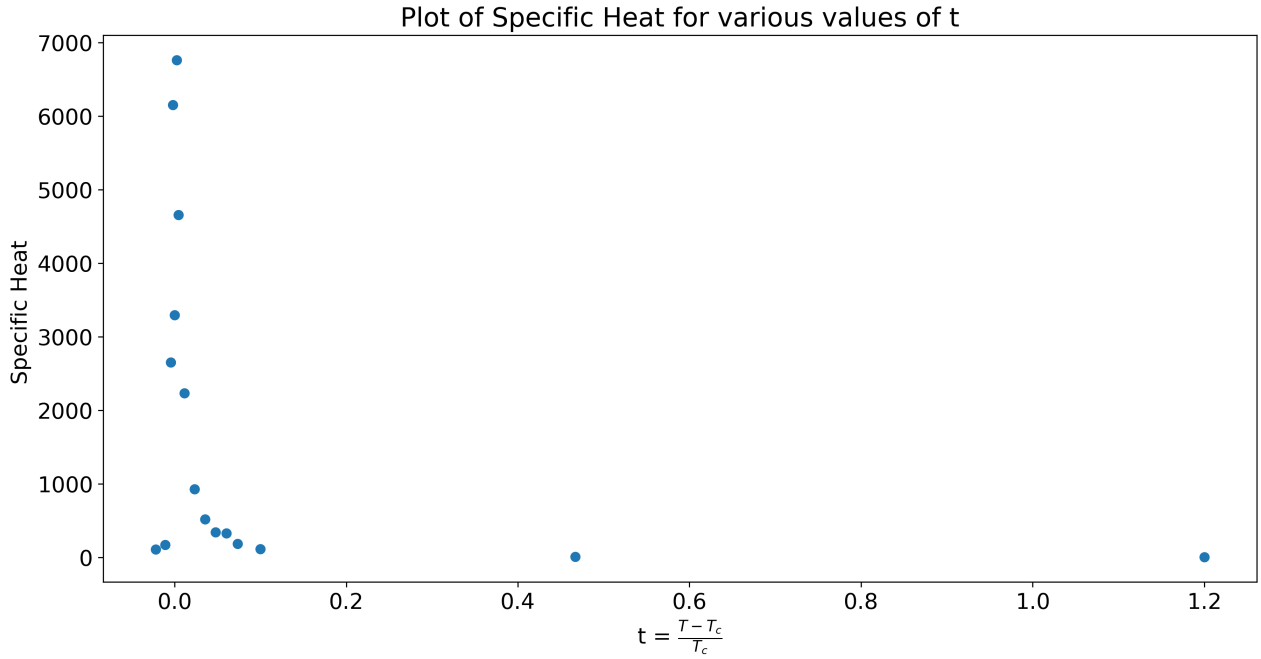
2.1.2 Magnetic Susceptibility

The magnetic susceptibility $J\chi$ is plotted here as a function of t for various values of βJ ranging from 0.01 to 0.7. This data was again generated by taking 20000 sweeps across a 200 x 200 lattice for each value of βJ. This method is used for all future graphs of magnetic susceptibility as well. It is also used for the graphs of the specific heat.



2.1.3 Specific Heat

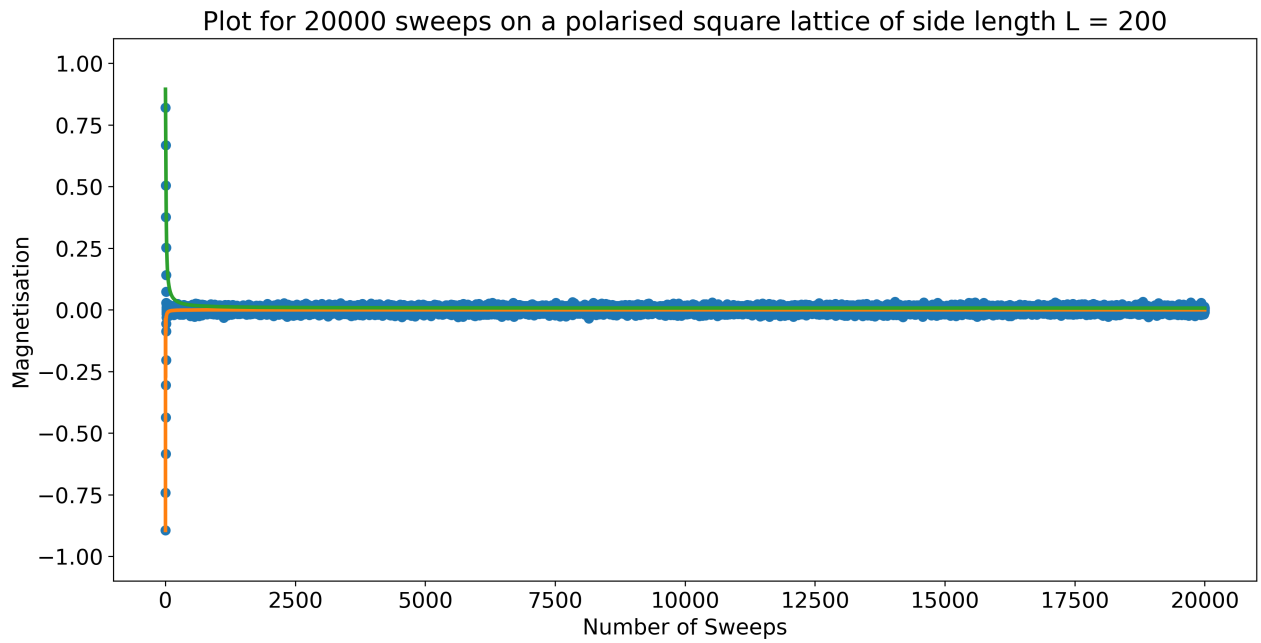
The specific heat is plotted here as a function of t for various values of βJ ranging from 0.01 to 0.7. This data was again generated by taking 20000 sweeps across a 200 x 200 lattice for each value of βJ.



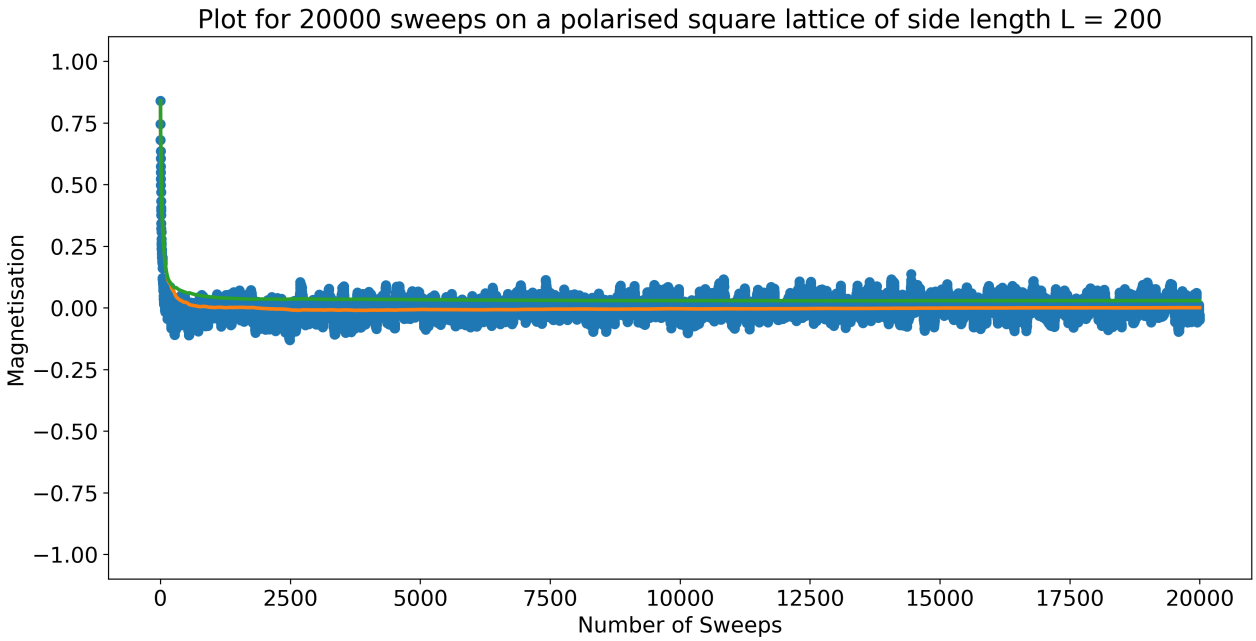
2.2 Polarised Boundary Conditions

2.2.1 Average Magnetisation per Spin

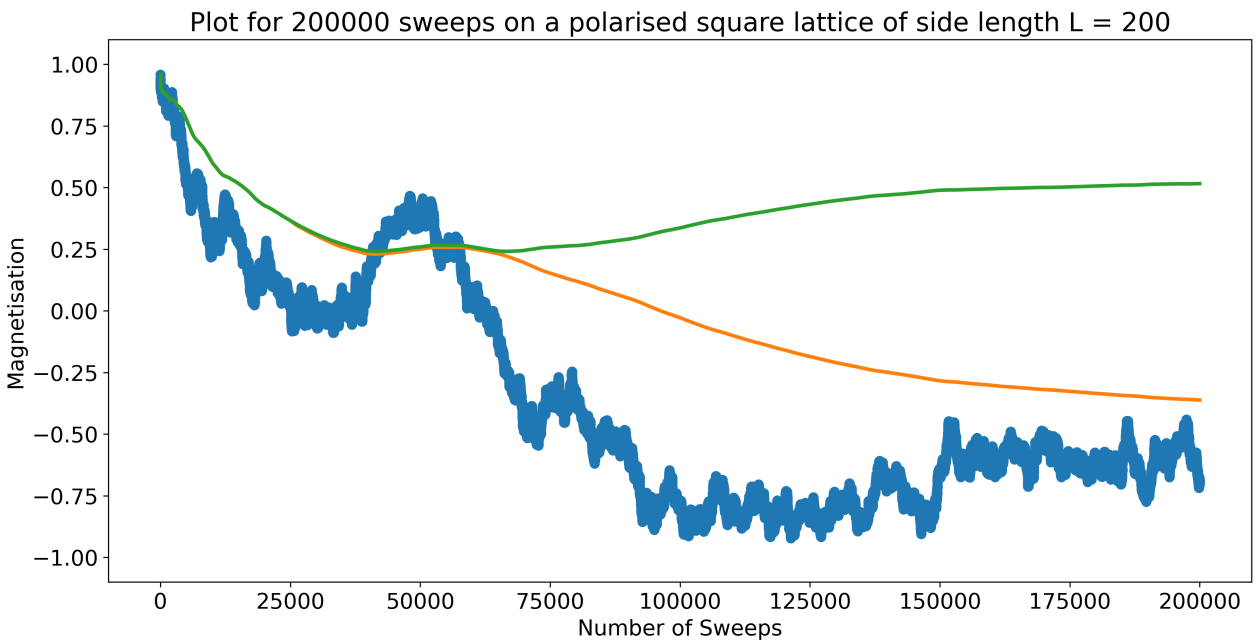
Case 1: $\beta J = 0.2$



Case 2: $\beta J = 0.4$



Case 3: $\beta J = 0.6$



The first two graphs look very similar to the graphs for the periodic boundary conditions so this analysis is limited to the third graph. Note that the third graph has been extended to include data up to 200 000 sweeps. This shows the system's behaviour over a very long period of time.

For the system with periodic boundary conditions, the phase transition is clear and the average magnetisation stabilises at 1 where all the spins are aligned spin up. However, this does not occur in the case of the polarised boundary conditions due to the fact that the spins on one edge of the lattice are fixed to be constantly spin down so it is impossible for all the spins to be aligned spin up.

Looking at the graph, it is apparent that the average magnetisation per spin is initially very close to 1 (as would be expected if a phase transition had occurred) but the magnetisation of the system slowly decreases over time. This curve is not smooth and has some outlying peaks (for example, at around 50 000 sweeps) which is indicative of some erratic behaviour in the system but the overall trend is clear. After about 100 000 sweeps, the average magnetisation per spin is nearly -1 (as will be seen later, this occurs for semi-polarised conditions where one edge's spins are all fixed spin down) but it is impossible for all the spins to be aligned spin down due to the fact that some of them are constantly fixed spin up. Thus, the data still varies a much more than in the system with periodic boundary conditions but the system seems to have stabilised between a magnetisation of - 0.5 and -1.

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This instability is indicative of what will be labelled an "unstable" phase transition. There is a clear change in the
magnetic behaviour of the system at temperatures below the critical temperature but this change does not lead to a constant
magnetisation after the phase transition (as was the case for the periodic boundary conditions): instead there is erratic
behaviour.
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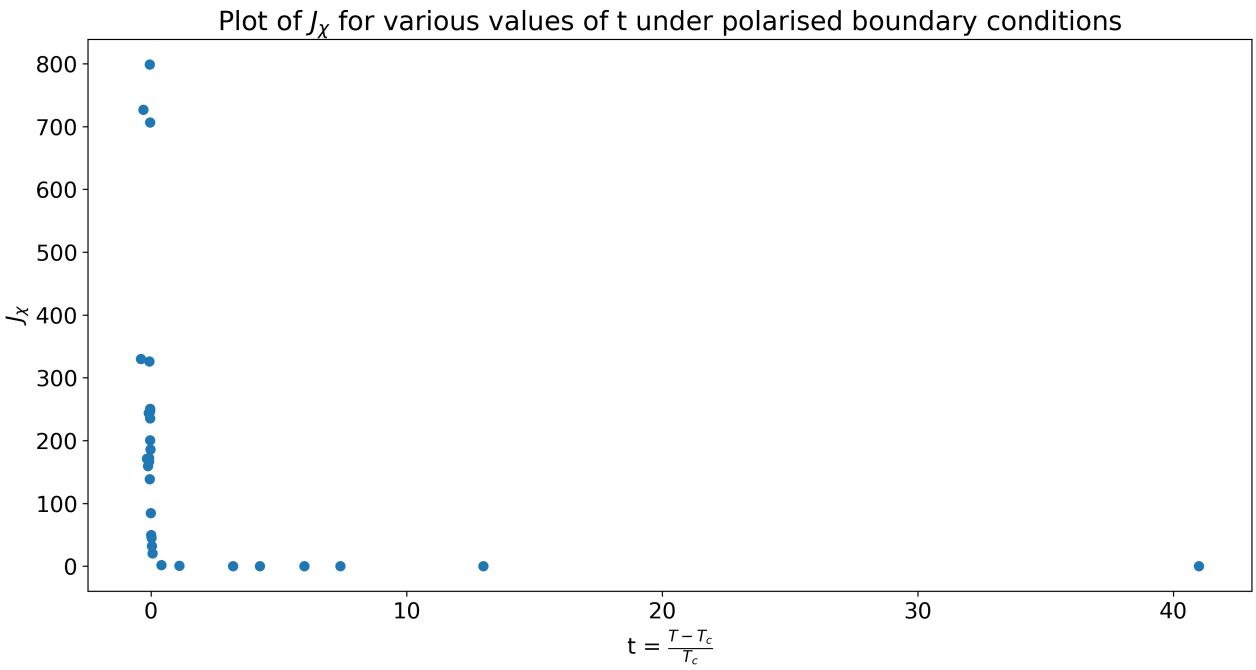
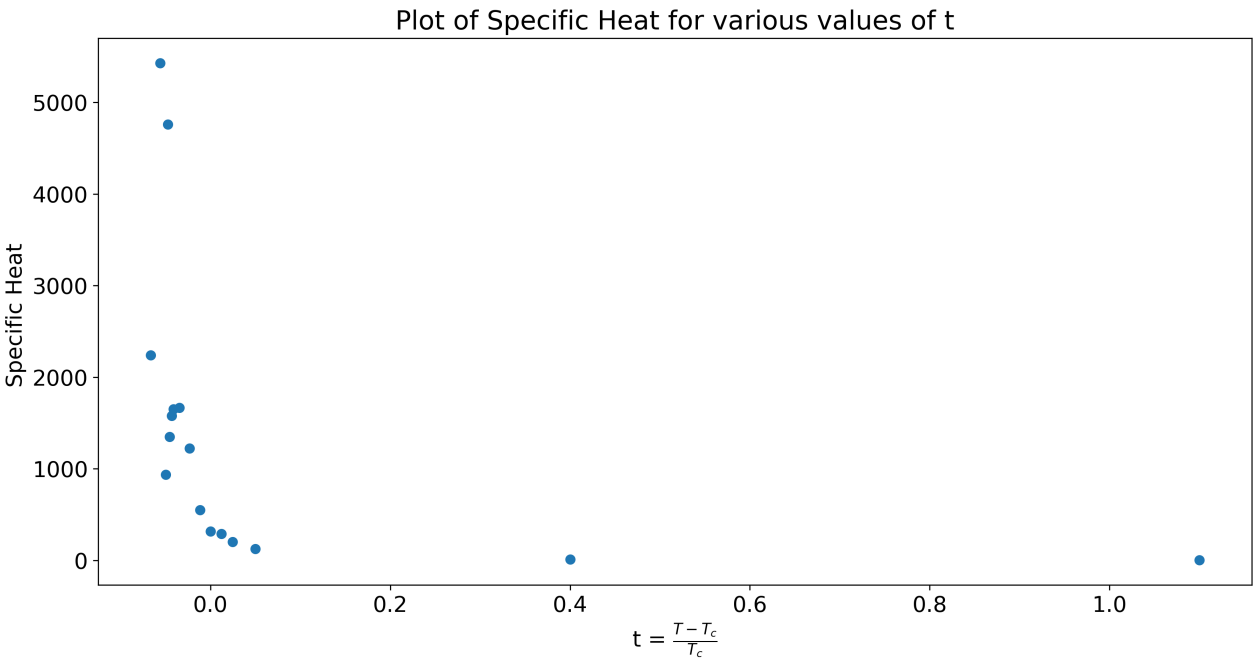
2.2.2 Magnetic Susceptibility



2.2.3 Specific Heat

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From the graphs for the magnetic susceptibility and specific heat, some differences are evident for both. The graph of the
magnetic susceptibility seems to not have as clear a decline at temperatures below the critical temperature as it did for
the periodic boundary conditions. This sustained period of high magnetic susceptibility may be able to explain the erratic
behaviour of the graph for the average magnetisation per spin of the system.

Now, the specific heat seems to not be peaked around zero in this case. In fact, the peak is below zero, meaning that the
specific heat peaks at temperatures below the critical temperature. For the periodic boundary conditions, the specific heat
peaked at or near the critical temperature. This was also where the magnetic susceptibility peaked. However, the magnetic
susceptibility for these polarised boundary conditions remains high even at temperatures below the critical temperature.
This may help to explain the shift in the peak of the specific heat graph.
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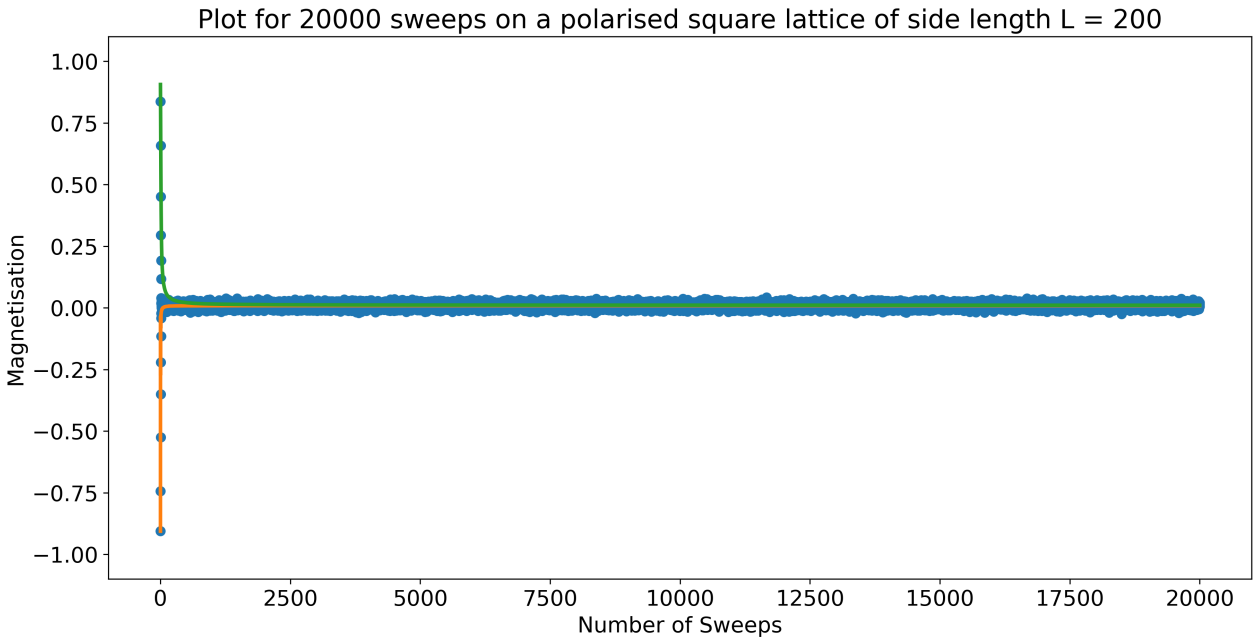
2.3.1 Semi-Polarised Boundary Conditions (all up)

In this case, all of the spins on one edge of the lattice were fixed in an all-up state for the duration of the simulation.

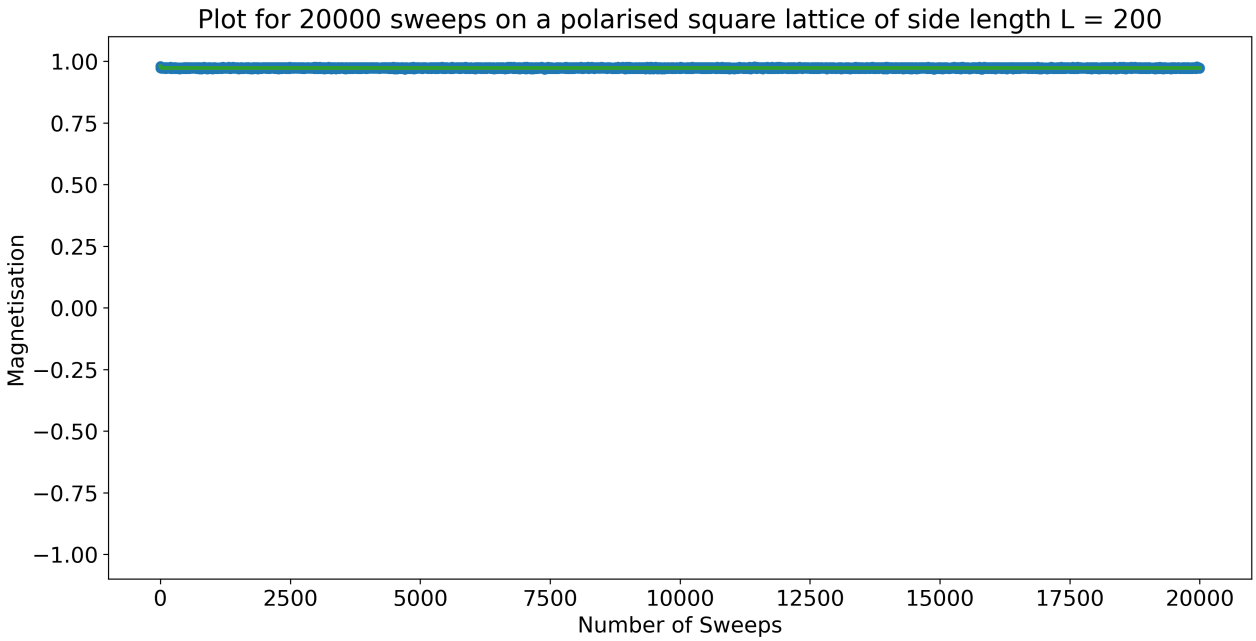
2.3.1.1 Average Magnetisation Per Spin

Case 1: βJ = 0.2



Case 2: βJ = 0.4

Case 3: βJ = 0.6

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In this case, the behaviour of the system's average magnetisation is very similar to what is observed for the standard
periodic boundary conditions. The phase transition is very clear because all the spins in the lattice can be aligned in a
spin up state unlike in the next case where one edge's spins were fixed to be all spin down. Thus, once the phase
transition has taken place, the spins don't change their alignment anymore, making the phase transition "stable". The
changed boundary conditions seem to have no effect on the average magnetisation in this case.
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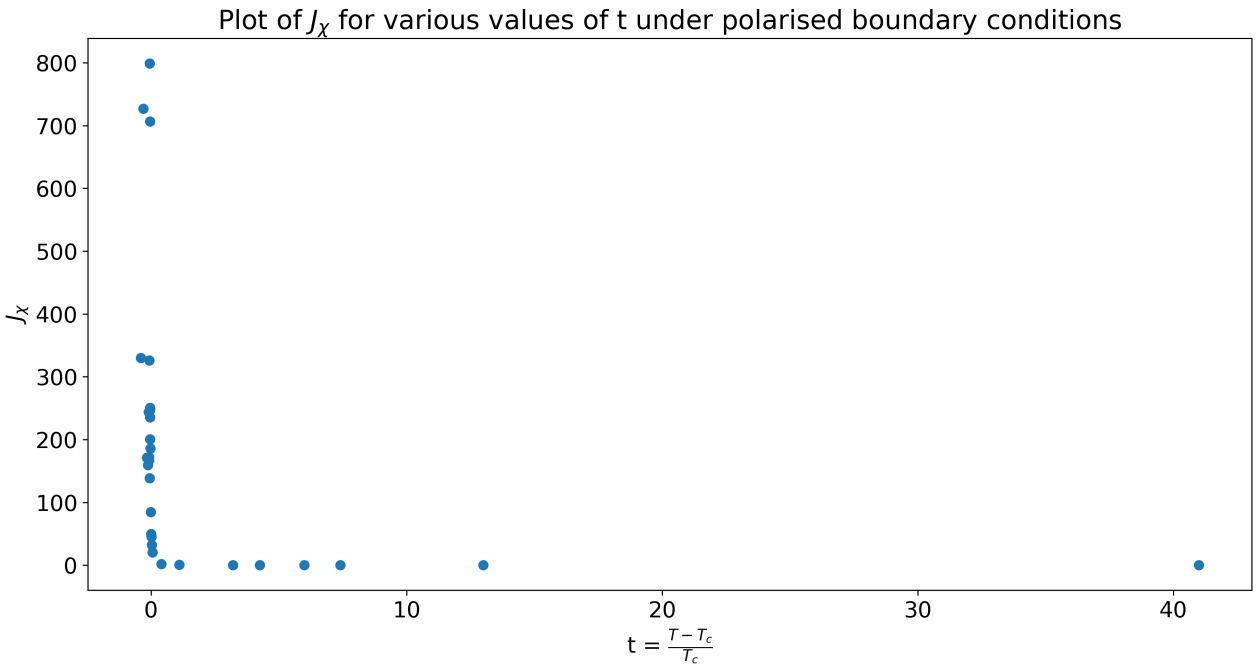
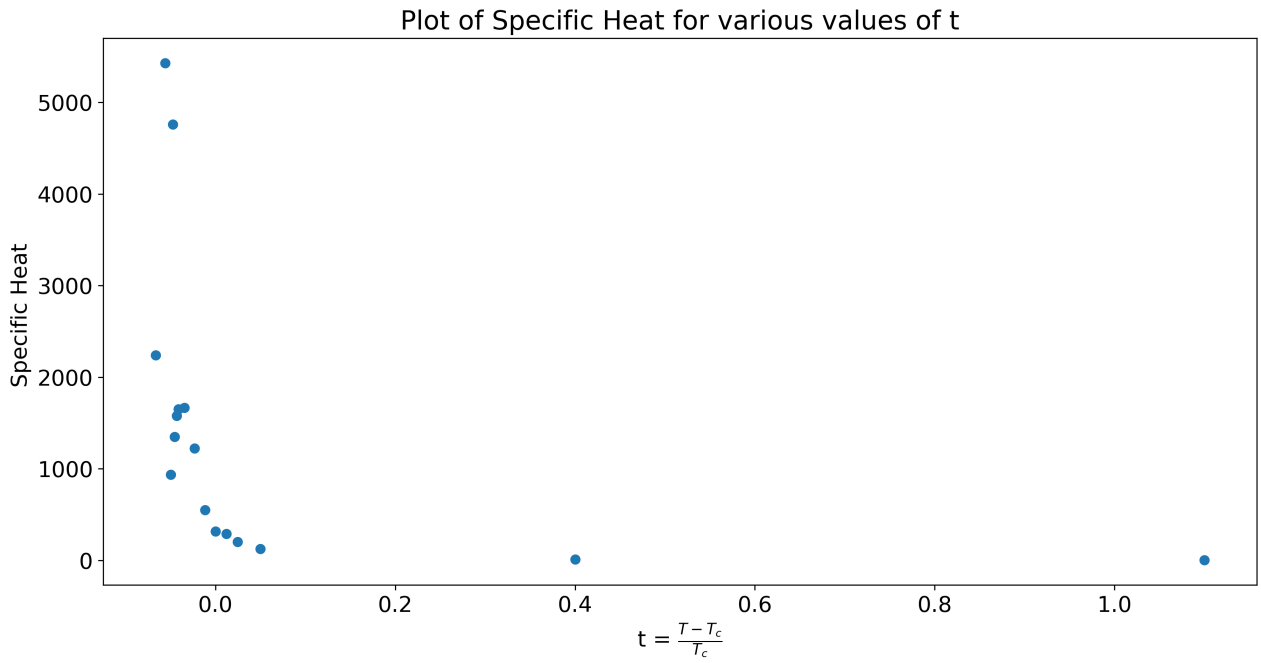
2.3.1.2 Magnetic Susceptibility



2.3.1.3 Specific Heat

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The graphs for the magnetic susceptibility and specific heat look very similar to the graphs for the polarised boundary
conditions. In short, it seems that this change to having only one polarised edge makes little difference. So, the same
analysis as before applies here again.
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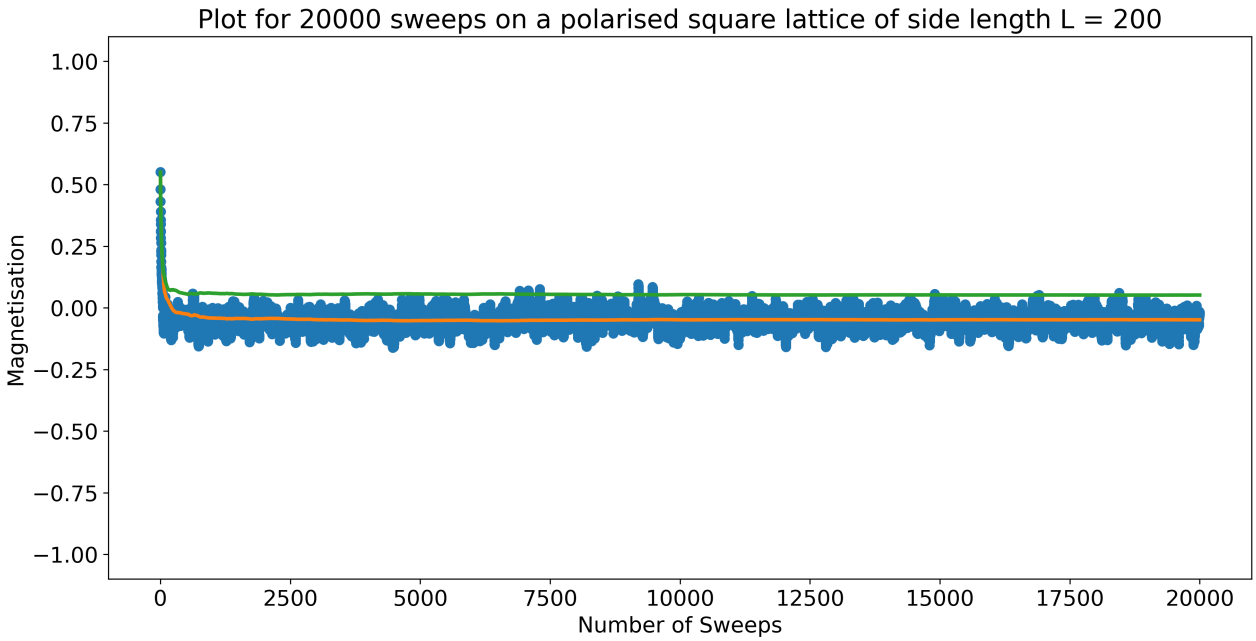
2.3.2 Semi-Polarised Boundary Conditions (all down)

This simulation is the same as the previous one but now all the spins on one edge are fixed as spin down instead of spin up.

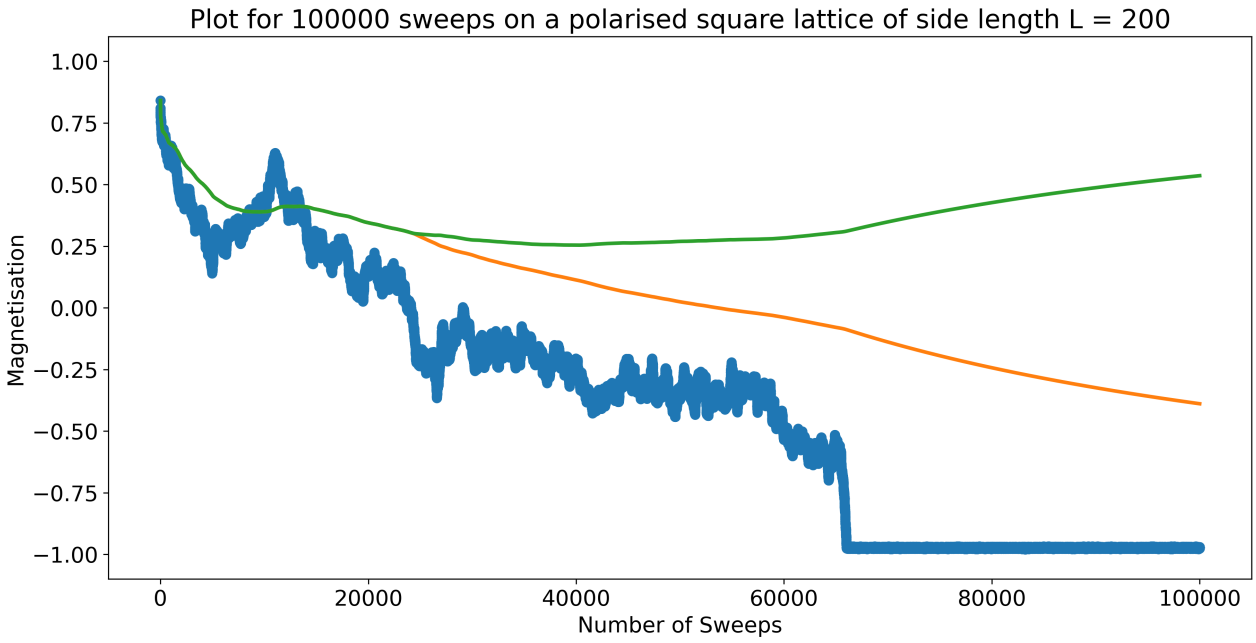
2.3.2.1 Average Magnetisation per Spin

Case 1: βJ = 0.2

Case 2: βJ = 0.4



Case 3: βJ = 0.6

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The first two graphs look very similar to the graphs for the periodic boundary conditions as well as the previous case
where one edge's spins were fixed as all up. However, it is in the third graph (that is, at temperatures below the critical
temperature) where there is a clear change in behaviour.

This is the temperature at which the effects of the phase transition would usually be seen. In the previous graphs, this
meant that the average magnetisation was constant and all the spins were aligned spin up. However, this alignment is
impossible in this case because 20 of the spins in the system are always aligned to be spin down. In this case, the
magnetisation is initially high (between 0.75 and 1) after a few sweeps but becomes lower as more sweeps are taken over the
lattice. Eventually, after about 65000 sweeps, all the spins are negatively aligned and the average magnetisation is a
constant -1.
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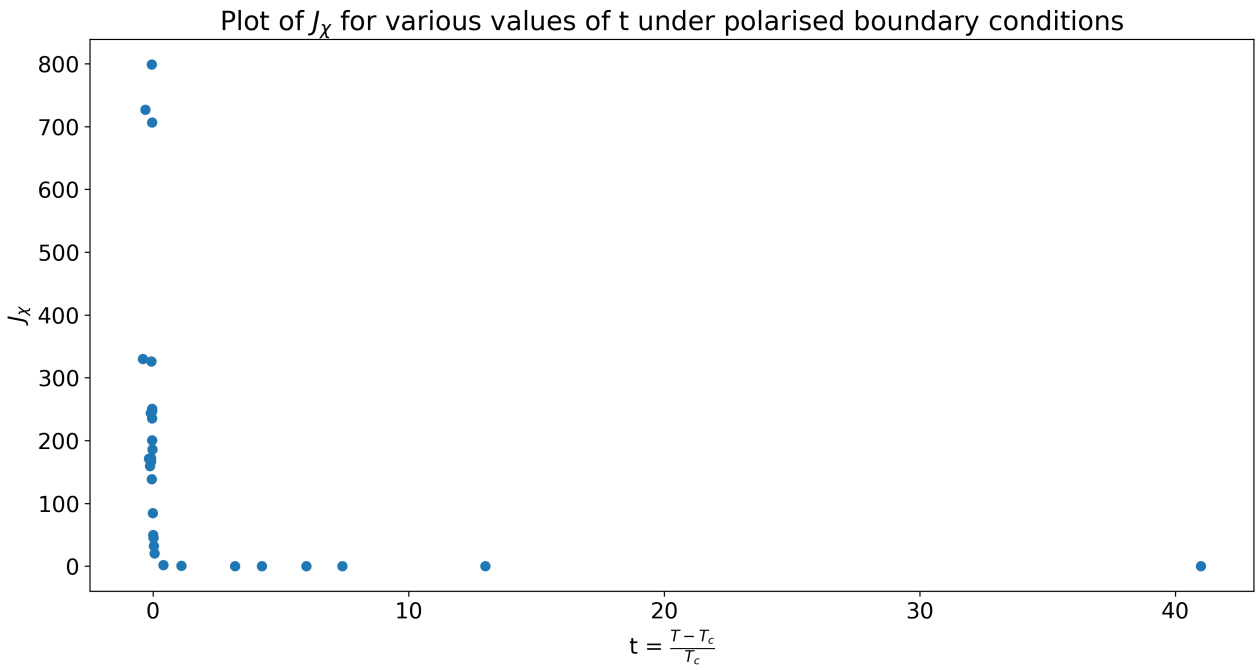
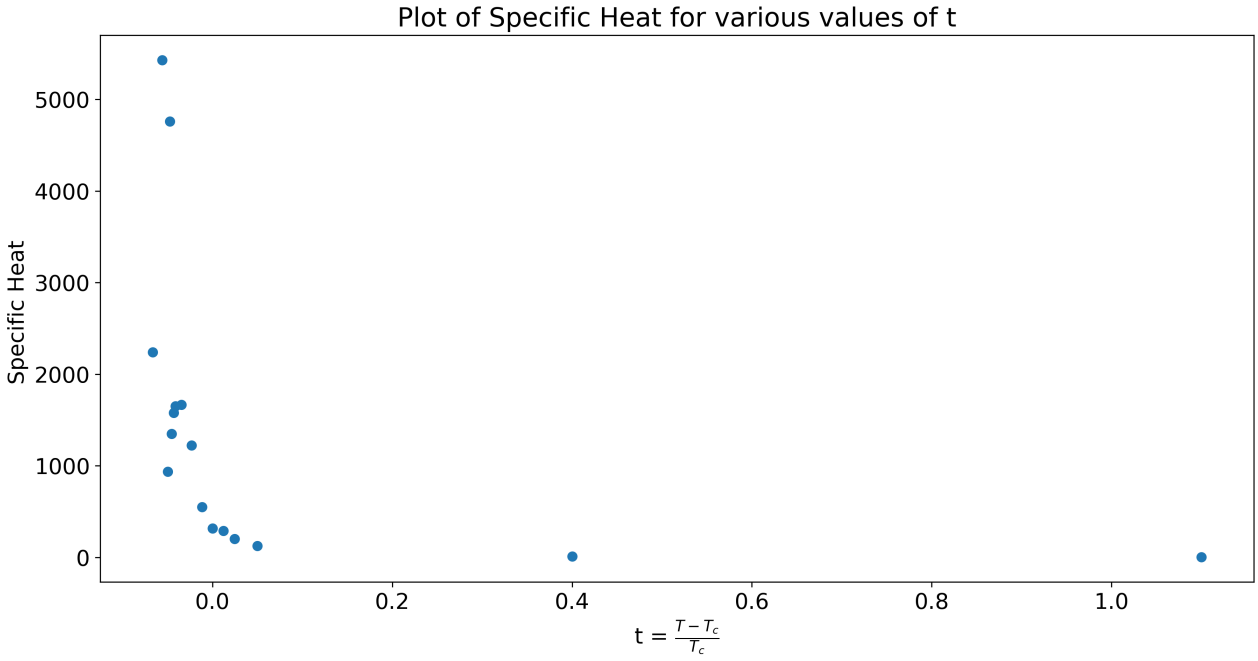
2.3.2.2 Magnetic Susceptibility



2.3.2.3 Specific Heat

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Once again, the graphs for magnetic susceptibility and specific heat seem to not be affected much by the change in
polarisation. It can be concluded that, while the changes in polarisation have a significant effect on how the average
magnetisation of the system changes over time, they seem to not have any noticeable effect on the specific heat or the
magnetic susceptibility of the system.
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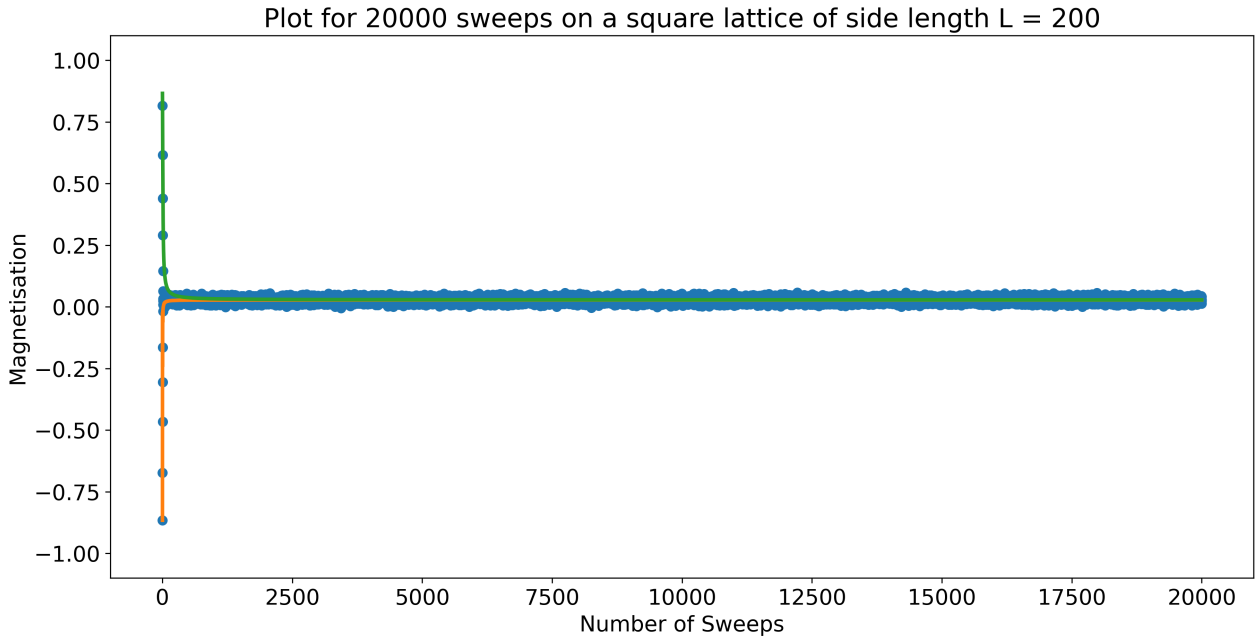
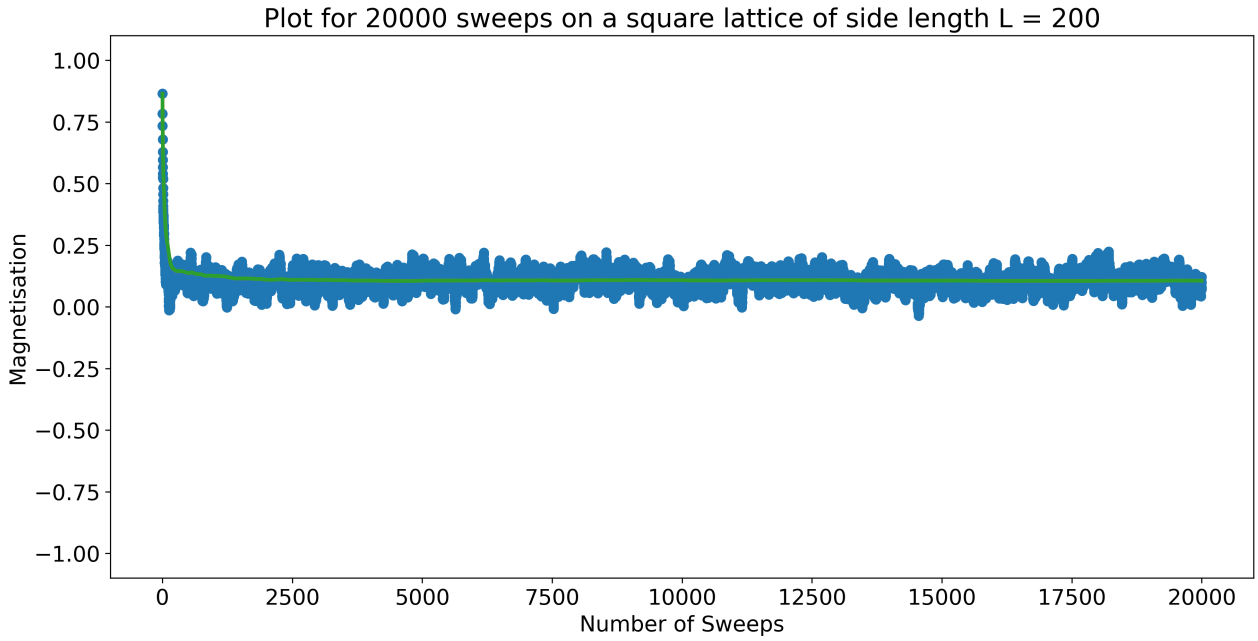
Section 2.4.1: Non-Interaction Boundary Conditions (all up)

2.4.1.1: Average Magnetisation per spin

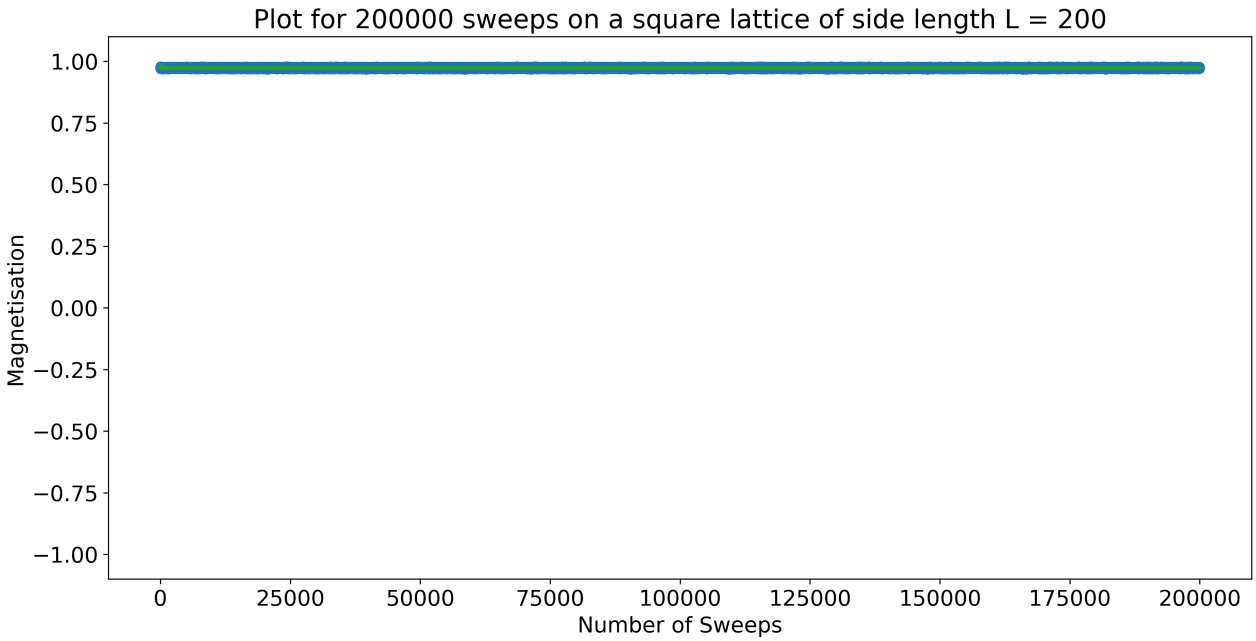
Case 1: $\beta J = 0.2$



Case 2: $\beta J = 0.4$



Case 3: $\beta J = 0.6$

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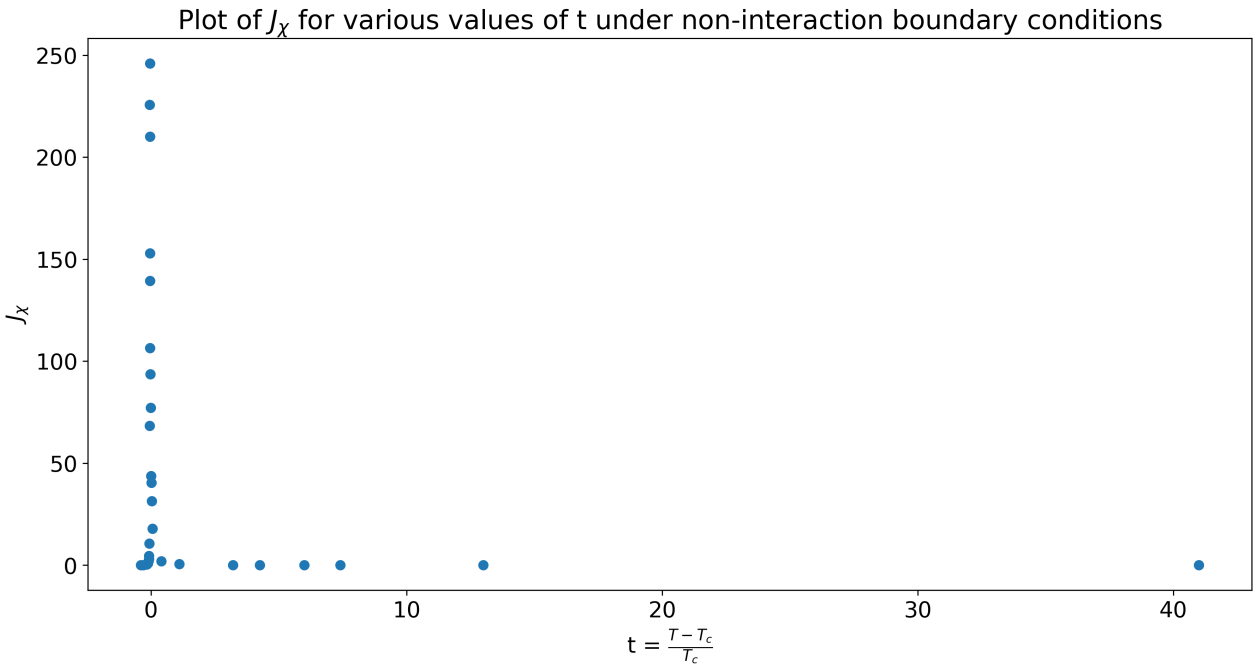
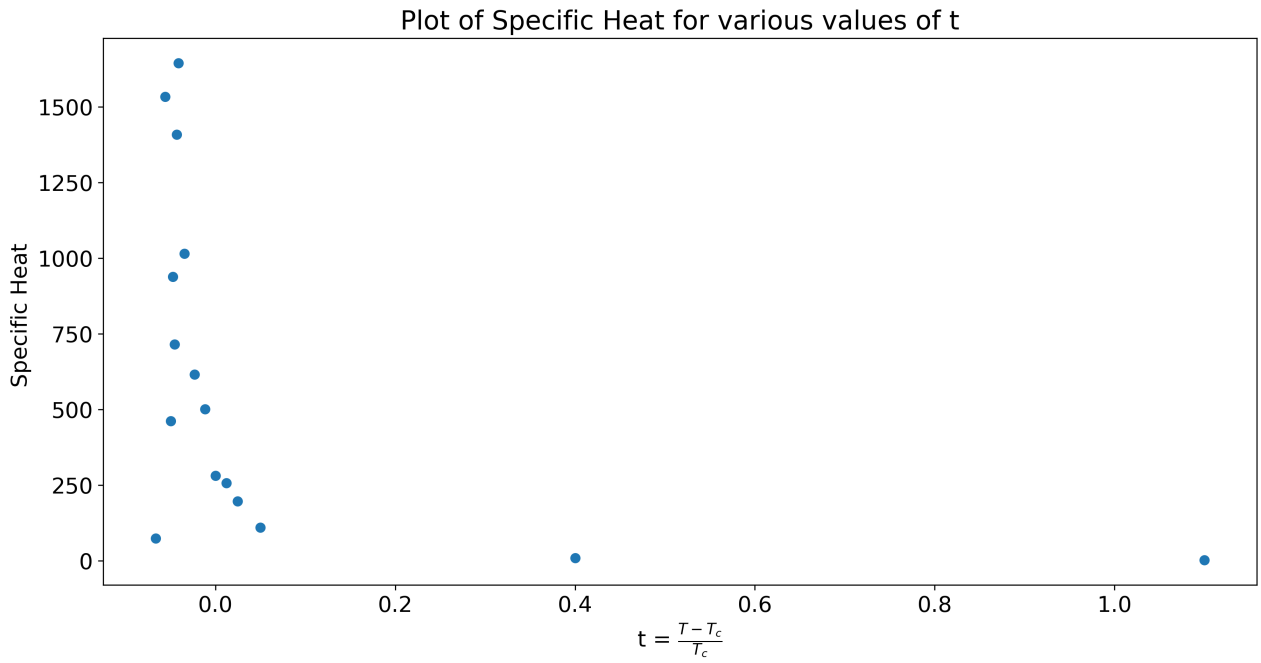
It is clear here that this set of non-interaction boundary conditions where all the outer spins are fixed spin up has
essentially no effect on the average magnetisation data. These graphs look exactly the same as the graphs for the periodic
boundary conditions. A phase transition has clearly taken place and it is stable with all the spins being aligned spin up.
This will not occur for the next case where all the outer spins are aligned spin down so that the "stable" phase transition
is impossible.
```

2.4.1.2 Magnetic Susceptibility



2.4.1.3 Specific Heat



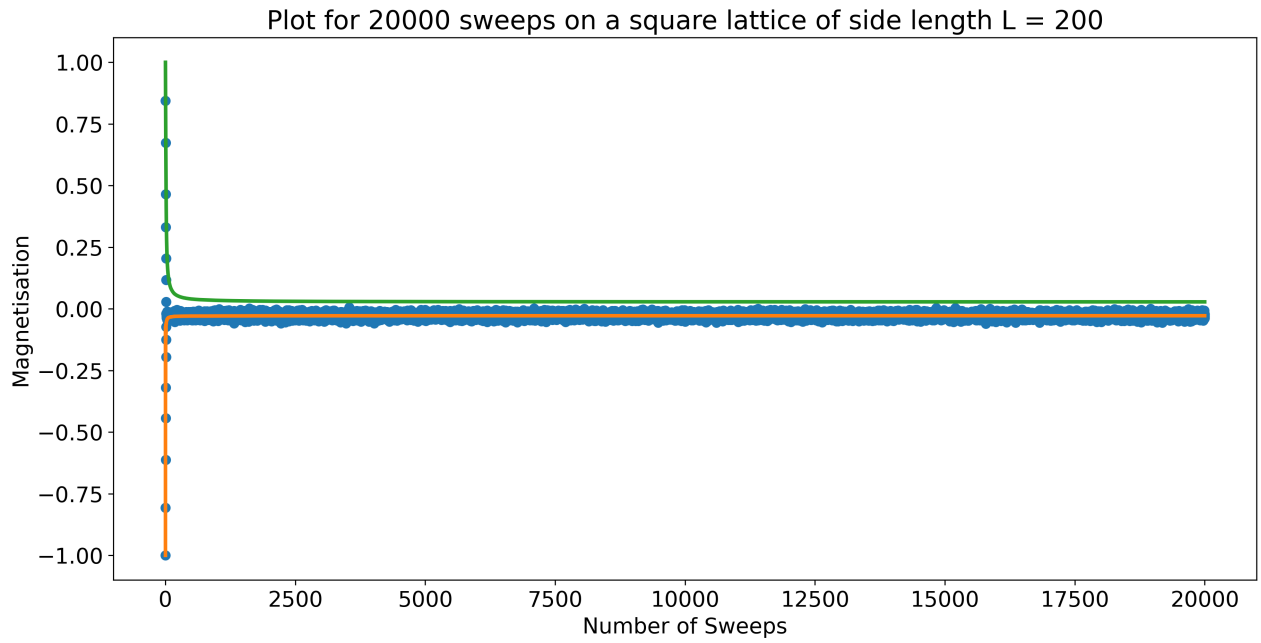
Again, the specific heat and magnetic susceptibility graphs look very similar to the graphs for the system with standard periodic boundary conditions.

However, there is one notable difference: the specific heat graph does not peak at the same critical temperature as in the periodic case. In fact, it peaks for lower temperatures. This is a possible indication that the critical temperature has actually been reduced by the effect of fixing the outer spins as all spin up.

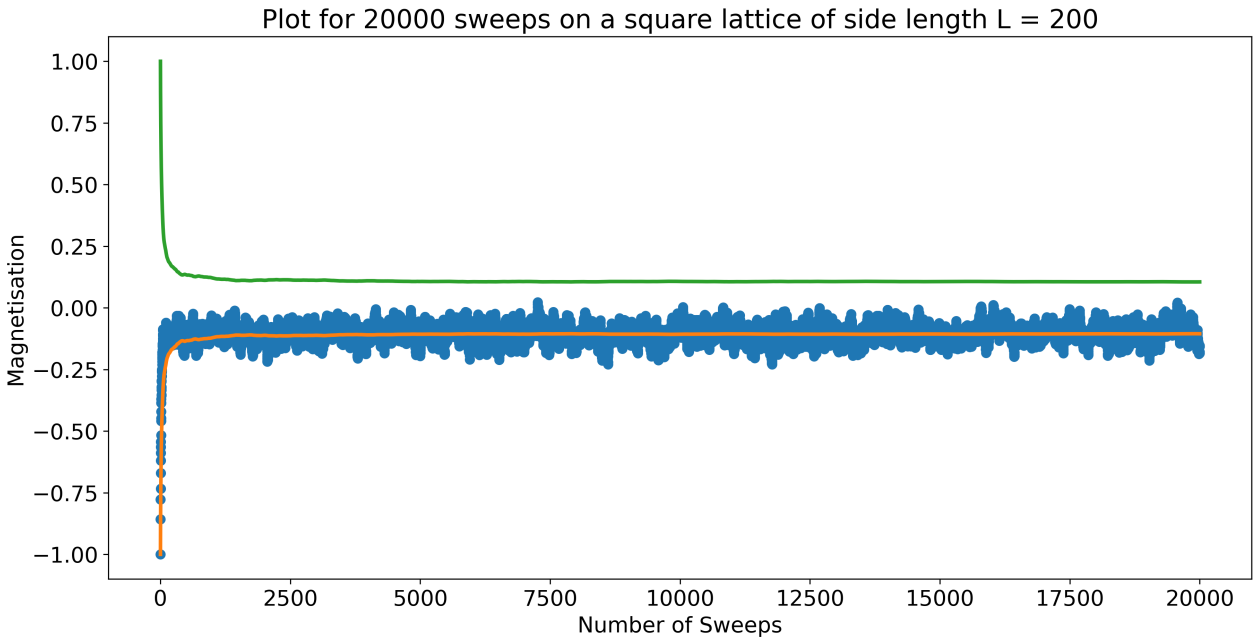
Section 2.4.2: Non-Interaction Boundary Conditions (all down)

2.4.2.1: Average Magnetisation per spin

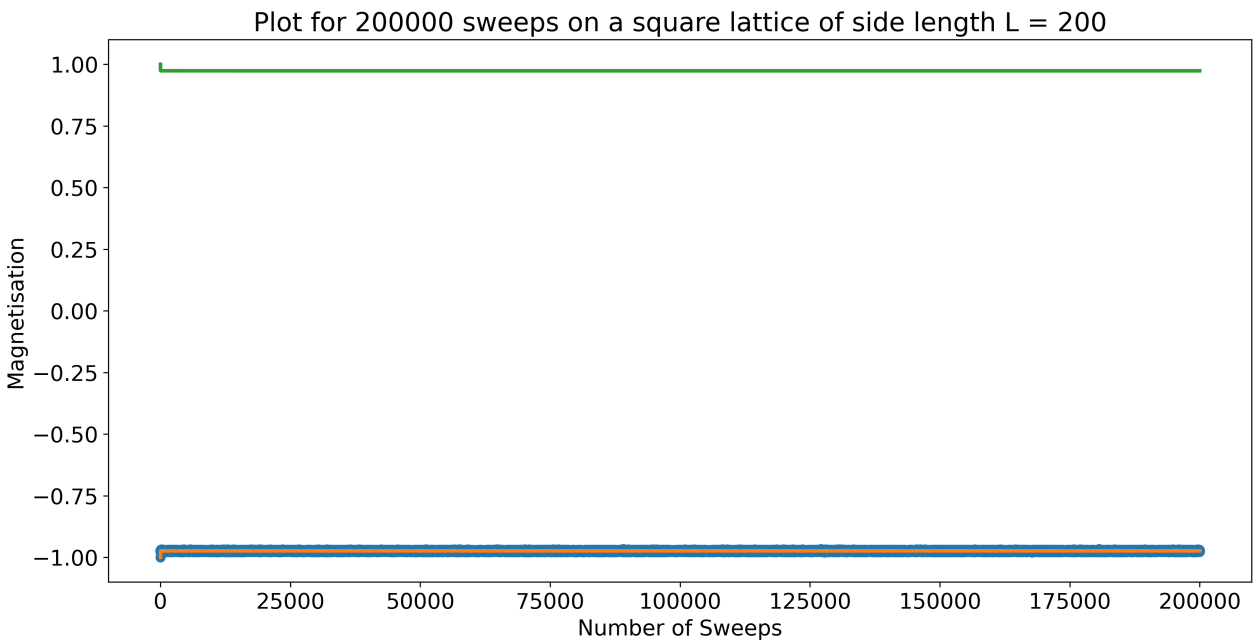
Case 1: $\beta J = 0.2$



Case 2: $\beta J = 0.4$



Case 3: $\beta J = 0.6$




```
The average magnetisation graphs for these boundary conditions are very different to the standard case. In fact, it is
clear here that a phase transition has taken place. However, this phase transition results in all the spins being aligned
spin down instead of spin up as usual. So, the average magnetisation becomes -1 instead of 1. Thus, it seems that the phase
transition has been "reversed" here: the spins are all spin down instead of spin up after the phase transition.
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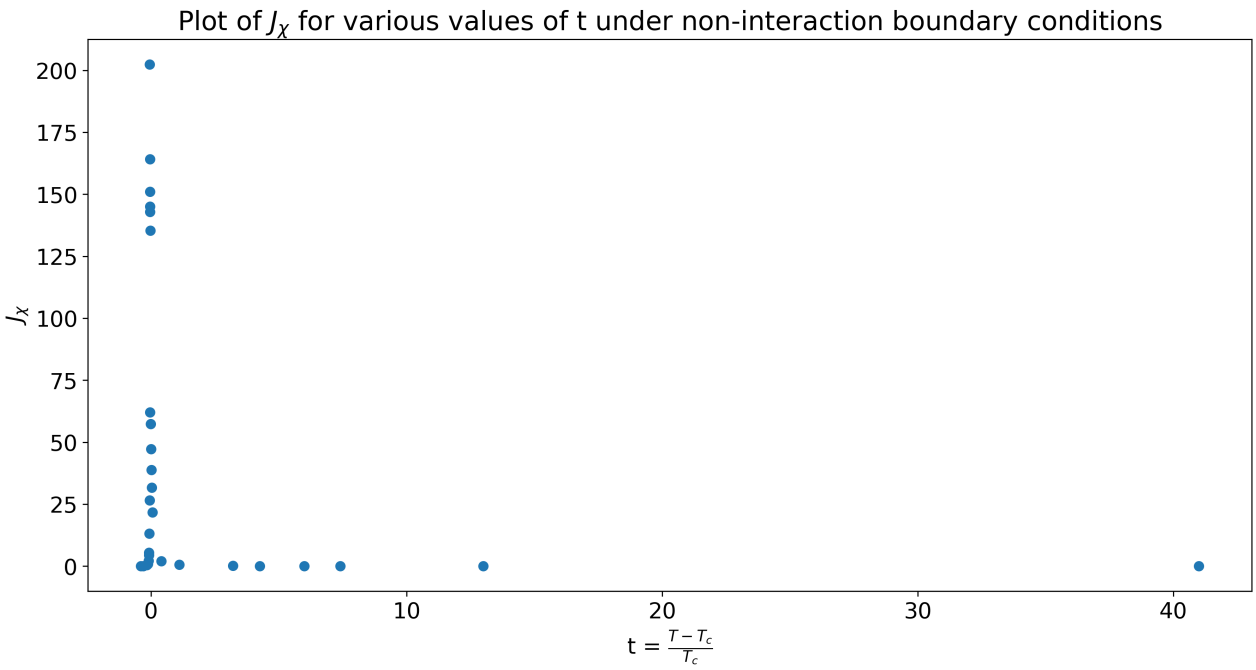
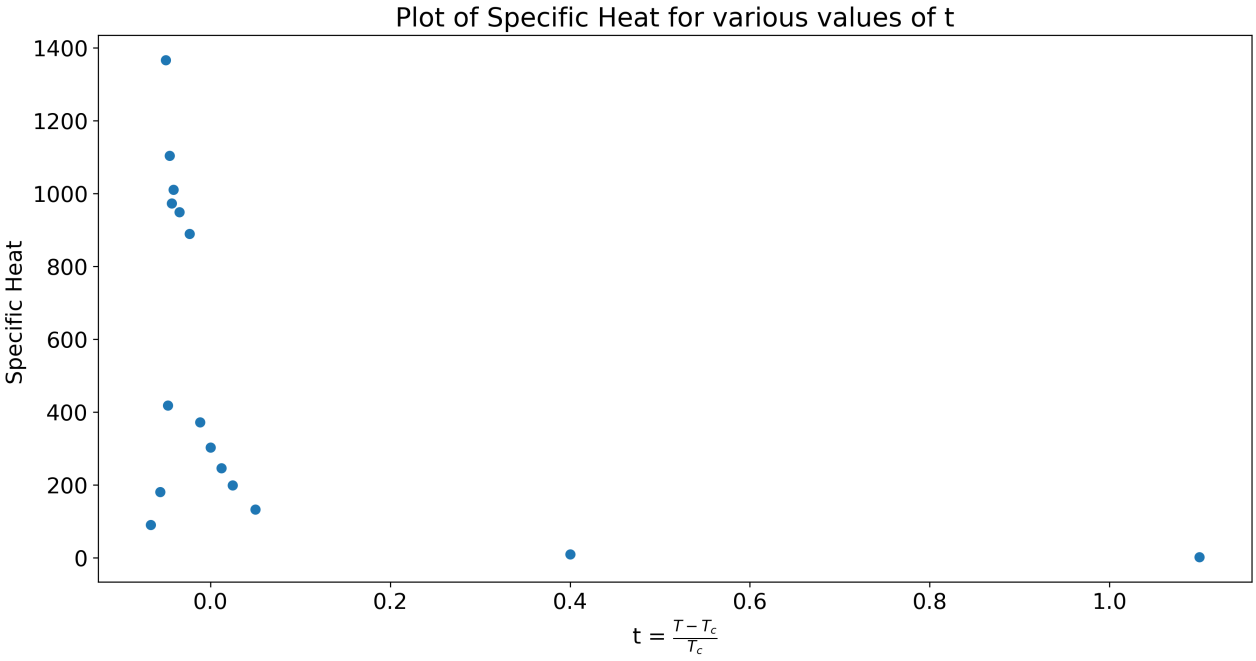
2.4.2.2: Magnetic Susceptibility



2.4.2.3: Specific Heat

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The magnetic susceptibility and specific heat graphs look almost exactly the same as the graphs for the periodic boundary
conditions. Thus, despite the phase transition being "reversed" and these boundary conditions having a significant impact
on the system's magnetisation, it seems that the change in boundary conditions has had no effect on the magnetic
susceptibility or specific heat.
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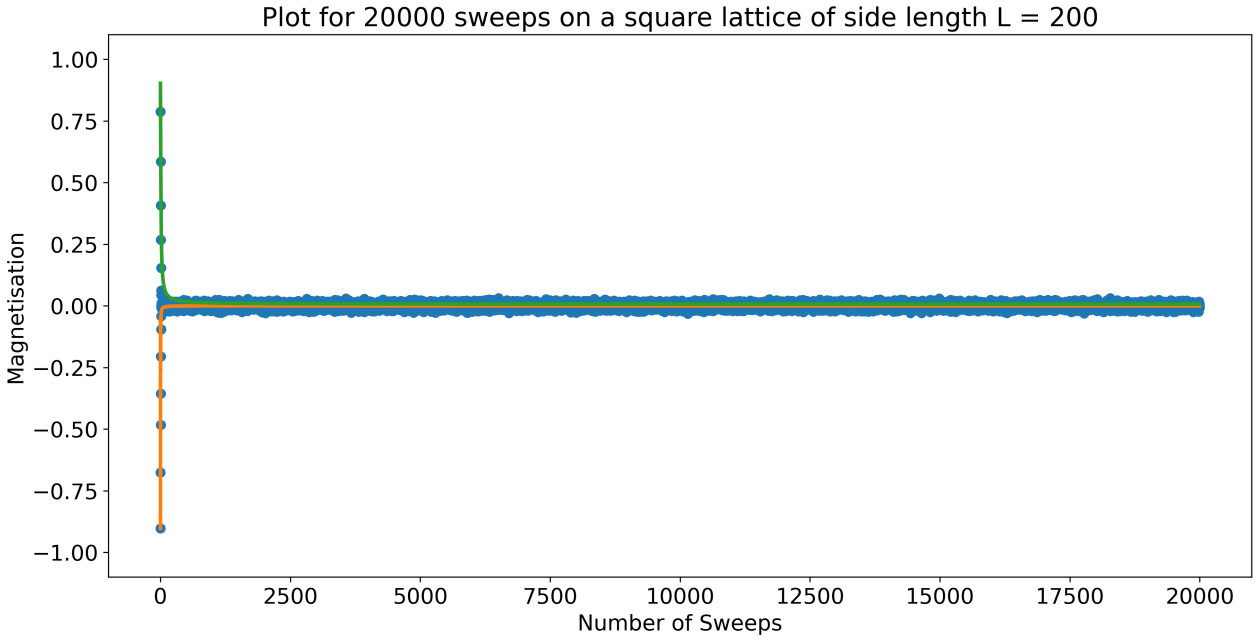
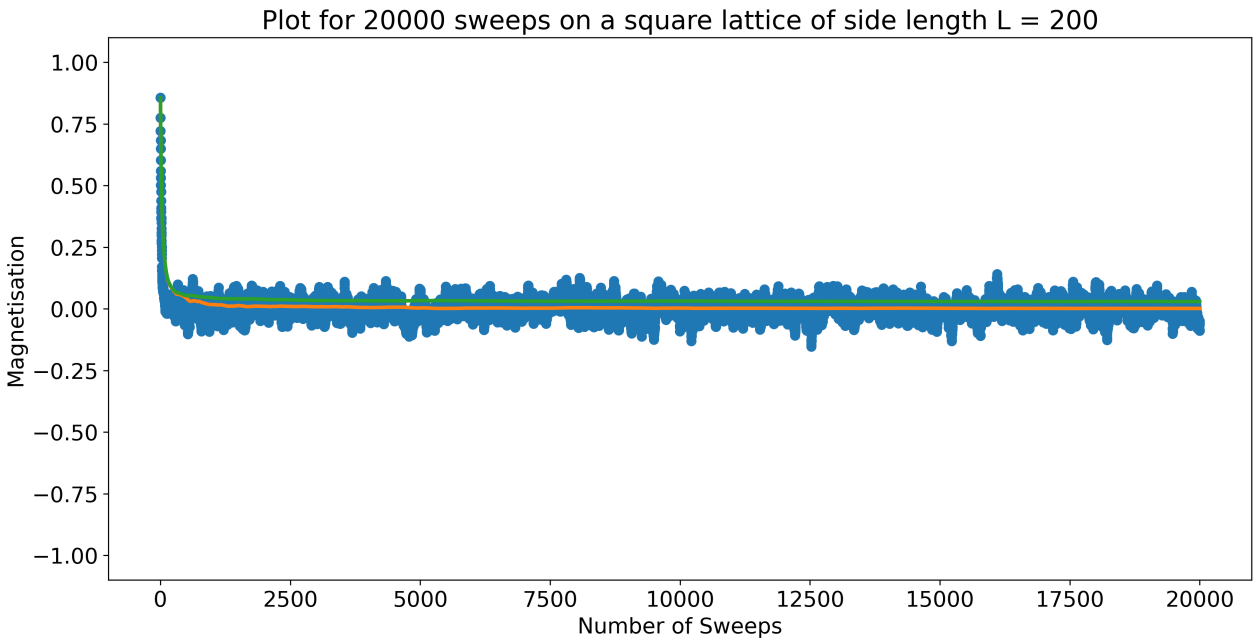
Section 2.5: Ferromagnetic Boundary Conditions

2.5.1: Average Magnetisation per spin

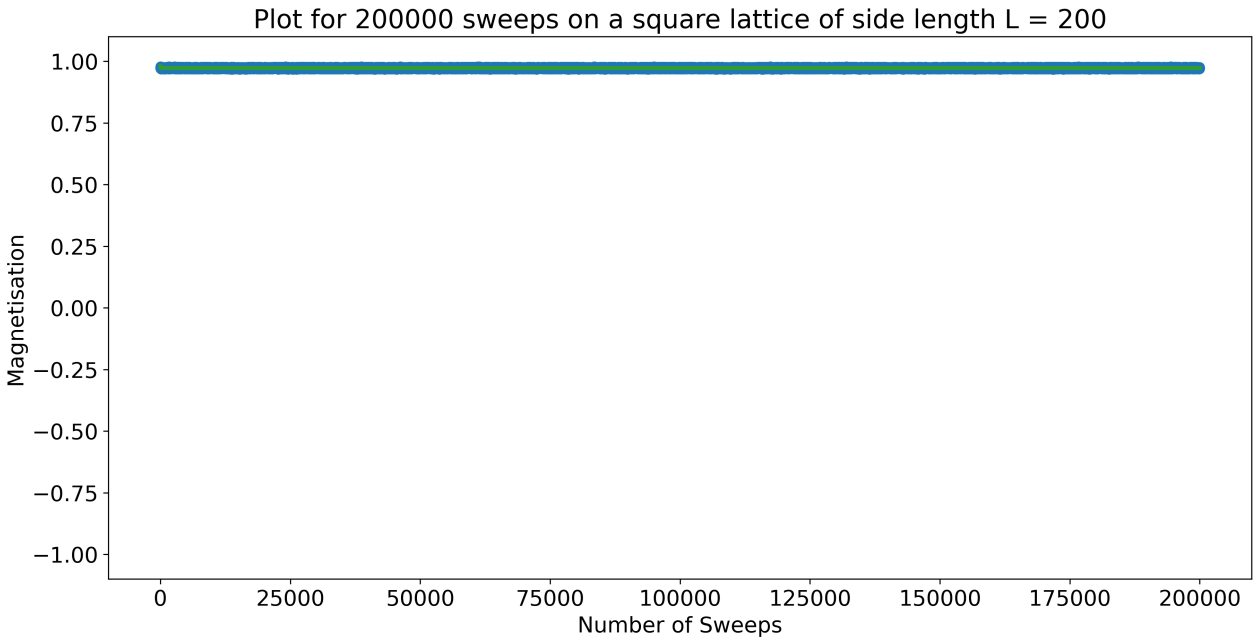
Case 1: $\beta J = 0.2$



Case 2: $\beta J = 0.4$



Case 3: $\beta J = 0.6$

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The graphs of the average magnetisation look very similar to the standard periodic boundary conditions. No significant
difference is made to the average magnetisation per spin by imposing these new boundary conditions.
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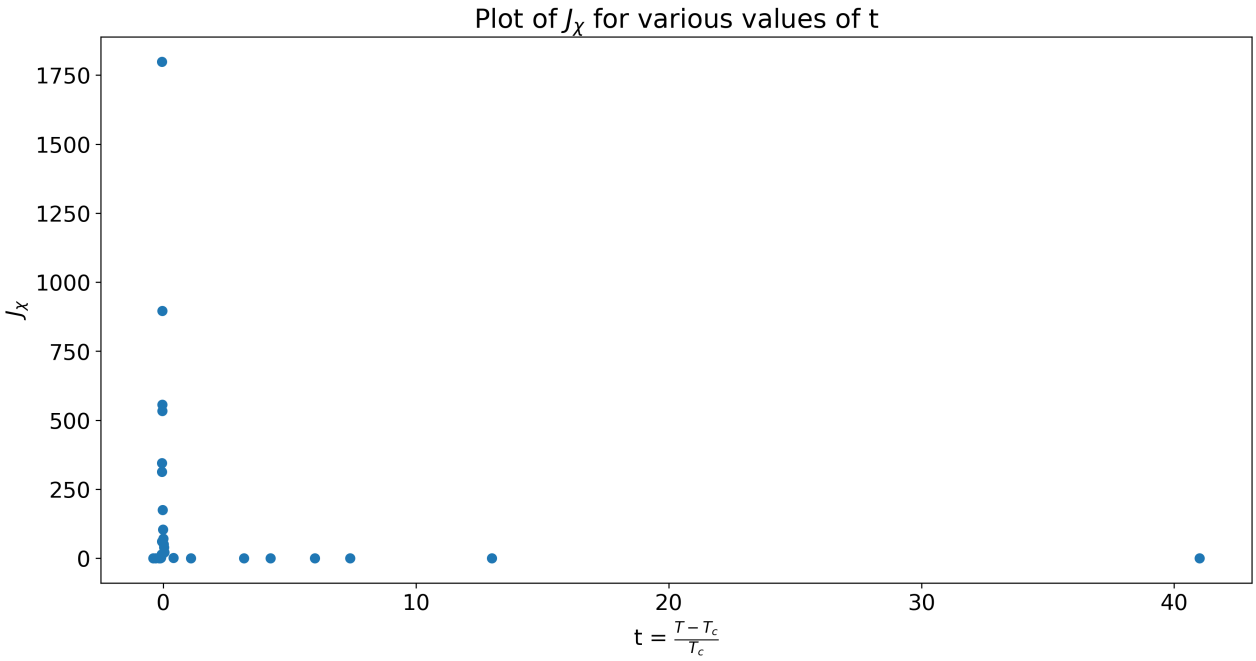
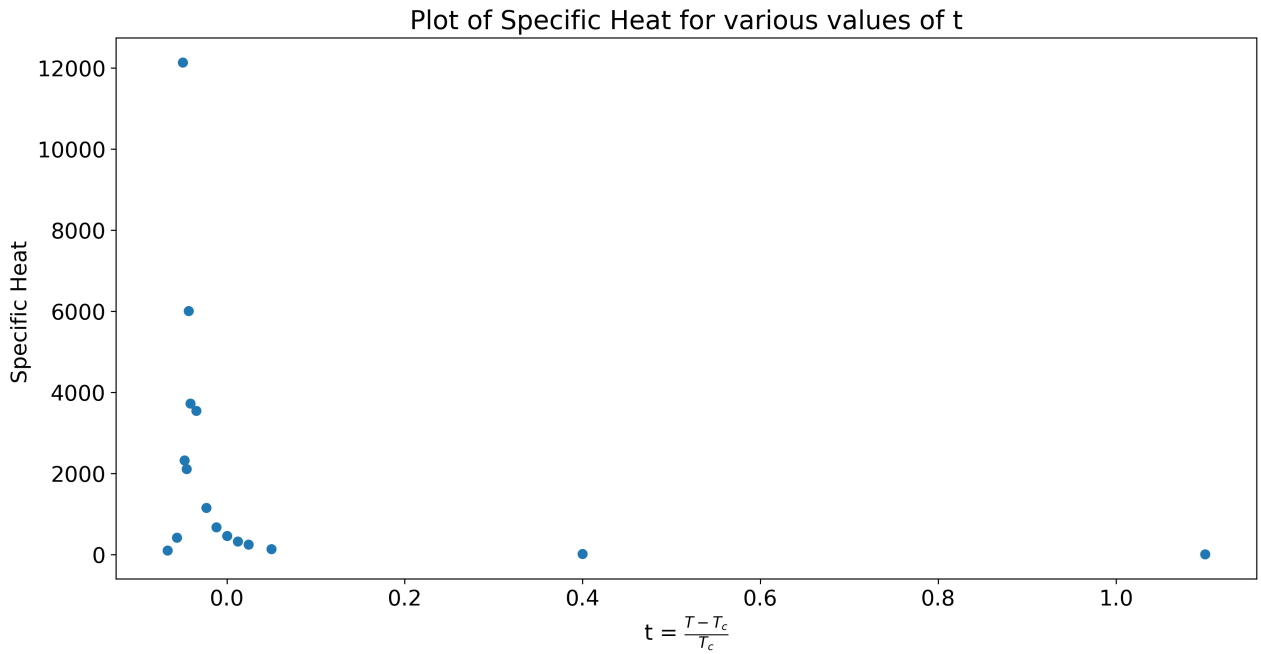
2.5.2: Magnetic Susceptibility



2.5.3: Specific Heat

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Despite the fact that the majority of the spins are now interacting anti-ferromagnetically, the graphs for the magnetic
susceptibility and specific heat still have the same shape as those of the periodic boundary conditions. The only change is
that the peak of the specific heat graph is shifted to the right once again.
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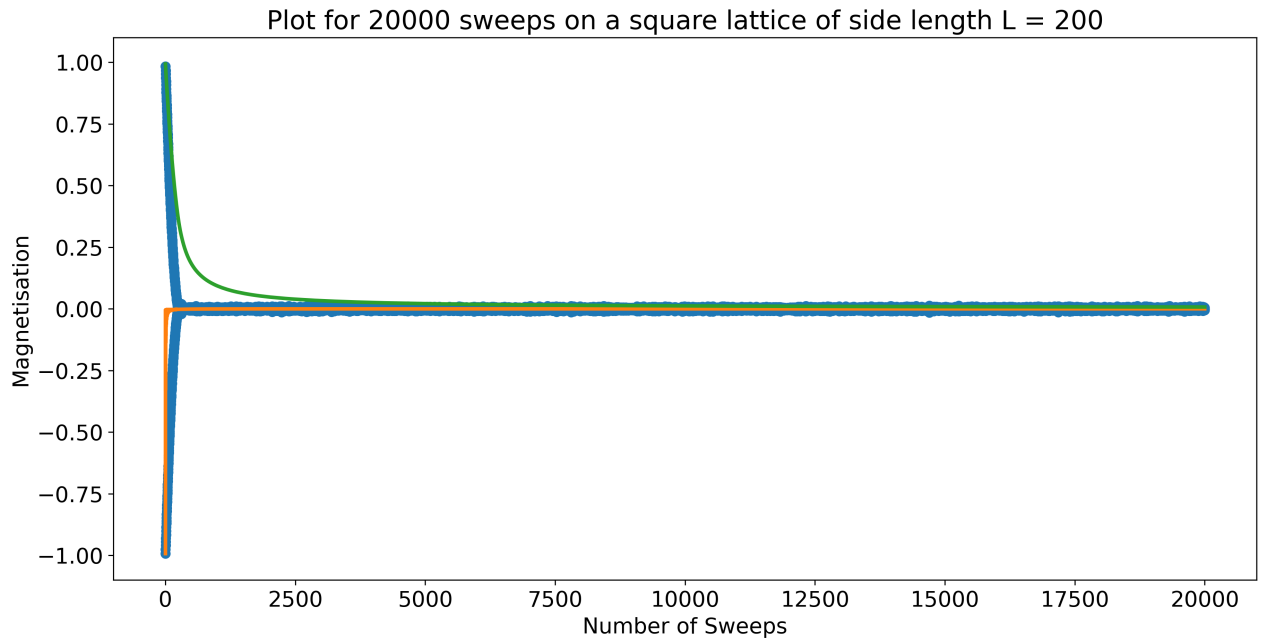
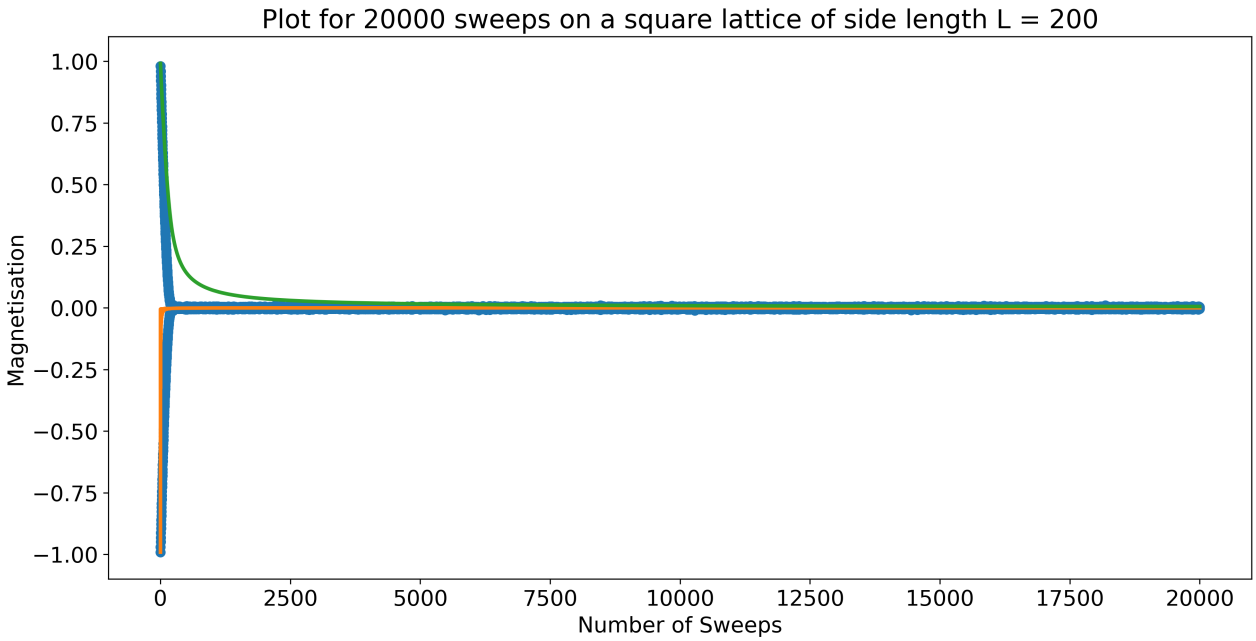
Section 2.6: Anti-ferromagnetic Boundary Conditions

2.6.1: Average Magnetisation per spin

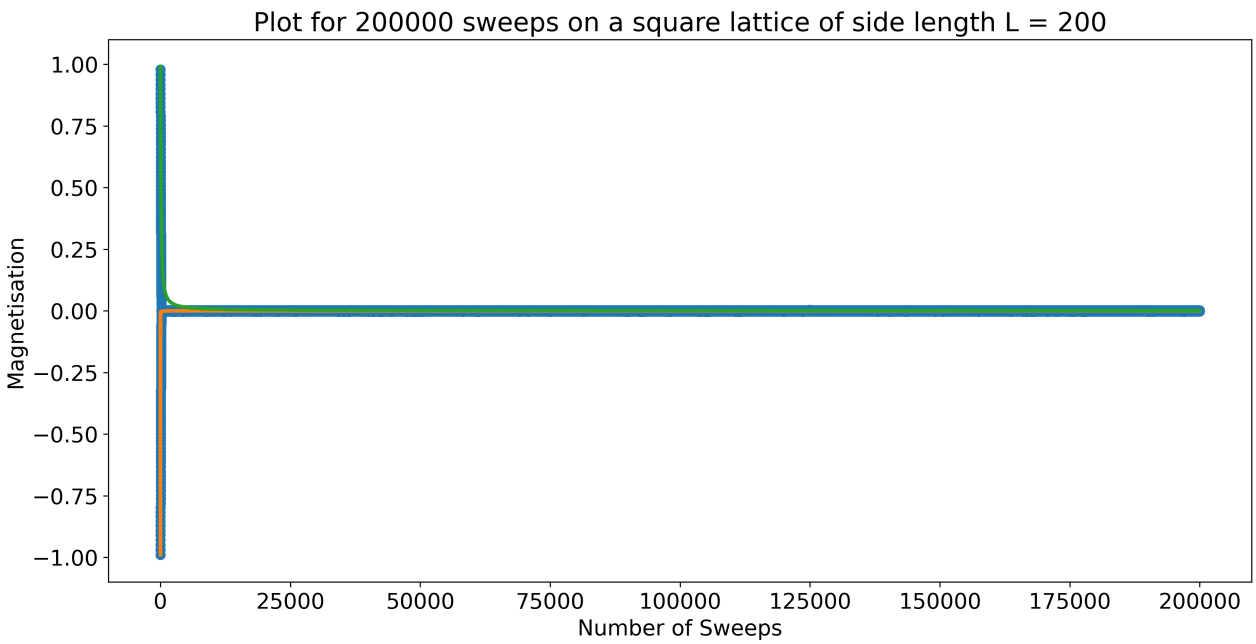
Case 1: $\beta J = 0.2$



Case 2: $\beta J = 0.4$

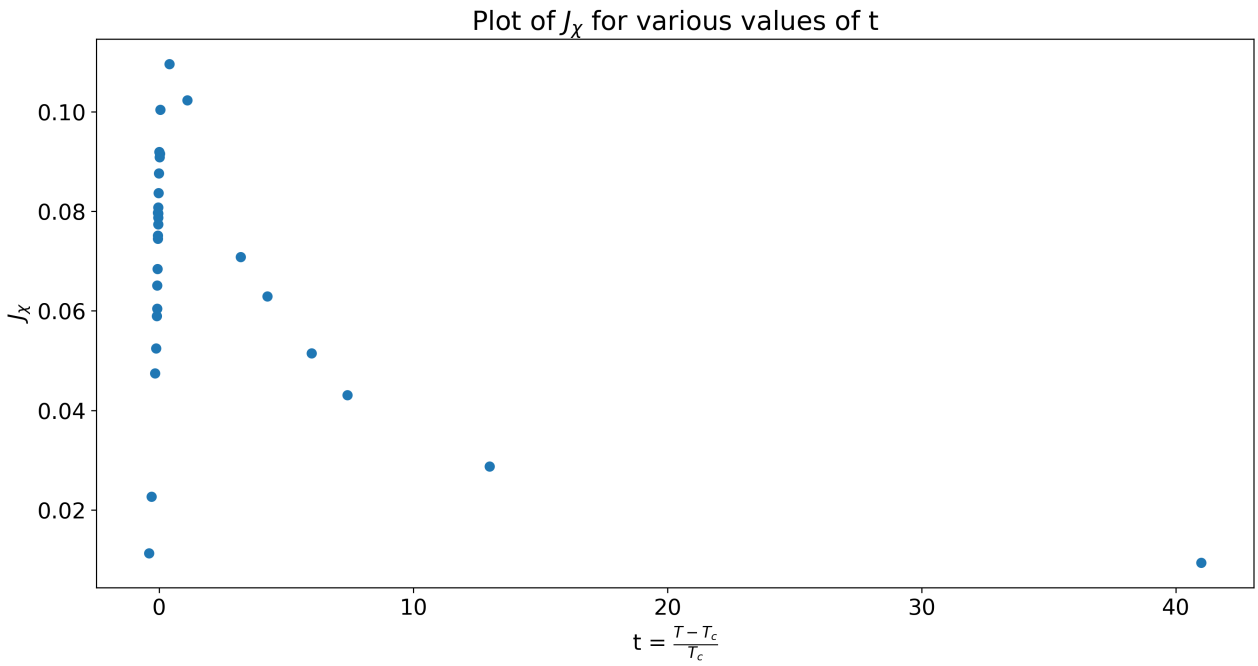


Case 3: $\beta J = 0.6$

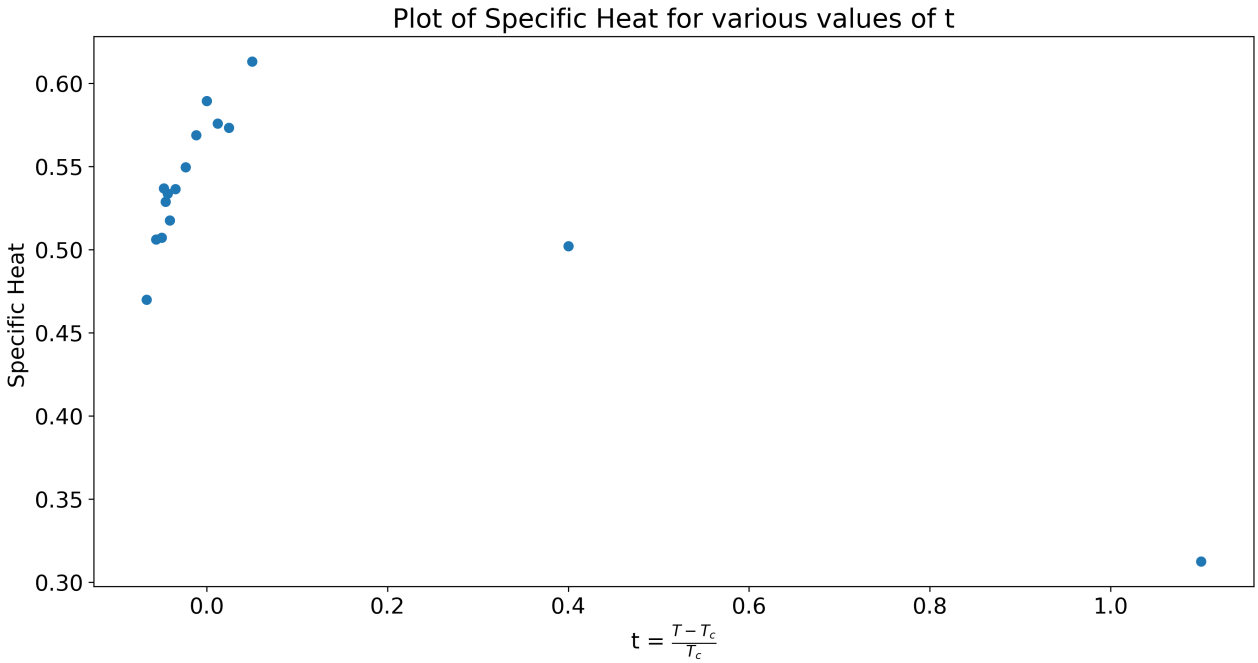



```
In this case, there is a significant change from the system with periodic boundary conditions. It seems that there is no
phase transition in this case. This is possibly due to the anti-ferromagnetic interactions on the edges of the lattice
preventing the phase transition from taking place. In all the above graphs, the magnetisation converges to 0 after a large
number of sweeps.
```

2.6.2: Magnetic Susceptibility



2.6.3: Specific Heat




```
Due to the lack of phase transition in this case, the graphs for magnetic susceptibility and specific heat look completely
different.

For the magnetic susceptibility, there is a clear peak with an almost immediate drop near the critical temperature. The
magnetic susceptibility slowly decreases as the temperature increases above the critical temperature. "Critical
temperature" here refers to the temperature at which a phase transition would occur for the periodic boundary conditions.

The specific heat graph follows no real discernible pattern. It does not have any clear peak or trough. At first, it seems
to increase as the temperature increases above the critical temperature but the furthest right data point seems to show
that this trend will not hold.
```

Section 3: General Conclusions

For the boundary conditions which involved fixing some of the spins as either spin up or spin down, a clear pattern emerges. Fixing the spins as spin up has essentially no effect on the system because the standard phase transition (where all the spins are aligned spin up) can still take place.

However, fixing spins as spin down has a significant impact on the behaviour of the system and leads to "unstable" or "reversed" phase transitions as described above. This is because the presence of negative spins makes the usual phase transition impossible so the system starts to behave in a very different manner.

Overall, it seems that fixing the alignment of certain spins had very little effect on the magnetic susceptibility or specific heat except for moving the peak of the specific heat graph.

For the last two sets of boundary conditions, no spins were fixed but the outer edge spins interacted differently to the rest of the lattice. In the ferromagnetic case, this made no difference but the anti-ferromagnetic case had a huge impact on the magnetic susceptibility and specific heat.

This huge difference was made solely by allowing the edges to interact anti-ferromagnetically while the rest of the magnet was the same as in the periodic case. When the edges interacted ferromagnetically, this difference was not seen. This shows that the spins on the edges of the lattice are clearly the most important in determining the system's behaviour in these cases.