Computational Methods Assignment 3

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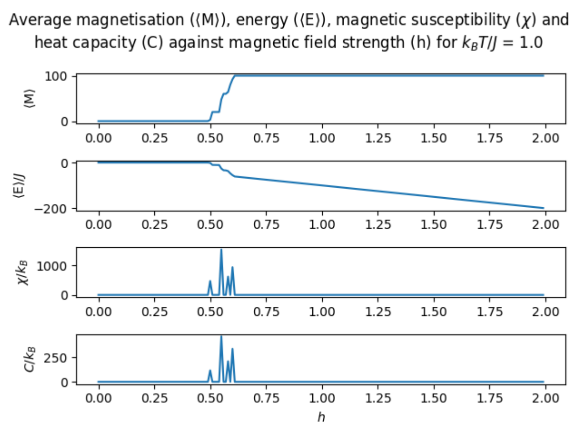
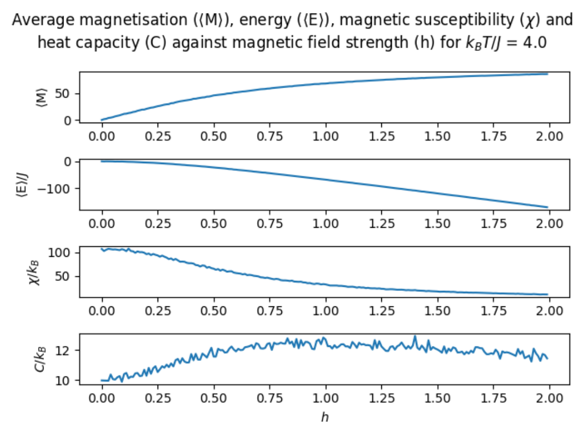
1 Varying the magnetic field

The average magnetisation, $\langle M \rangle$, average energy, $\langle E \rangle$, magnetic susceptibility, χ, and heat capacity, C, for the Ising model on a 10×10 periodic grid were calculated for a range of magnetic field strengths (h) by a metropolis algorithm for two temperatures, $k_B T/J = 1.0$ and $k_B T/J = 4.0$. This was repeated for ten random initial states and the average was taken.

The plots are shown in figures 1a and 1b respectively below. The same random starting state is used for each loop over the h values.



(a) $\langle M \rangle$, $\langle E \rangle$, χ, and C against h for $k_B T/J = 1.0$.



(b) $\langle M \rangle$, $\langle E \rangle$, χ, and C against h for $k_B T/J = 4.0$.

Figure 1: $\langle M \rangle$, $\langle E \rangle$, χ, and C against h for two different temperatures.

It can be seen in figure 1a that for $k_B T/J = 1.0$ C and χ are only non-zero when $\langle M \rangle$ changes, at which point their values spike upwards. $\langle E \rangle$ changes with h once it passes the threshold at which $\langle M \rangle$ is non-zero, and when $\langle M \rangle$ changes suddenly so too does $\langle E \rangle$.

Figure 1b shows that $\langle M \rangle$ increases steadily with h for $k_B T/J = 4.0$. At the same time $\langle E \rangle$ decreases steadily as h increases.

The graphs behave very differently for the two different values of $k_B T/J$. This suggests that they are observations of the behaviour of the system in both the ferromagnetic and paramagnetic phases i.e. below (figure 1a) and above (figure 1b) its critical temperature. As such the critical temperature likely lies between $k_B T/J = 1.0$ and $k_B T/J = 4.0$

2 Varying the temperature

The average magnetisation, $\langle M \rangle$, energy, $\langle E \rangle$, magnetic susceptibility, χ, and heat capacity, C, for the Ising model on a 10×10 periodic grid were calculated for a constant magnetic field $h = 0$ and the temperature was varied, from $k_B T/J = 0.01$ to $k_B T/J = 4.0$. The graphs are shown in figure 2.

As can be seen in figure 2 the magnetisation of the system remains mostly consistently at its most negative until the critical temperature T_C, which is found to be approximately $T_C = 2.00\ J/k_B$ where its absolute magnitude decreases and it begins to fluctuate around 0. At higher temperatures it fluctuates around zero with low magnitude.

Appendix A shows other graphs generated for this exercise. Before T_C some graphs, such as figure 12a show positive $\langle M \rangle$ while others, such as figures 2 and 12e show negative $\langle M \rangle$.

This again shows the ferromagnetic and paramagnetic behaviour of the system at different temperatures below and above the critical temperature respectively.

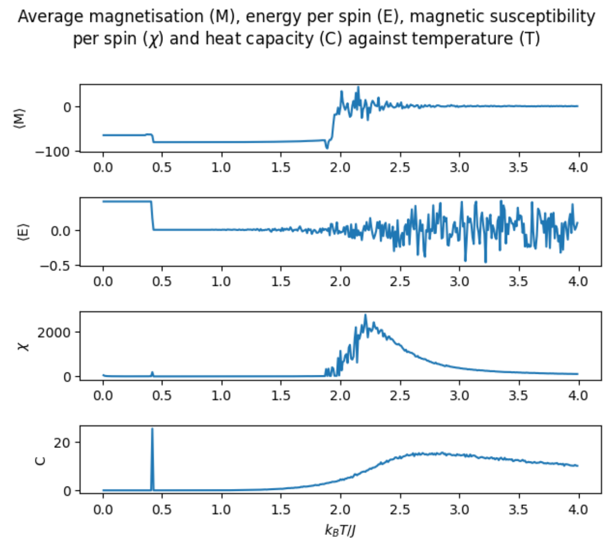


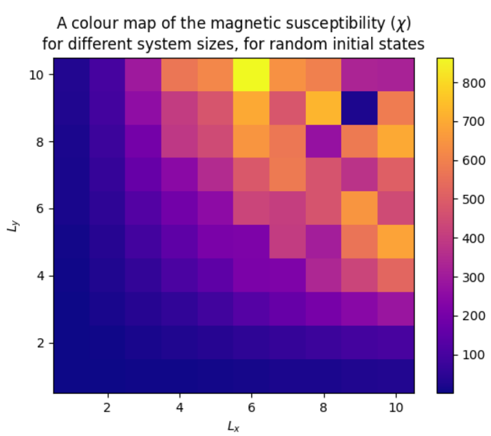
Figure 2: $\langle M \rangle$, $\langle E \rangle$, χ, and C against $k_B T/J$ for $h = 0.0$

3 Varying the system size

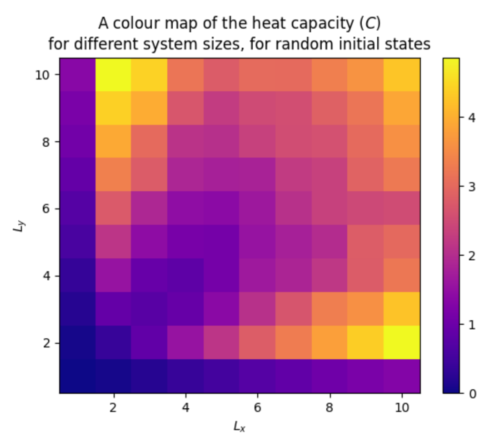
The magnetic susceptibility and heat capacity of the system at T_C and for $h = 0$ were found for different rectangular system dimensions, from a 1×1 grid to a 10×10 grid, by varying the x and y lengths, L_x and L_y respectively.

This was done for a variety of different initial conditions, each one being repeated 10 times and the average being taken.

The initial conditions investigated were: random initial state (figure 3), an initial grid of all 1s (figure 4), an initial grid of all -1s (figure 5), alternating rows of 1s and -1s (figure 6) and a "checkerboard" of alternating 1s and -1s (figure 7).



(a) χ for a random initial grid of -1s and 1s.



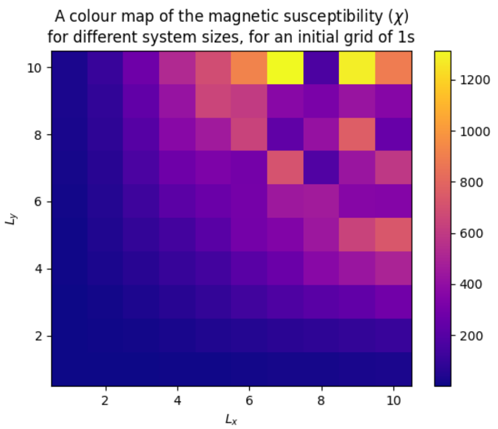
(b) C for a random initial grid of -1s and 1s.

Figure 3: The magnetic susceptibility (χ) and heat capacity (C) for a random initial grid of -1s and 1s.

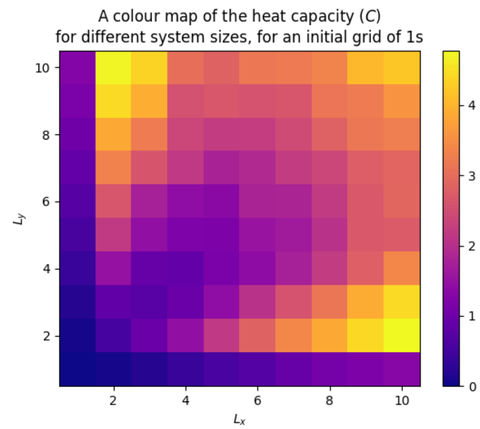
The information is displayed in a series of colour maps in figures 3 to 7.

As can be seen in all figures there is a general trend whereby χ tends to increase with increasing system size. Of course this program relies heavily on randomness in all cases, so the increasing trend is not uniform and is often violated, but it is generally true.

The case of C is more interesting. As with χ it tends to increase with increasing system size. However it is also higher for systems with large differences in sizes between dimensions. For example in figure 3b the

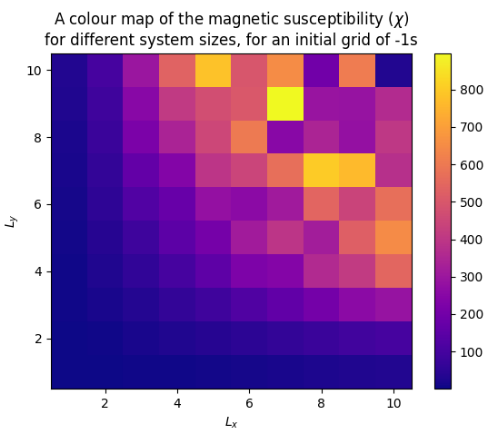


(a) χ for an initial grid of 1s.

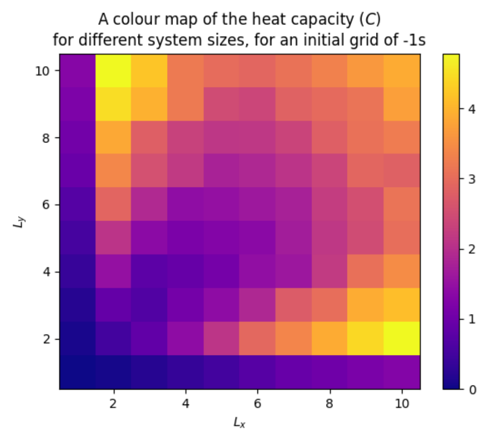


(b) C for an initial grid of 1s.

Figure 4: The magnetic susceptibility (χ) and heat capacity (C) for an initial grid of 1s.



(a) χ for an initial grid of -1s.



(b) C for an initial grid of -1s.

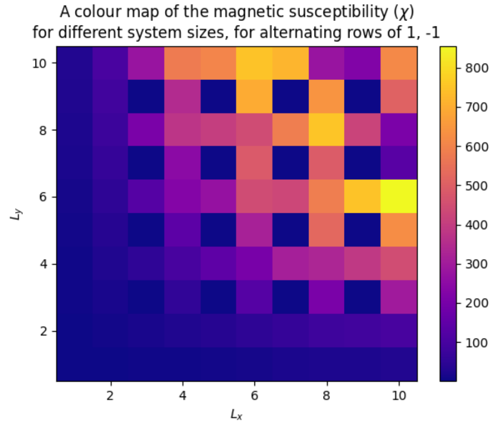
Figure 5: The magnetic susceptibility (χ) and heat capacity (C) for an initial grid of -1s.

two points with the highest values of C are $(2, 10)$ and $(10, 2)$ - this holds for all initial conditions.

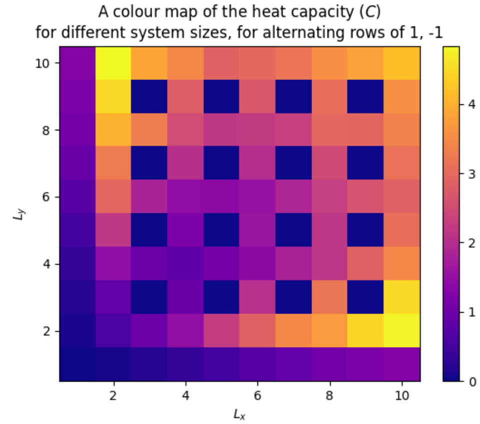
As seen in figures 3, 4 and 5, after the metropolis algorithm is carried out the systems which start off randomly, with all 1s or with all -1s appear to behave approximately the same.

The cases of initial states of alternating rows or points behave similarly to one another. In general χ and C are much lower than is to be expected based on the previous starting conditions and the surrounding system sizes when both L_x and L_y are equal to an odd number, as can be seen in figures 6 and 7.

The one-dimensional systems are exceptions to all of these patterns, other than the fact that χ and C increase with increasing system size, and even this is notably slower than is observed in the two-dimensional systems. This is likely because the one-dimensional Ising model is paramagentic while in two dimensions it undergoes a phase transition at $T = T_C$ between the ferromagnetic and paramagnetic phases, and this system is studied at approximately the critical temperature, so it is approximately in the ferromagnetic phase.

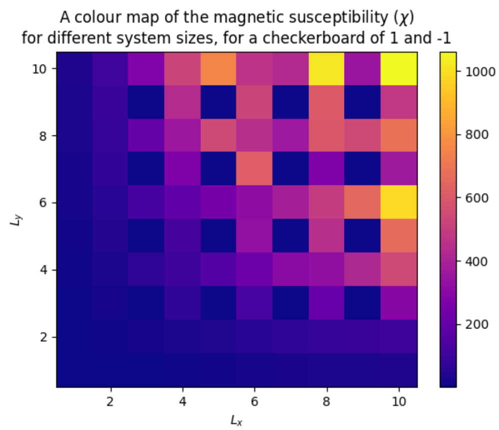


(a) χ for an initial state of alternating rows of 1s and -1s.

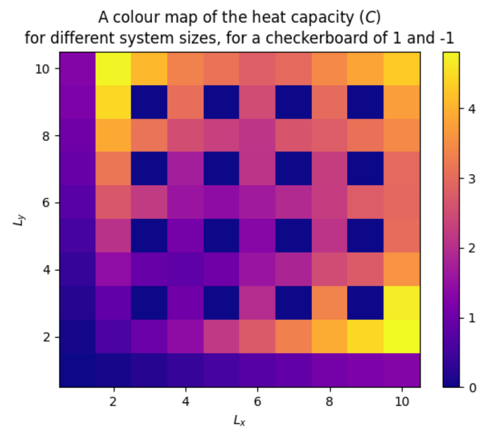


(b) C for an initial state of alternating rows of 1s and -1s.

Figure 6: The magnetic susceptibility (χ) and heat capacity (C) for an initial state of alternating rows of 1s and -1s.



(a) χ for an initial "checkerboard" of alternating 1s and -1s.



(b) C for an initial "checkerboard" of alternating 1s and -1s.

Figure 7: The magnetic susceptibility (χ) and heat capacity (C) for an initial "checkerboard" of alternating 1s and -1s.

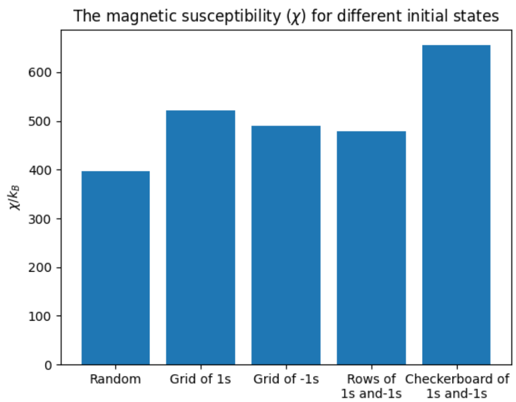
4 Varying the initial state

The magnetic susceptibility and heat capacity of the system at T_C and for $h = 0$ were found for a 10×10 grid for the list of different initial conditions investigated in 3, each one being repeated 100 times and the average being taken. The results were plotted in bar charts which are shown in figure 8

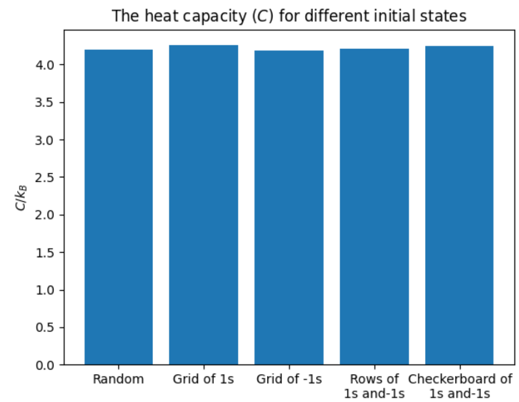
As can be seen from figure 8b at least among the chosen states for this investigation the initial state has very little effect on the value obtained for C. There is only a small variation in the value obtained for C for each initial state. This can also be observed in figures 3b, 4b, 5b, 6b and 7b. Which, apart from the "holes" in figures 6b and 7b are all largely similar, especially the value obtained for a 10×10 grid.

This is not precisely the case for χ. A random initial state appears to give a lower value of χ, while the "checkerboard" arrangement gives a higher value of χ than the uniform grids of 1s or -1s, or the alternating rows of -1s and 1s. However, if this calculation is repeated, different results are observed, see figure 9.

In the case of figure 9a the opposite relation is seen, and a random initial state appears to give a *higher*



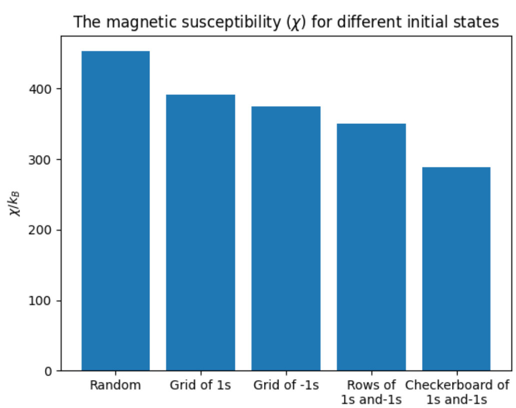
(a) A comparison of the different values of χ obtained for different starting conditions for a 10×10 grid.



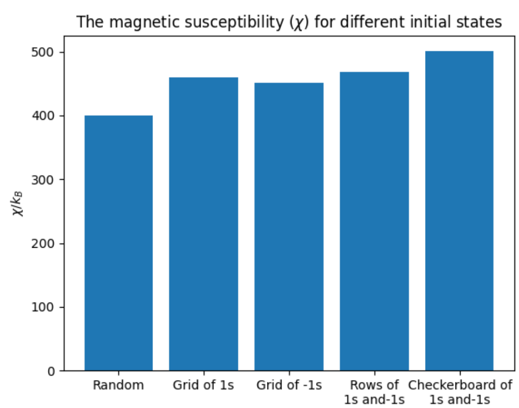
(b) A comparison of the different values of C obtained for different starting conditions for a 10×10 grid.

Figure 8: A comparison of the magnetic susceptibility (χ) and heat capacity (C) obtained for different starting conditions for a 10×10 grid.

value of χ, while the "checkerboard" arrangement gives a *lower* value of χ, while figure 9b yields the same results as in figure 8a. This all suggests that for larger sample sizes (i.e. larger numbers of repetitions) the initial state is is irrelevant (at least as long as it is one of the five chosen states in this investigation) to the average value obtained for χ.



(a) A comparison of the different values of χ obtained for different starting conditions for a 10×10 grid repeated one hundred times and averaged.



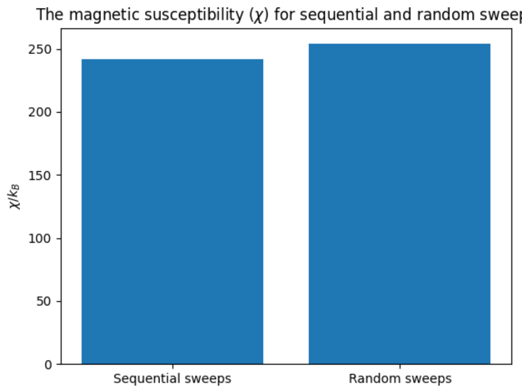
(b) A comparison of the different values of χ obtained for different starting conditions for a 10×10 grid repeated one thousand times and averaged.

Figure 9: A comparison of the magnetic susceptibility (χ) obtained for different starting conditions for a 10×10 grid, repeated a different number of times.

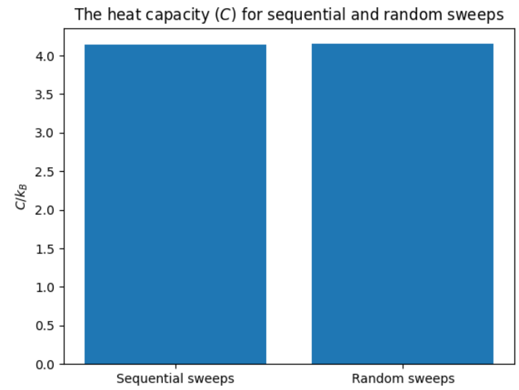
5 Varying the sweeping process

Additional methods were defined in the Ising Lattice class to sweep through the lattice sites randomly rather than sequentially as was done previously, and then carry out a metropolis algorithm in this random order.

The values of χ and C were found for both of these methods of sweeping. This was done one hundred times and the average was taken, with the results plotted on bar charts, as shown in figure 10.



(a) A comparison of the different values of χ obtained for the different sweeping methods.



(b) A comparison of the different values of C obtained for the different sweeping methods.

Figure 10: A comparison of the magnetic susceptibility (χ) and heat capacity (C) obtained for the different sweeping methods.

As is obvious from figure 10 the method of sweeping through the lattice points, sequentially or randomly is irrelevant and has no appreciable effect on the obtained value of χ or C.

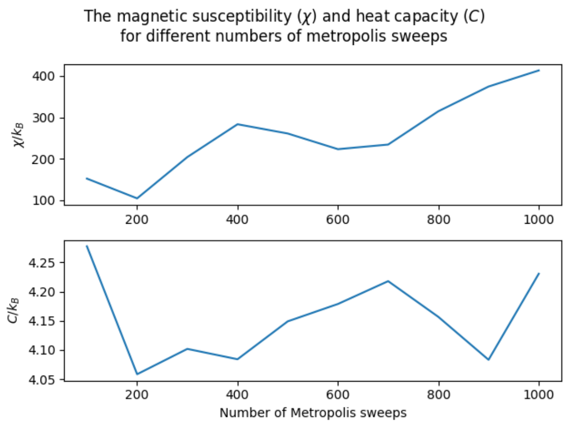
6 Varying the number of Metropolis samples

Before this all calculations were carried out with 200 initialising sweeps of the lattice and a further 1000 metropolis samples.

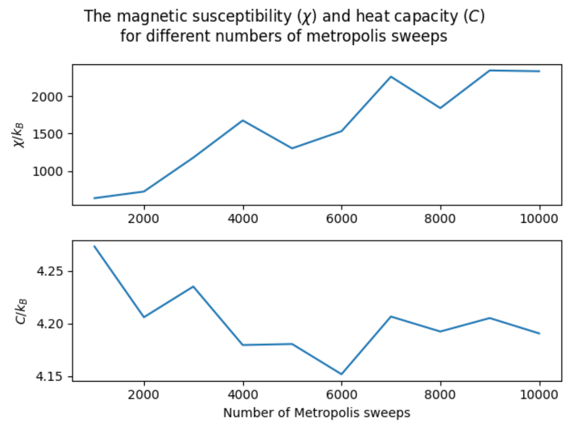
The values of χ and C were found for varying numbers of metropolis samples with random initial conditions, sequential sweeps and a 10×10 grid. This was repeated 100 times for each number of sweeps and the values were averaged to account for the random variation in the calculated values. The results are plotted below in figure 11.

For χ it appears that its value tends to increase as the number of metropolis samples increases, while it appears that the value of C tends to decrease as the number of sweeps increases. The graphs do not, of course, show strictly increasing or decreasing trends, they are both very bumpy. This is likely due to random sampling that hasn't been smoothed out, even by 100 iterations.

However I believe that if this were allowed to repeat for a significantly large number of times and the average taken what would be found is a general increase in χ and decrease in C with increasing numbers of metropolis samples.



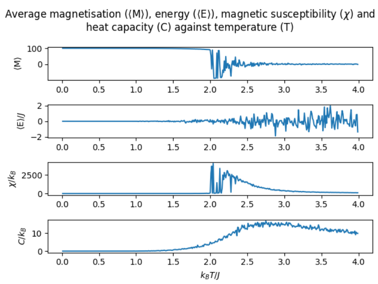
(a) The values of χ and C after a number of metropolis samples from 100 to 1000 samples, measured for every 100 samples.



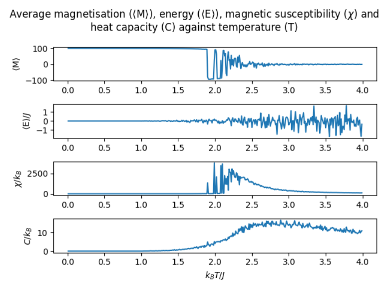
(b) The values of χ and C after a number of metropolis samples from 1000 to 10000 samples, measured for every 1000 samples.

Figure 11: The values of χ and C after a number of metropolis samples measured at two different precisions.

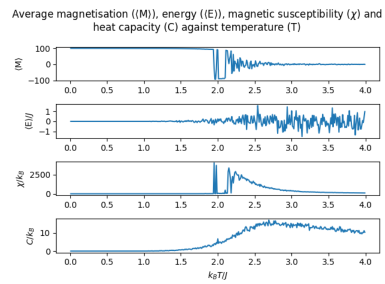
A Extra graphs of varied temperature



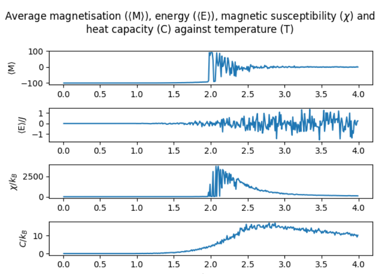
(a)



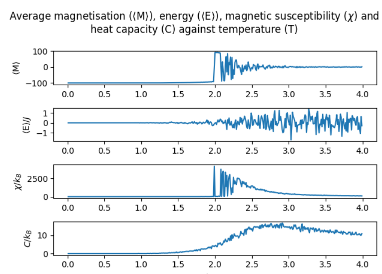
(b)



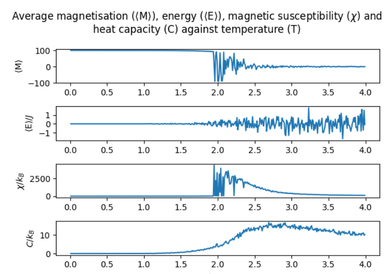
(c)



(d)



(e)



(f)

Figure 12: A collection of graphs showing $\langle M \rangle$, $\langle E \rangle$, χ, and C against $k_B T/J$ for $h = 0.0$