Problem: 1

Plot $\langle M \rangle$ vs T for and compare with the results from the text and lecture.

Below are the images from lecture and the text, respectively:

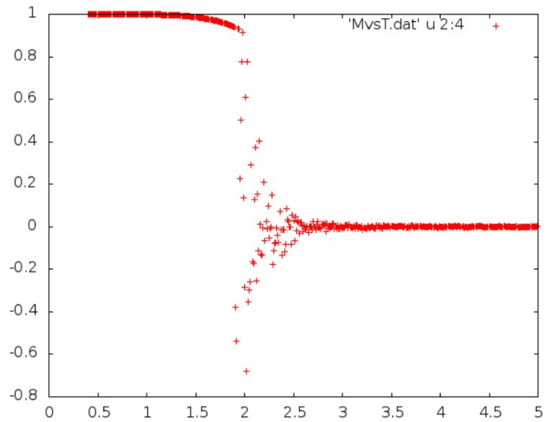

Figure 1: The plot from lecture

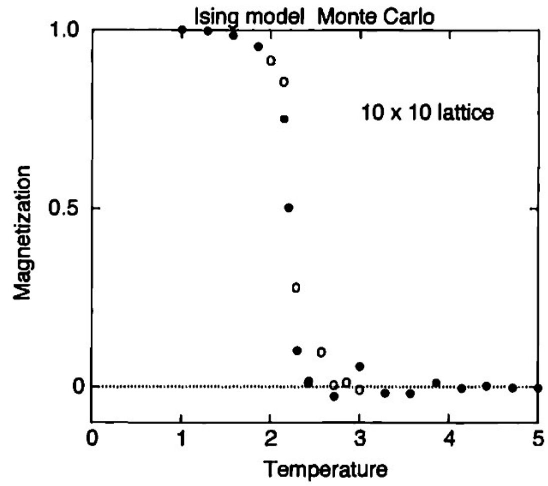

Figure 2: The plot from the text

Below are the images that I was able to produce (both coarse and fine):

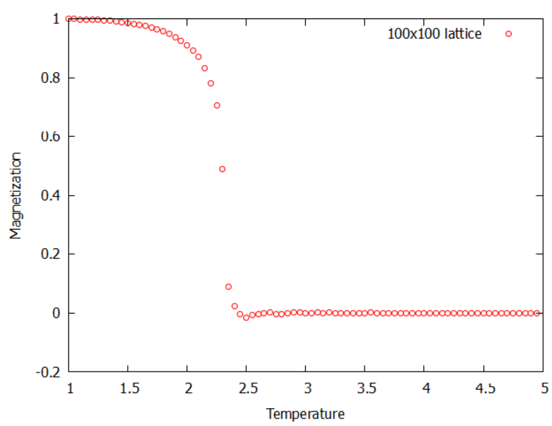

Figure 3: The coarse plot

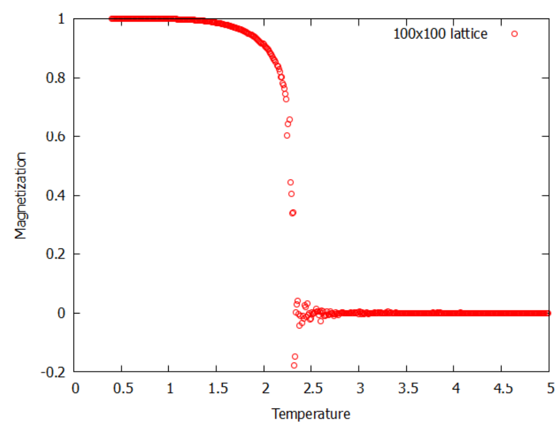

Figure 4: The fine plot

From my plots, we can see that the magnetization stays around 1 at lower temperatures (e.g., $T < 1$) and 0 around higher temperatures (e.g., $T > 2.5$). As the temperature approaches ≈ 2.27, we can see that the magnetization drops very steeply and the plot resembles very closely to that of a waterfall. I.e., near the critical temperature T_C, we have very large fluctuations with the magnetization. This makes sense to see as the text notes that a system at its critical point is extremely sensitive to small perturbations; thus, we should expect to see large fluctuations around T_C.

Furthermore, we see that the fluctuations around T_C in the plot given in lecture are much larger than what we observed, and our plot resembled the one given in the text much more closely. I think that this is most likely due to the fact that I reduced the number of Monte Carlo steps (I brought it all the way down to 2000 to save time, which is much closer to the 1000 that the text used), which essentially means that the system had less time to evolve.

Problem: 2

Plot $\langle E \rangle / N$ vs T. Compare and discuss the results for the high and low temperature regimes.

Below shows the plot that I was able to produce:

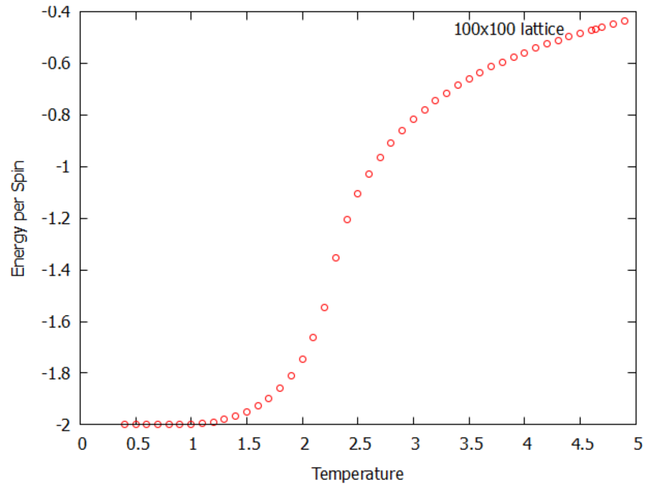

Figure 5: My plot for $\langle E \rangle / N$ vs T

From this plot, we can see that the energy per spin at low temperatures is essentially -2. We expect this to be the case since the energy function of our system is given as follows (assuming no external magnetization – i.e., $H = 0$):

$$E = -J \sum_{\langle ij \rangle} s_i s_j$$

where the sum is over all pairs of nearest neighbor spin $\langle ij \rangle$, and J is the exchange constant that we are assuming to be positive. At lower temperatures, we expect these spins to mostly stay in the same direction. Since we take each spin to have a magnitude of 1, we find that each particle has an energy contribution of 4 (one for each of its nearest neighbor), which results in the sum to be the following:

$$T \text{ low} \implies E = -J \sum_{\langle ij \rangle} s_i s_j = -J \frac{4N}{2}$$

Note that we included the fact of 2 since we would be double counting the energy contributions otherwise. Taking $J = 1$, results in the energy per spin to be -2.

Once the temperature starts increasing, we expect the energy to increase, which is what we do end up seeing in the plot. Notice that we see the most rapid increase in energy per spin near the critical temperature, and we continue to see that energy increases (although at a lower rate) as temperature further increases. As noted in lecture, the energy does not tend to 0 as T increases to larger values, meaning that relative spin order must not be random.

Problem: 3

Determine T_C from the specific heat per spin, C/N. Do this for lattice sizes of 20×20, 50×50, 100×100, and combine the results in a single plot. Comment on how the T_C values you obtain compare.

Below shows the plot that I was able to produce:

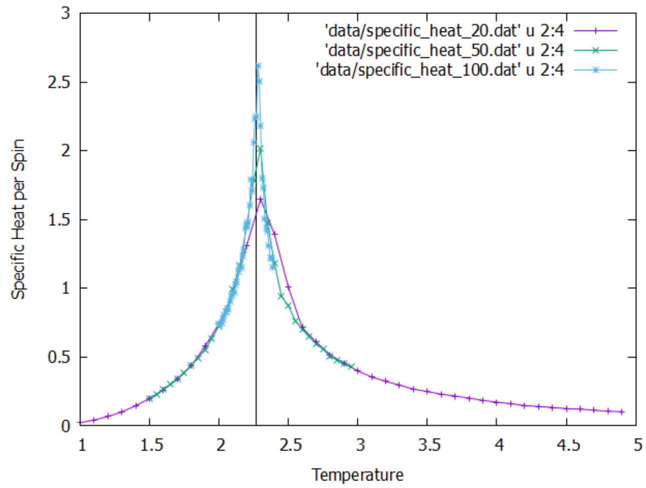

Figure 6: My plot for C/N vs T with a vertical line around T_C

From the plot above, we can see that

$$20 \times 20 : T_C \approx 2.30 \qquad 50 \times 50 : T_C \approx 2.29 \qquad 100 \times 100 : T_C \approx 2.27$$

Notice that as the lattice size increases, we have the peak to both be closer to T_C as well as larger and sharper. We expect this to be the case since the peak in C/N becomes sharper as lattice size increases – in fact, $C_{\text{max}}/N \sim \log(L)$ as noted in lecture. If we were to continue with larger lattice sizes, then we should expect the peak to be almost asymptotic.

Problem: 4

Plot the "reduced" correlation function, $f(i) - \langle s \rangle^2$, at $0.5 \times T_C$, $0.95 \times T_C$, and $2 \times T_C$. Determine the corresponding correlation lengths.

Below are the plot and fitted plot:

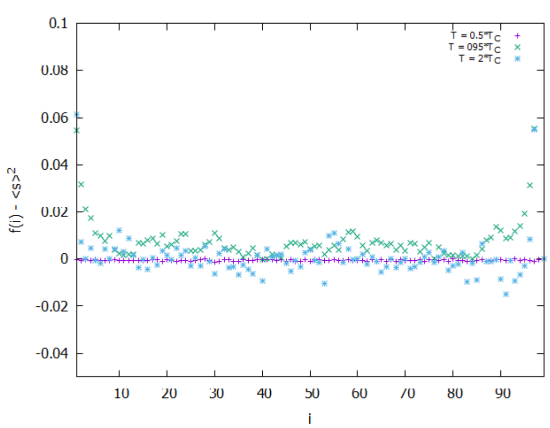

Figure 7: The plot of the "reduced" correlation function

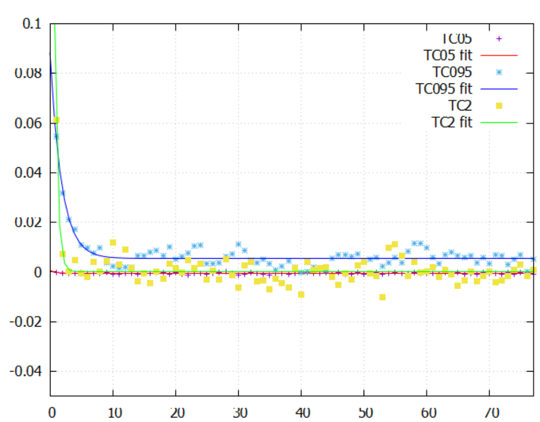

Figure 8: The fitted plot

As for the fitted values, I got:

$$
\begin{aligned}
0.5 \times T_C &: \xi \approx 0.99533 \pm 7232.49268 \\
0.95 \times T_C &: \xi \approx 1.84513 \pm 94.85100 \\
2 \times T_C &: \xi \approx 0.46289 \pm 42.46746
\end{aligned}
$$

For the full logs on these fits, they can be found under the log folder.

I should note that the fitted values have *very* large uncertainties, so we should take these values with a grain of salt (also, the chi-square values for these fits were *very* small – around the order of 10^{-6}). For how I could have made the fitting better, I think that including weights to these data point (which is very doable since we are doing many sweeps) would result in a fit that has a lower uncertainty; for this fit, I took the weights to be 0.5 for all the points (similar to what was done for the weighted vs. non-weighted exponential fits back in lecture 12). If given more time, I think that I could have implemented this into the fit.

However, we see the general relationship between these values to be expected; as we approach T_C, we should expect ξ to get larger and larger (eventually tending to ∞ as $T \to T_C$). Indeed, we do see this occurring as ξ is largest at $0.95 \times T_C$ when compared to the other two correlation lengths. Furthermore, we see that the correlation length does seem to be decreasing with increasing T, which is what we expected.

As for the correlation length at $0.5 \times T_C$ (and its absurdly high uncertainty), I think that the value should be more close to 0 than what is found through the fit. This is because $e^{-r_i/\xi} \approx 0$ for very small ξ, which is the trend that we see in the plot. Furthermore, we know from lecture that the range and magnitude of the correlation length is small at low T, which makes the argument for ξ being closer to 0 more likely.

One final notable trend we see from the plot is that for temperatures near T_C, we see that we start with a positive correlation that eventually becomes a negative correlation.

Problem: 5

Produce several snapshots of the spin structure at $0.95 \times T_C$. Relate these observations to the correlation lengths you previously obtained.

Below are some snapshots of the spin structure at $0.95 \times T_C$:

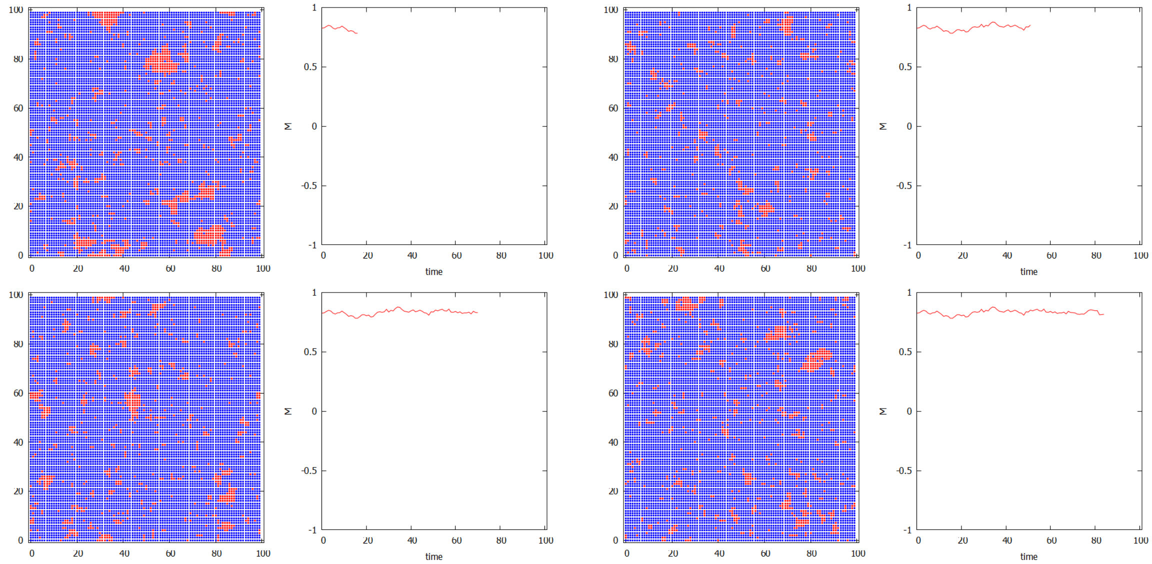

Figure 9: Some snapshots of the spin structure at $0.95 \times T_C$

A gif can be found under the img folder.

From these snapshots, we see that there are clusters forming, which is a result of the spins being correlated to each other. Thus, the higher the correlation length we obtain, the larger we expect these clusters to be. Since $0.95 \times T_C$ is near the critical temperature, we should expect clusters to form, which is indeed what we see.

However, the correlation length that we found seems to be too small compared to the size of the clusters that are shown in the snapshots above; I think that we should instead expect a correlation length of around 10 based off the size of the clusters. The difference in the expected correlation length with the fitted correlation length is not a major concern for me since the fitted values have such a high uncertainty attached to them. If I were to refine the fitting some more (e.g., include weights to the data points, and maybe increase the number of sweeps), then I believe that we would see a more accurate value for the correlation length.

Remark: On How I Implemented magnetism.c

I have implemented the energyFunction function to return the corresponding energy value for a certain spin; this means that I kept the spin as-is (that is, I did not flip the spin as shown in lecture), and I did not return twice the energy value. As for how the energy of a particular spin is calculated, it is using the following:

$$E_i = -J(s_i s_{\text{left}} + s_i s_{\text{right}} + s_i s_{\text{above}} + s_i s_{\text{below}}) - \mu H s_i$$

It is in the boltzmannFlip function that I introduced the factor of -2.0 attached to the energyFunction; this factor of -2.0 is what will give ΔE_{flip}. With this, the implementation of the boltzmannFlip is exactly the same as provided in lecture as well as the text.

As for the getEnergyPerSpin and getEnergySquaredPerSpin functions, I instead opted to make these into getEnergy and getEnergySquared functions, which will return the total energy and total energy squared for the system, respectively. My reasoning for doing so was that it made it easier to implement problems 2 and 3 of this assignment as it made it easier to keep track of the factors of 2 as well as the scaling factors (i.e., dividing/multiplying by the lattice size). This meant that I had to slightly change the main files provided in lecture to accommodate for these changes.

Lastly, the getMagnetization was implemented using the fact that

$$M_\alpha = \sum_i s_i$$

which is the magnetic moment for a given microstate. To find the magnetization, we need to take the sum over the magnetic moment for a microstate multiplied by the probability of such a microstate to occur; this is where the many sweeps for our Monte Carlo simulation comes into play. The getCorrelationInfo function was implemented using what was given in lecture.