PHY407: Lab 11

Date: December 3rd. 2021

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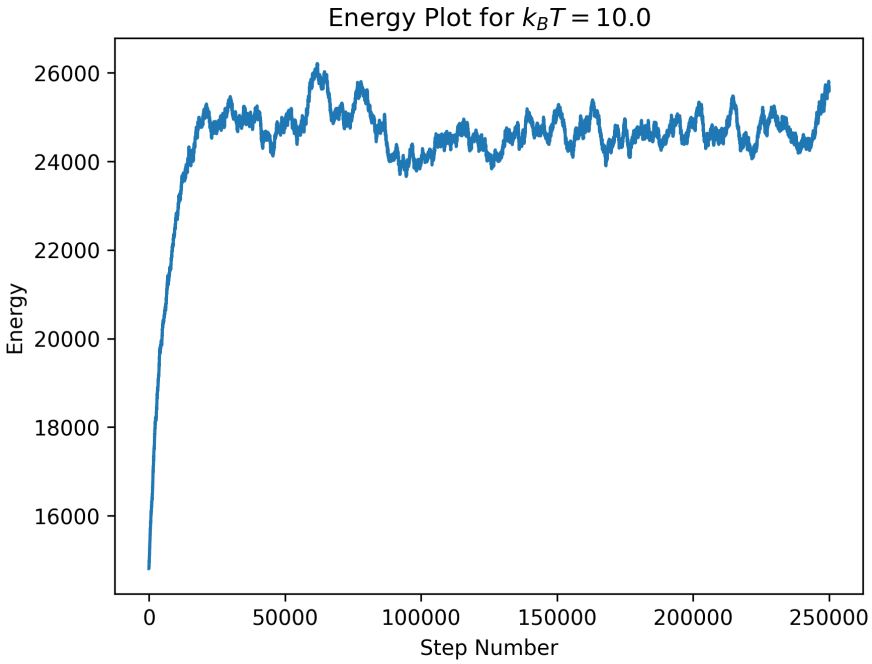
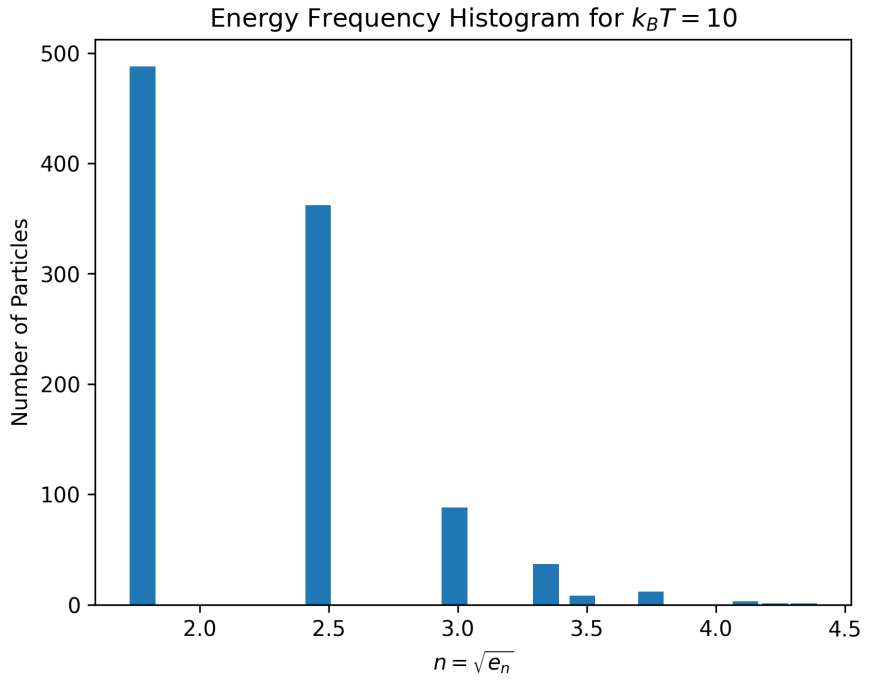
Contributions:

- Q1. and Q4. - Brendan
- Q2. and Q3. - Nikolaos

Q1.a.

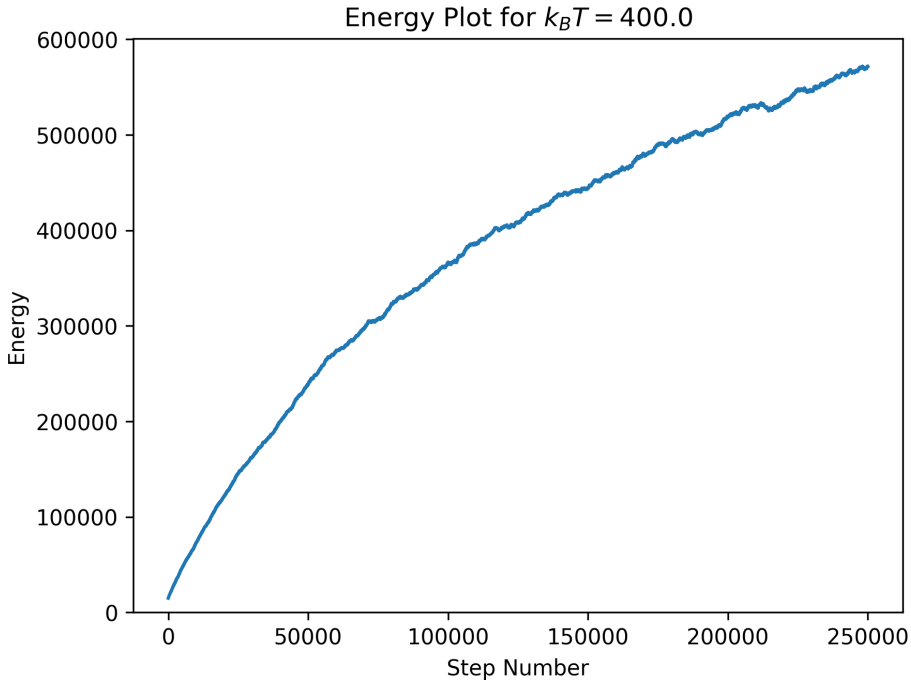
The following are the plots for total energy of the gas and the associated energy frequency distribution.



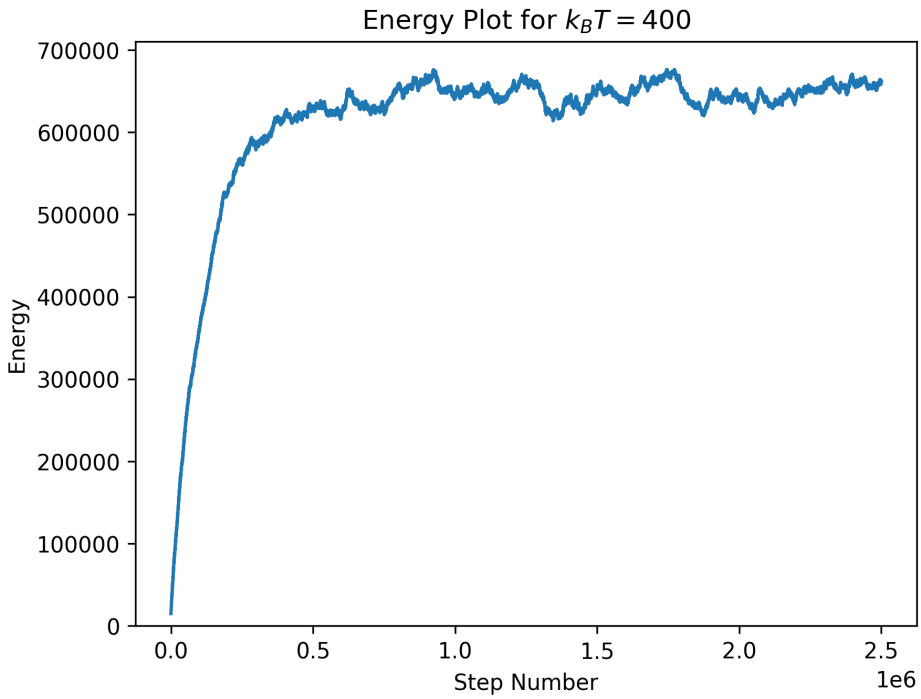


Q1.b.

The plots for energy as a function of step size were plotted each for each value of k_BT at constant step size 250000. As k_BT increased, the energy plots took longer to plateau and hence to reach equilibrium. Specifically, for $k_BT = 400$, 1200, I used 2500000 steps and for $k_BT = 1600$ I used 2750000. The graph below is for $k_BT = 400$ for 250000 steps, an instance where equilibrium was not reached.

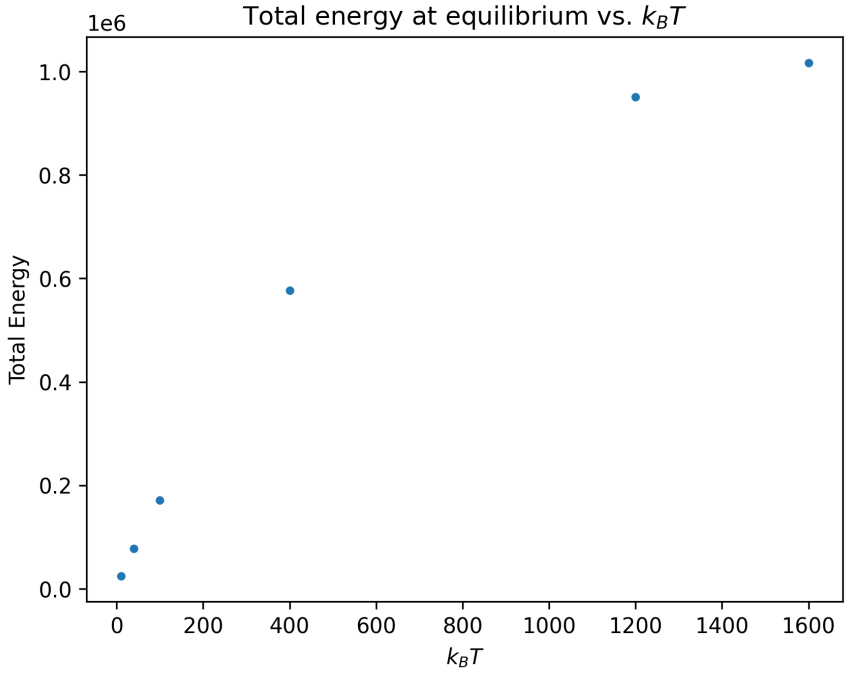


Increasing the step size to 2500000 gives the following graph:

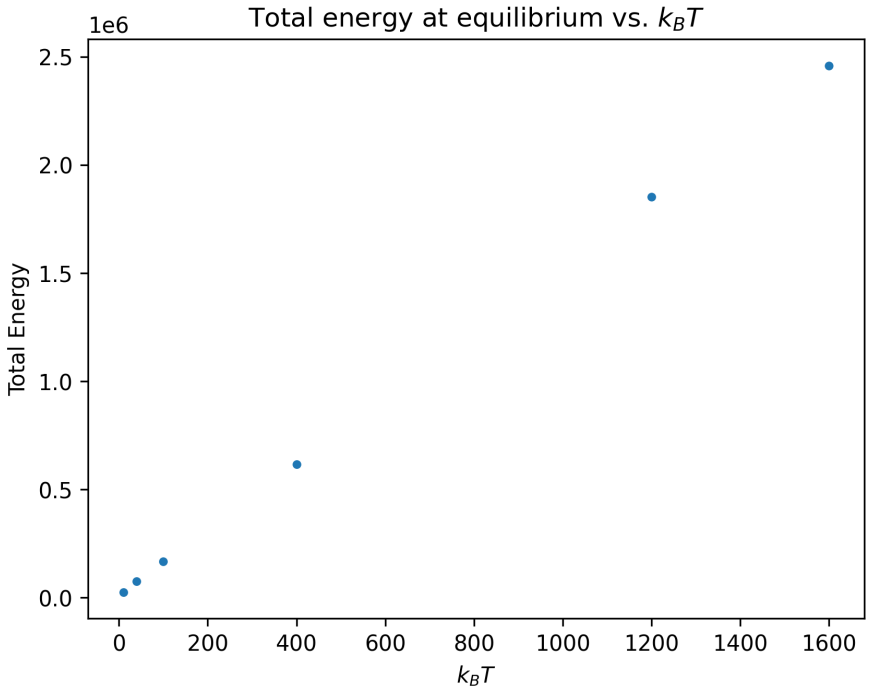


Here, it is clear that equilibrium has been reached.

If step size was left at 250000 for each case, and the "equilibrium" energy was taken to be the last value of total energy attained, then the energy temperature plot would look like this:

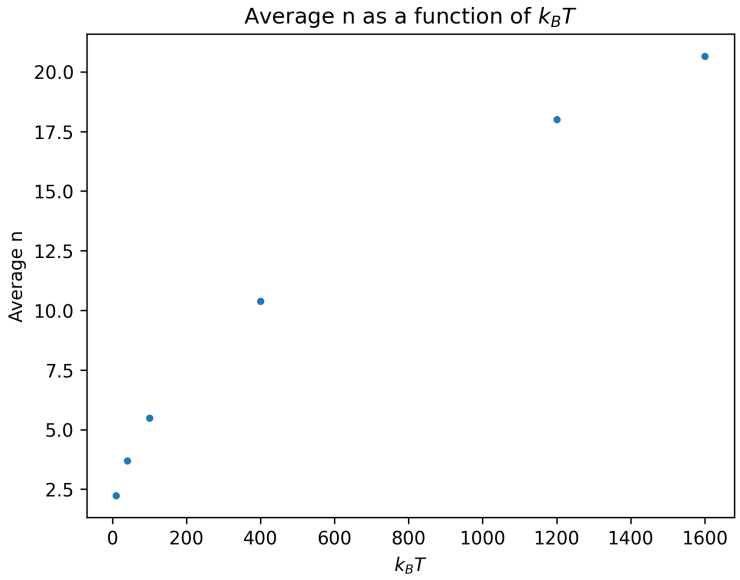


The above graph appears to be proportional to the square root of k_BT. If we increase the step size as mentioned earlier, we get the following graph:



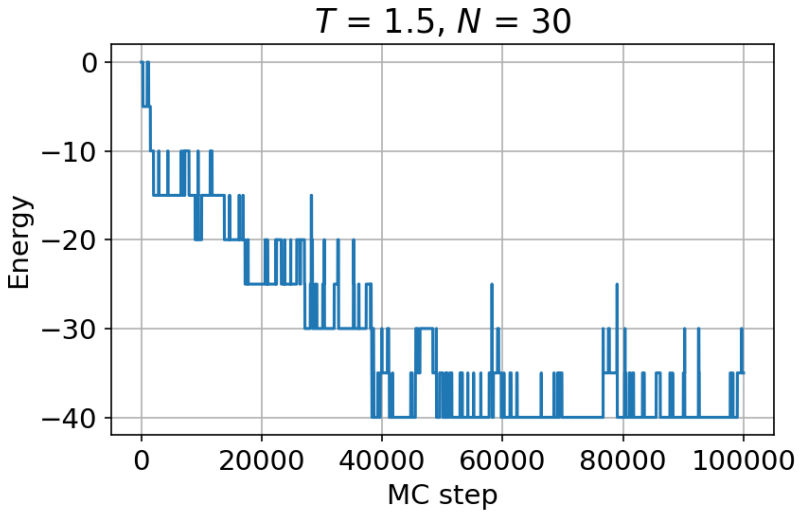
Which appears linear and we can use linear regression to find the value of the slope $\Delta E/\Delta T$. However a rough eyeball estimate of the slope gives an approximate value of the heat capacity to be $\Delta E/\Delta k_B T = 1562$ with $k_B = 1$.

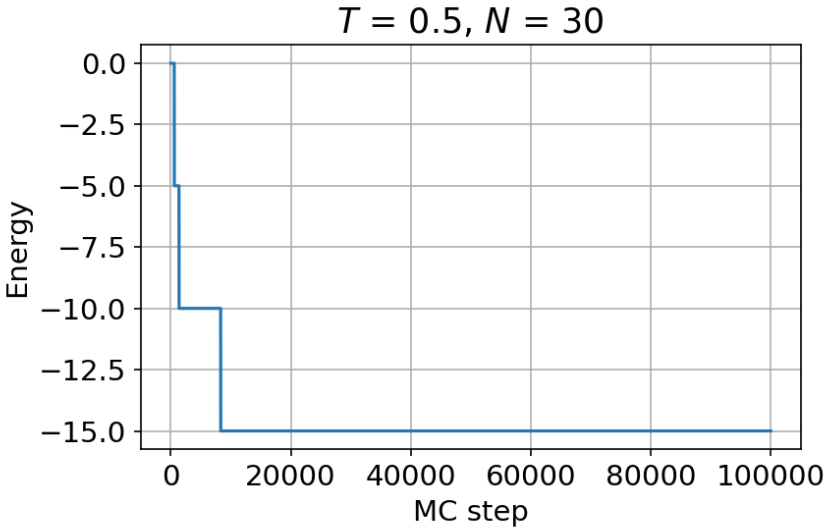
Below is the plot for the average value of n:

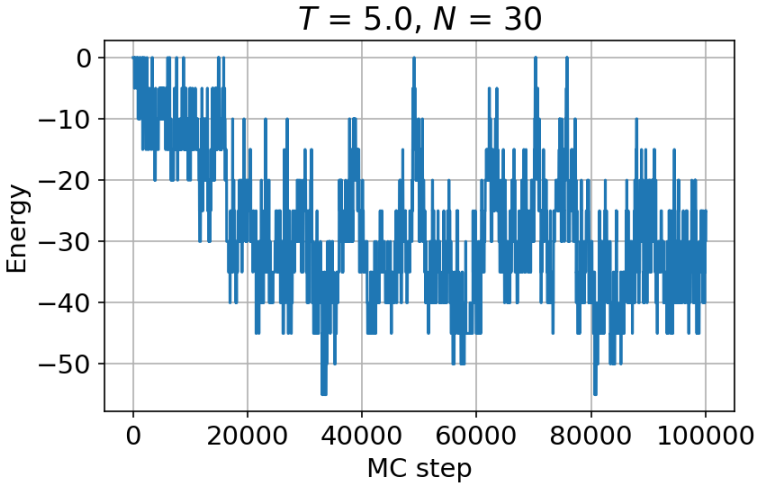


Q2.a.

Running the provided script and plotting the energy as a function of the Monte Carlo step, we get the following 3 plots, corresponding to 3 temperatures of T = 1.5, T = 0.5, T = 5.


$T = 1.5, N = 30$
0
−10
−20
−30
−40
Energy
0
20000
40000
60000
80000
100000
MC step


$T = 0.5, N = 30$
0.0
−2.5
−5.0
−7.5
−10.0
−12.5
−15.0
Energy
0
20000
40000
60000
80000
100000
MC step



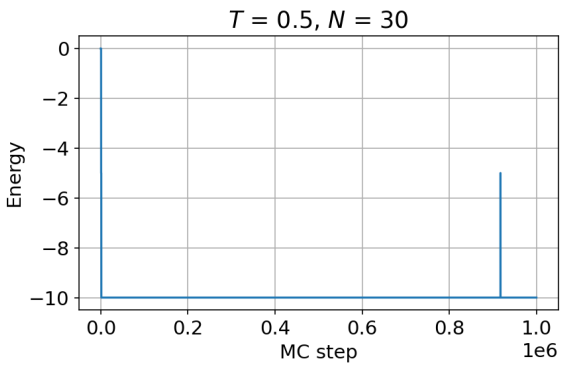
In the first (base) case, we observe an overall decreasing pattern in the energy throughout the Monte Carlo process. It seems that as the steps increases, the energy values fluctuate up and down. For large step values, the energy seems to tend closer to the -35 range.

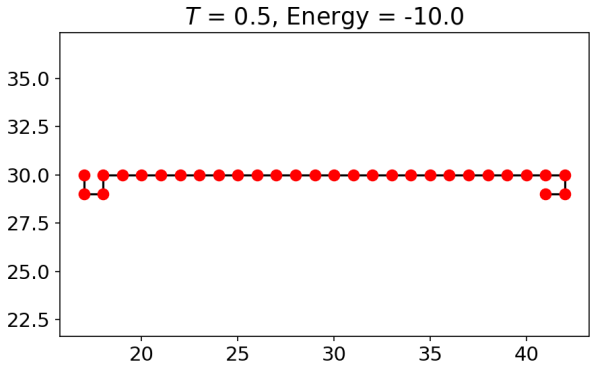
In the case where T = 0.5, we notice a very dramatic and fast reduction of the energy, and it seems that the simulation results in a constant -15 value for the energy for the majority of the steps.

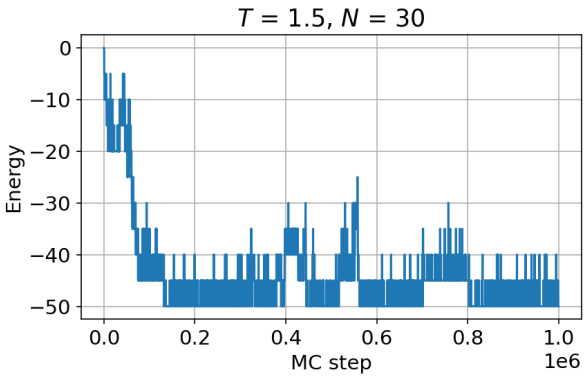
In the case where T = 5, we notice that the energy initially decreases and then fluctuates almost sinusoidally around the -30 mark for the remainder of the steps (MC > 20000).

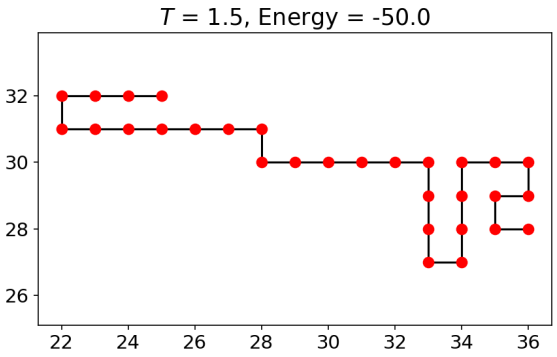
Q2.b.

Running the simulation for n = 1.e6 steps, we provide the energy, as well as the final structure of the protein plots, for T = 0.5, T = 5.









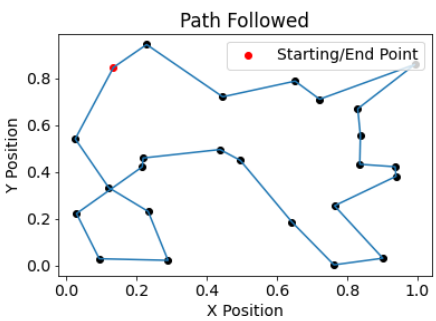
Looking at the energy plots for these two cases, we notice that during the second half of the simulation, the energy is typically lower for the T = 1.5 case. This is something we expect, as the system starts with higher T, it will go through a larger amount of processes than the one which started at T = 0.5, which is closer to the end value. Thus, in the T = 1.5 case, there is less available energy as we just take a larger picture of the behavior of the system. This causes the 2nd half of the simulation to have smaller energy values.

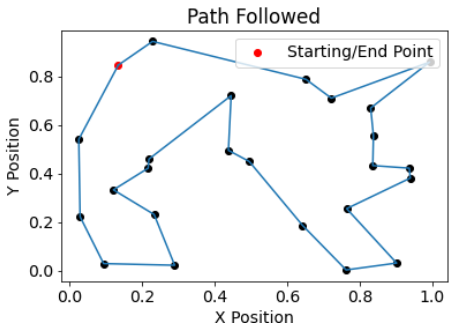
In the case where T = 0.5, we observe that the final form of the protein is almost unchanged compared to the initial condition of a simple horizontal line. The reason for this is that we start close to the T = 0 (end of simulation) value, thus the protein does not have time to change drastically compared to its initial arrangement, and thus we only observe a small folding on its edges. Significantly less dramatic than the case where T = 1.5 where the system has more time to evolve.

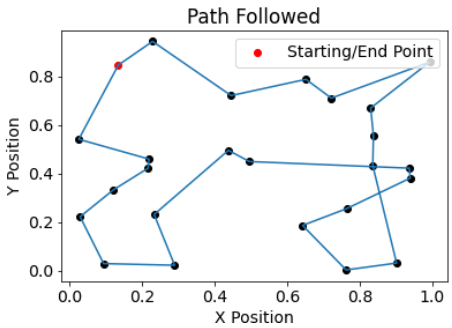
Q3.a.

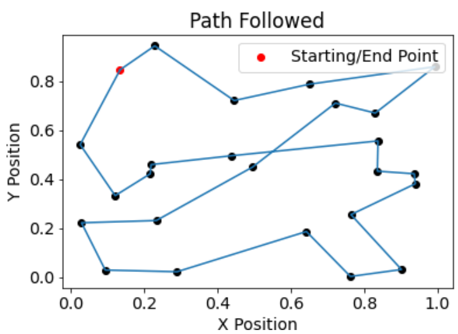
The base value for tau was 1.e4. In order to observe what effect changing the tau value has on the distance and the path taken, we plotted 3 different paths for each of the 3 different values of tau. These were: 1.e2 (smaller than baseline), and 1.e5 (larger than baseline).

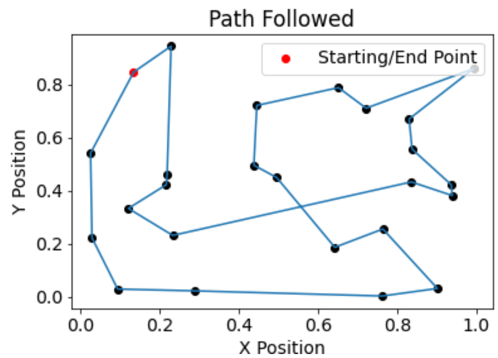
The baseline (tau = 1.e4) plot of path taken is presented below, for 5 different paths:





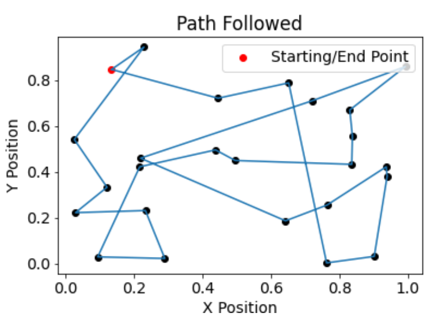


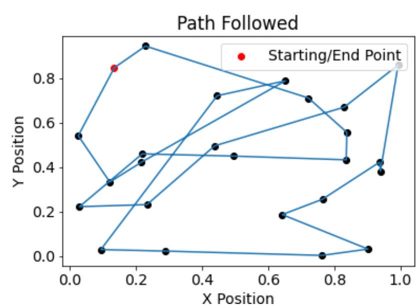


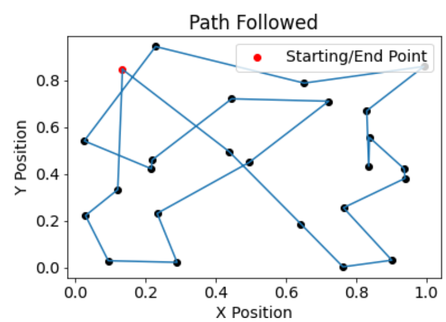


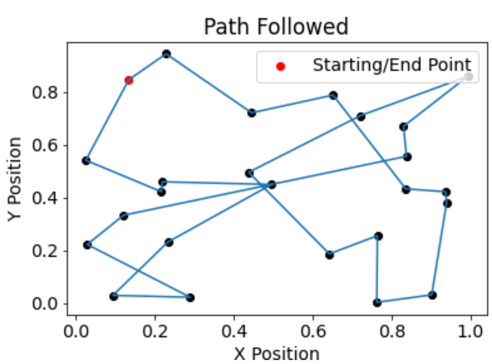
For each of these paths, the total distance traveled was determined to be around 5.2, fluctuating by approximately 0.4.

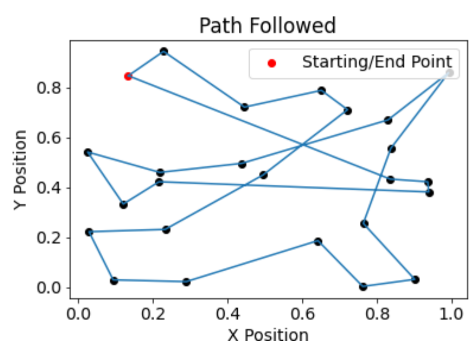
Plotting the same but with a smaller than baseline value of tau of tau = 1.e2, we get the following plots:



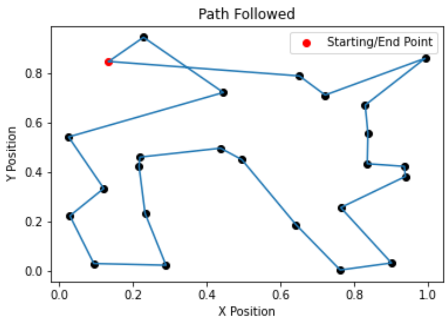


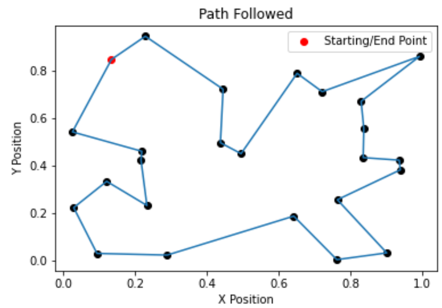


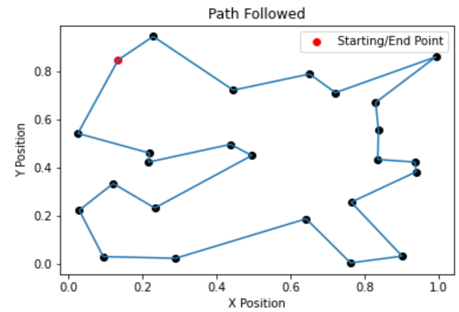


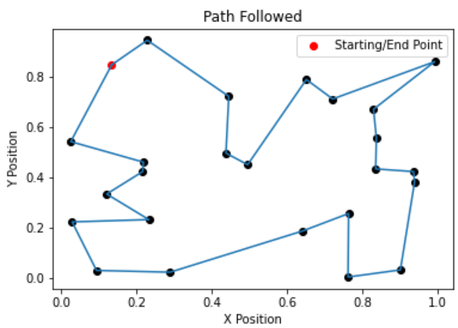


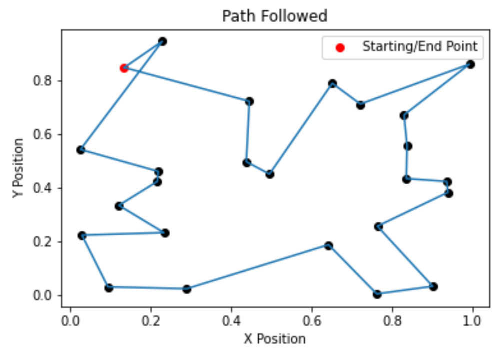
Plotting again the same but with a value of tau larger than baseline (tau = 1.e5), we get the following plots:











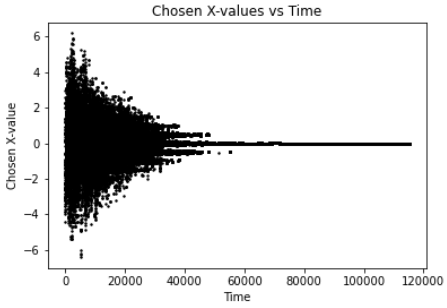
For the tau = 1.e2 case, the total travelled distance was larger than the baseline case, with a value of around 6.8, with a fluctuation of about 0.6.

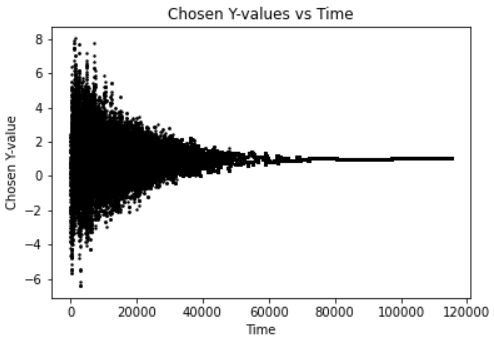
For the tau = 1.e5 case, the total traveled distance was slightly smaller than the baseline case, with a value of around 4.9, with a fluctuation of about 0.3.

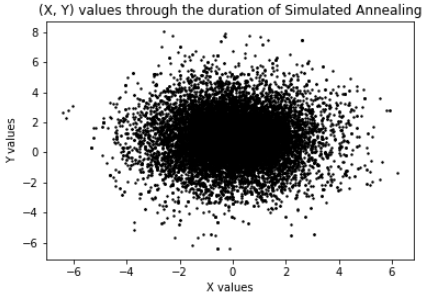
We observe that as tau increases, the total distance traveled becomes smaller, and more accurate. This makes sense, as the Annealing Optimization process yields more accurate results if we allow it to cool over a larger time period (larger tau). For the small value of tau, we observe that the system takes a much lengthier path, compared to the large value of tau, which is also consistent with the observation that total distance reduced for higher tau. In conclusion, higher tau means more accurate results.

Q3.b.i

Using an exponential cooling schedule with Tmax = 10, Tmin = 1.e-3 and tau = 1.e4, we evaluated the minimum of the given function, and constructed the plots of the x values sampled vs time of simulation, the y values sampled vs time of simulation, and the (x, y) plot of sampled values vs time of simulation. The starting x, y values were equal to 2 for both.







From the above plots, we observe that the points x, y are randomly scattered around the 0, 0 point (which we should expect from random sampling), while their individual sampling values vs time look bell shaped (which we should also expect as we random sampled from a normal distribution). It seems that for both x and y, the sampled values seem to be quite similar for large time values, and very close to the mean of 0 (while in the beginning they had higher spread).

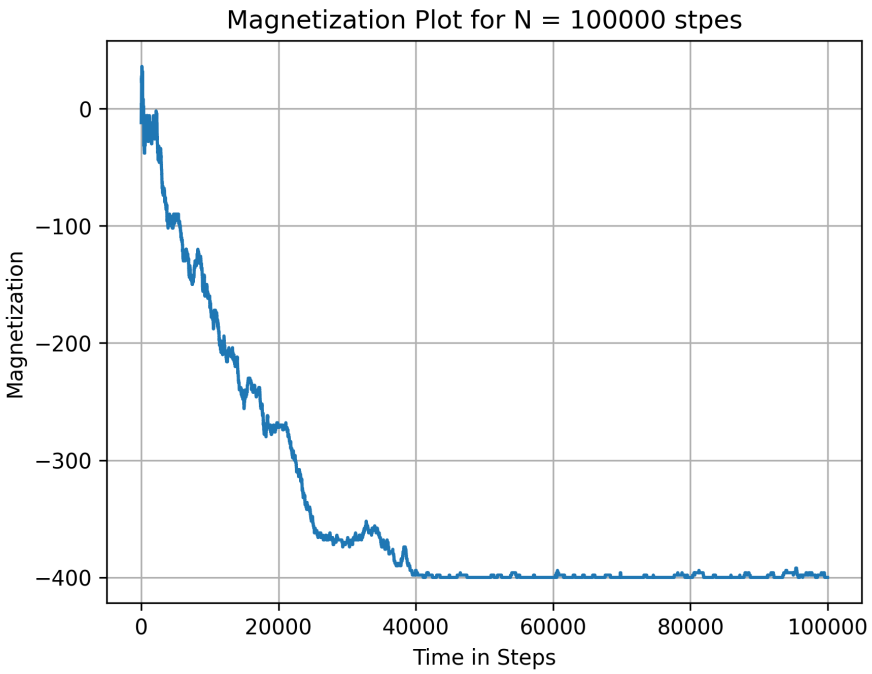
Using these x and y values and the method outlined above, we evaluated the global minimum of the given function to be approximately -0.999, which the function takes at the point (x, y) = (0.001, 1.017). Since we know the actual minimum to exist for (x, y) = (0, 1), our method's approximation was quite accurate.

Q3.b.ii.

Doing the same process for the other given function, but restricting ourselves in the range $0 < x < 50$ and $-20 < y < 20$, we evaluated the function's minimum to be approximately equal to -2.37, which the function takes at the point (x, y) = (2.16, 1.006). This is an acceptable result, as we are told that the function has competing minima, and the one we got is one of these minima. Thus, the method for this function could be more accurate (to capture the actual minimum at x = 16), but it is still reasonably accurate for estimating the location of the global minimum.

Q4.c.

Below is a plot of the magnetization for a trial:



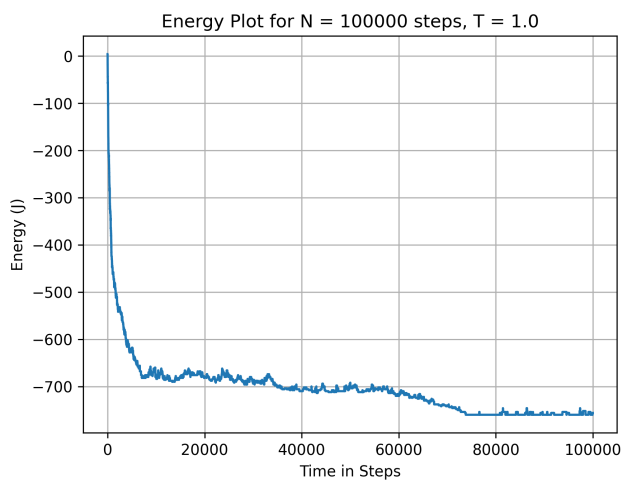
Here the system attains a spontaneous magnetization in the down direction, however magnetization in the up direction would have been equally as likely.

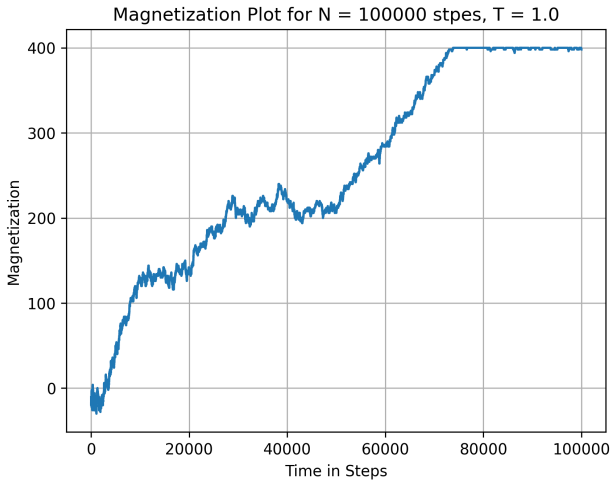
Q4.d.

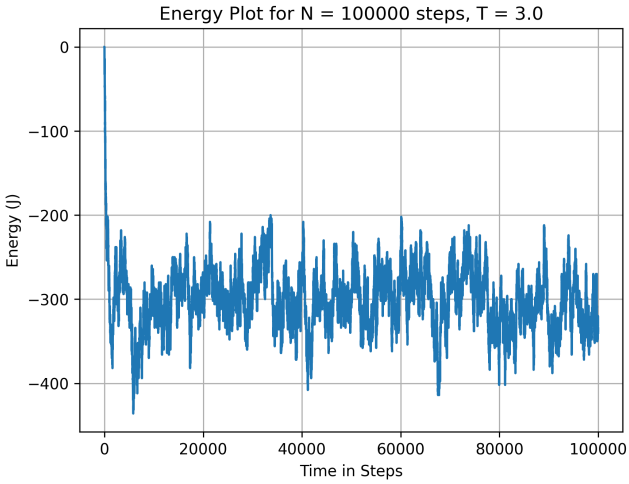
After several trials, the system's magnetization would have an equal probability of becoming spontaneously magnetized in one of the two directions. In each possible case, energy would always become negative and reach a minimum. Additionally, magnetization usually plateaued as energy plateaued dealing with a finite set.

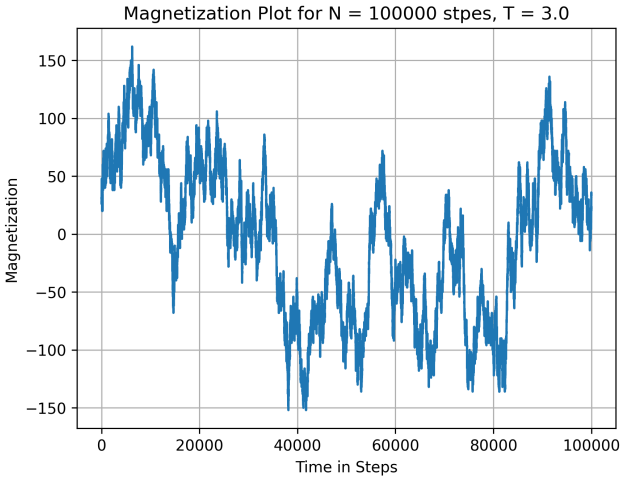
Q4.e.

As T increases the system's tendency to be uniformly magnetized in a preferential direction decreases. During the animations of increased T, the dipoles tend to flip back and forth more than with lower temperatures. This behaviour manifests itself in the energy and magnetization plots as well. For increased temperature, the total magnetization tends to oscillate more sporadically. Similarly, the energy plot tends to decrease far slower and it too oscillates more sporadically. Below is an energy and a magnetization comparison between T = 1.0 and T = 3.0:









The reason for this behaviour with increasing T is rooted in the acceptance function, specifically, in the Boltzmann distribution. In the acceptance function, the condition for accepting the new transition is if either the new energy is less than and or equal to the old, or if the new energy is greater than the old and R = random.random() is less than P = $\exp(-(E_{NEW} - E_{OLD})/k_BT)$ where R is uniformly distributed between 0 and 1. If $E_{NEW} - E_{OLD} > 0$, then increasing T will increase P since T is strictly positive. If P is larger, then it is more likely that R is less than P. This implies that the likelihood of accepting the new transition if $E_{NEW} - E_{OLD} > 0$ increases and hence the tendency for the system to decrease in energy decreases. This also means that since $E_{NEW} - E_{OLD} > 0$ is more likely than before to be accepted, sporadic oscillations in energy and magnetization will occur as the preference to magnetize in one direction decreases.