PHY407 Lab 11

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The workload was distributed as followings:

- **Sang Bum Yi did question 1 and 2**
- **Jianbang Lin did question 3**

Question 1

Part a)

The traveling salesman, which is an example of 10.4, was investigated as varying the cooling schedule time constant τ. The cooling rate was chosen to be an exponential form, in Equation 1.1. With the same constants defined in the exercise and the same number of cities to be visited, which was 25, the total distance traveled was compared for different paths taken. Figure 1.1, 1.2, and 1.3 show three different paths taken by the salesman and the total distance traveled in the bottom of the plot.

$$T = T_0 \exp\left(\frac{-t}{\tau}\right) \qquad \text{[Eq 1.1]}$$

where 't' refers to the time and T_0 refers to the initial temperature

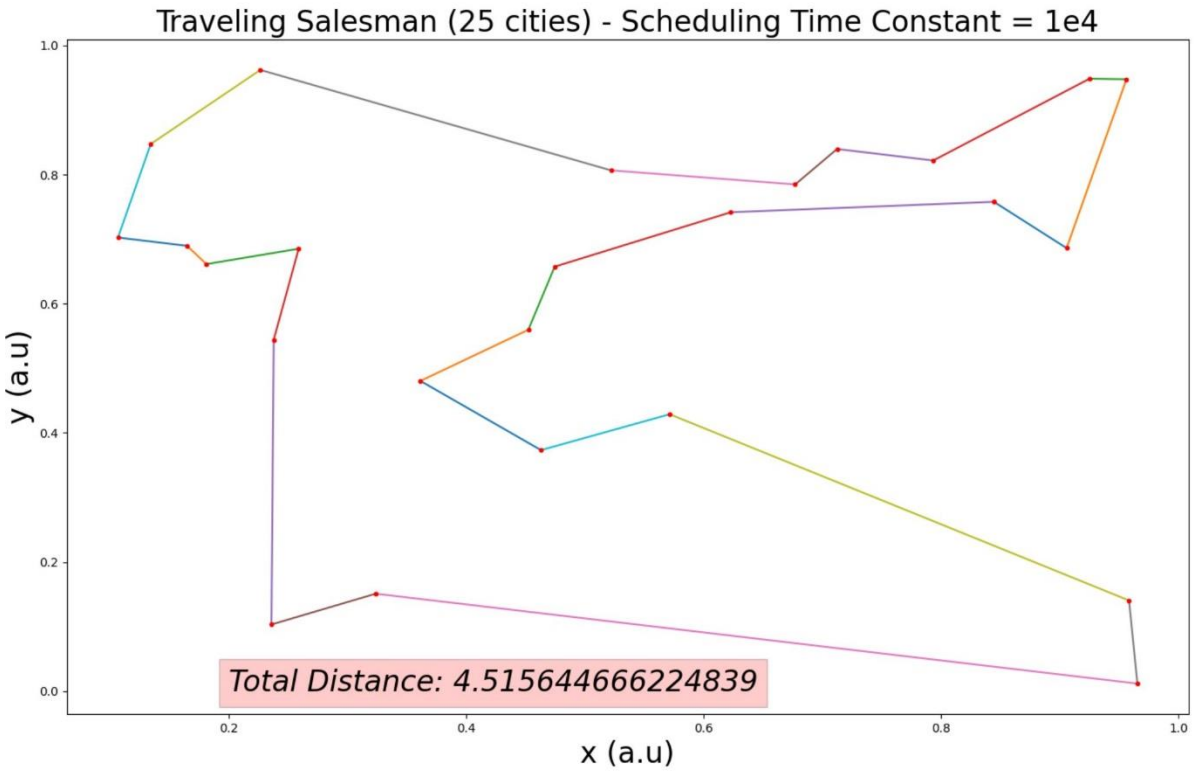

Figure 1.1: The path of travel taken by the salesman with the scheduling time constant being 10^4. Note that the total distance is approximately 4.52 (three sig fig).

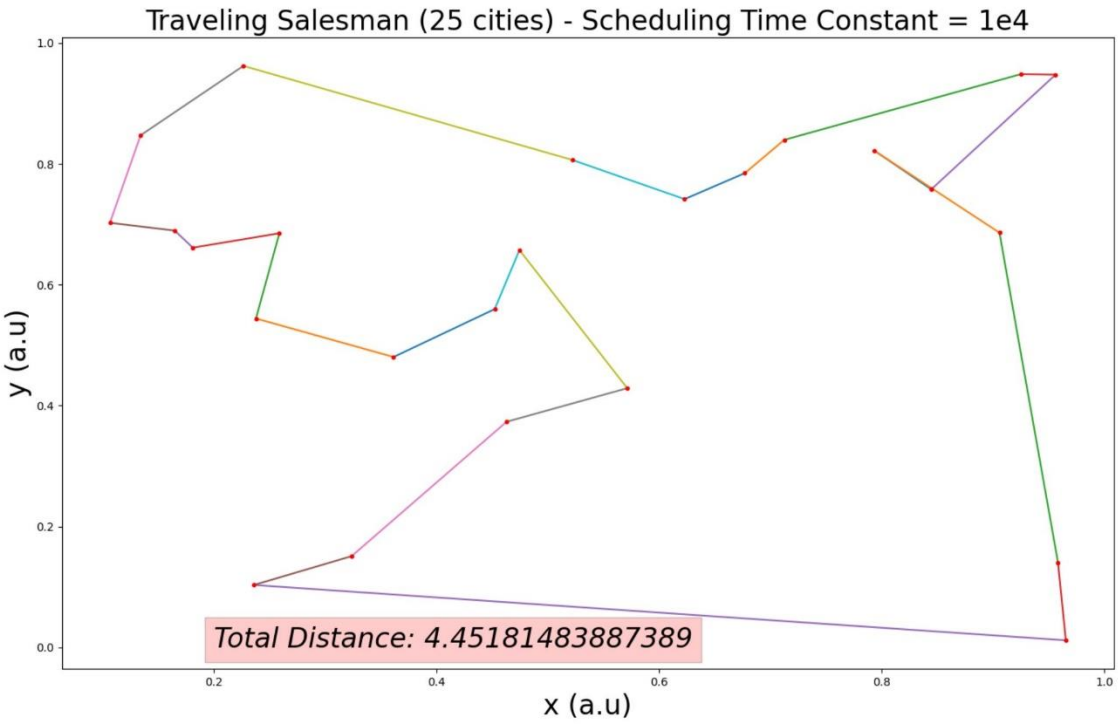

Figure 1.2: The path of travel taken by the salesman with the scheduling time constant being 10^4. Note that the total distance is approximately 4.45 (three sig fig).

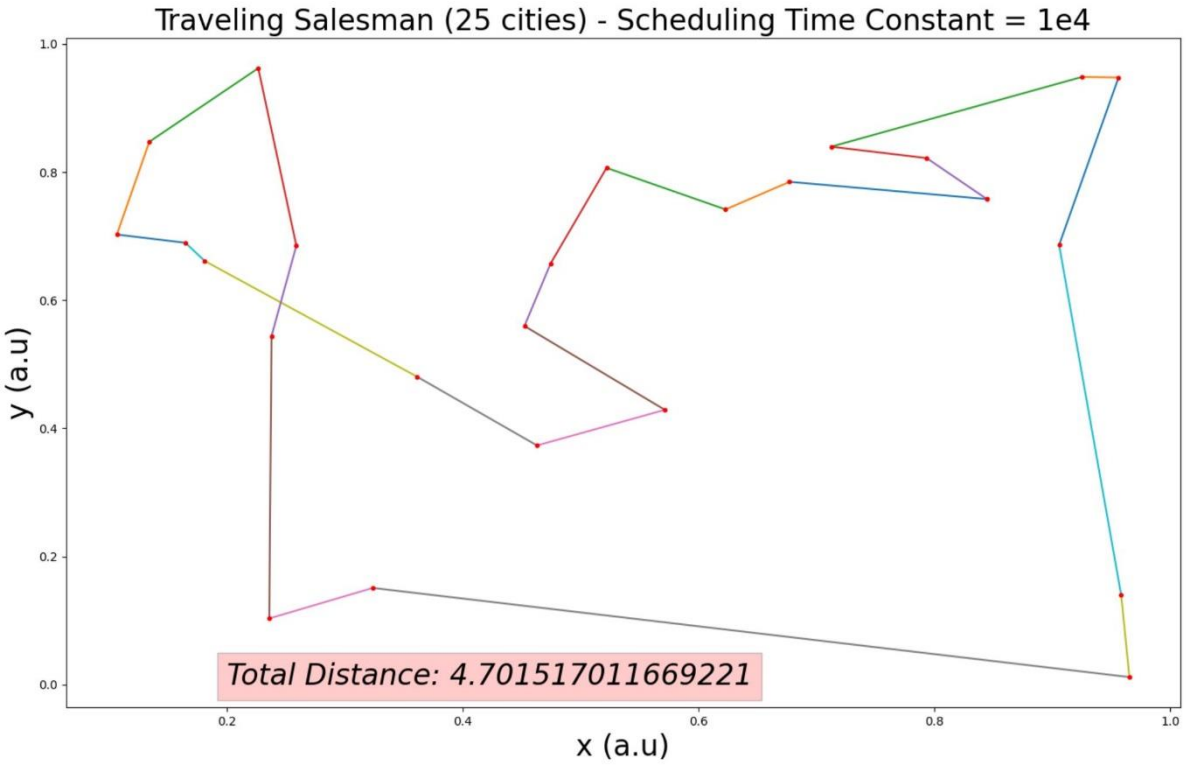

Figure 1.3: The path of travel taken by the salesman with the scheduling time constant being 10^4. Note that the total distance is approximately 4.70 (three sig fig).

As seen in three figures above, the same 25 cities were visited in three distinct paths at τ=10^4 and the total distances traveled were 4.52, 4.45, and 4.70 respectively. On the other hand, the total distances traveled were also investigated as τ decreased to 10^3, 10^2, and 10, as shown in figure 1.4, 1.5 and 1.6 respectively. In addition, the total distance traveled with the increased τ was also investigated in figure 1.7, with τ = 10^5.

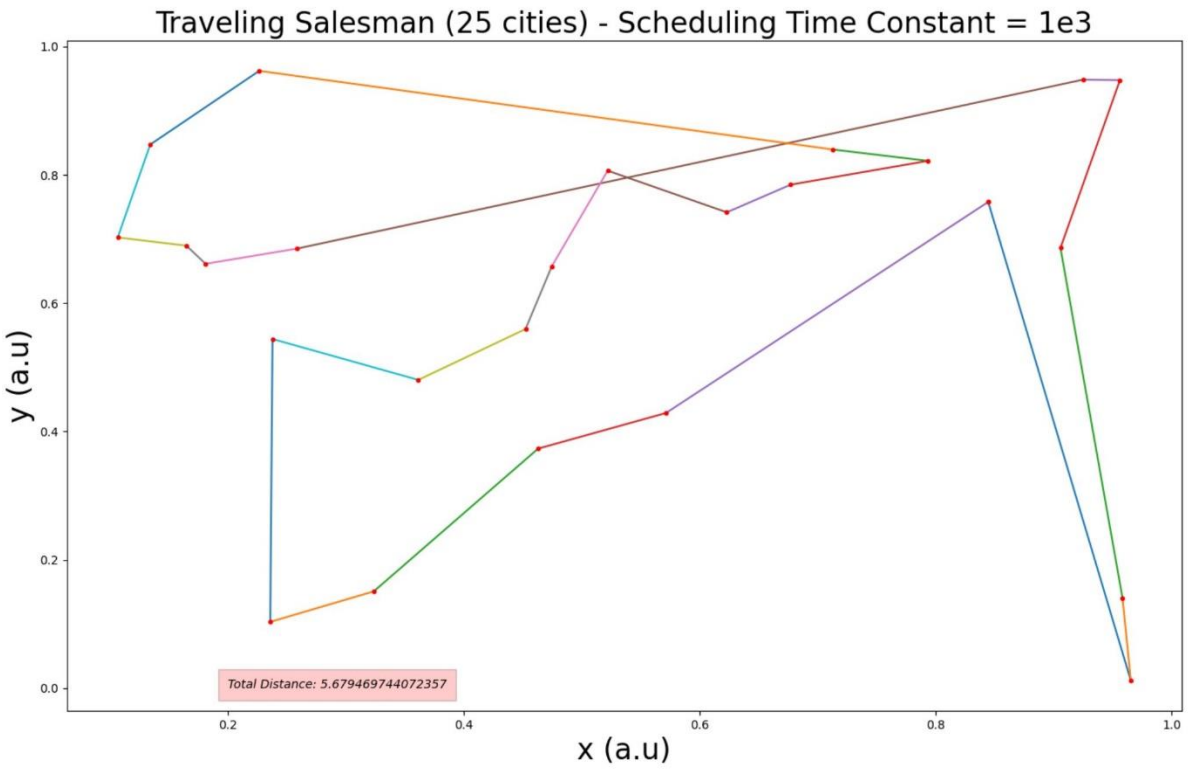

Figure 1.4: The path of travel taken by the salesman with the scheduling time constant being 10^3. Note that the total distance is approximately 5.68 (three sig fig).

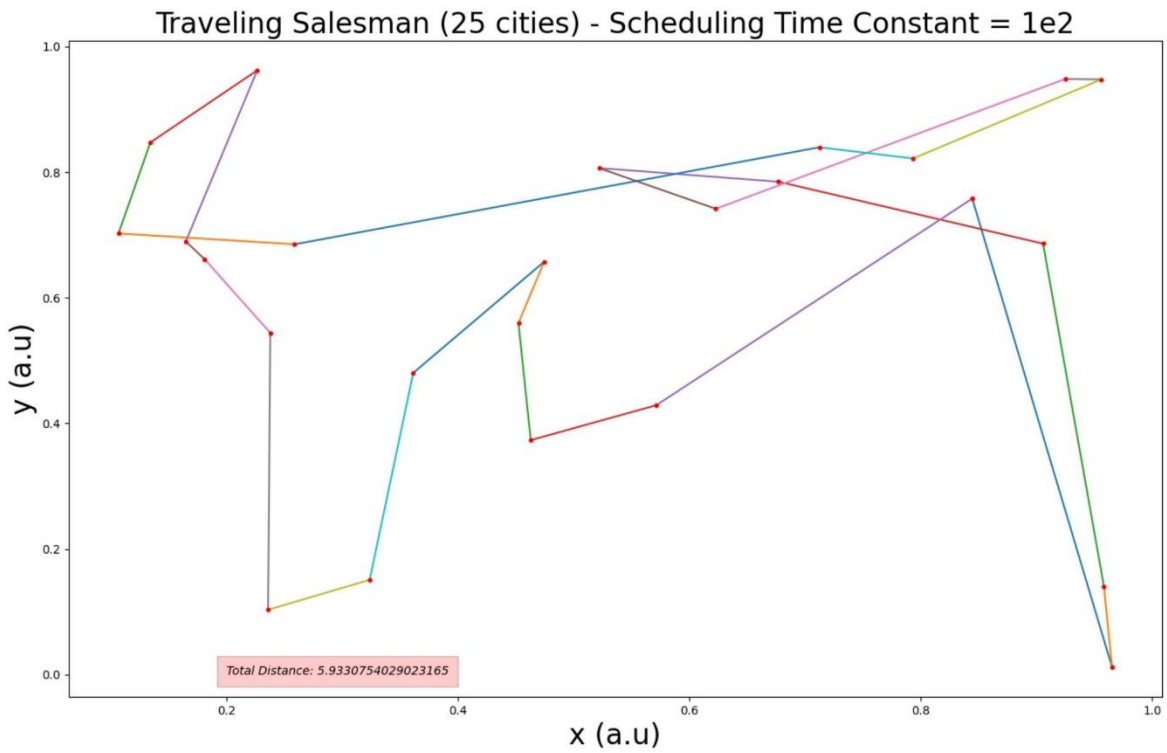

Figure 1.5: The path of travel taken by the salesman with the scheduling time constant being 10^2. Note that the total distance is approximately 5.93 (three sig fig).

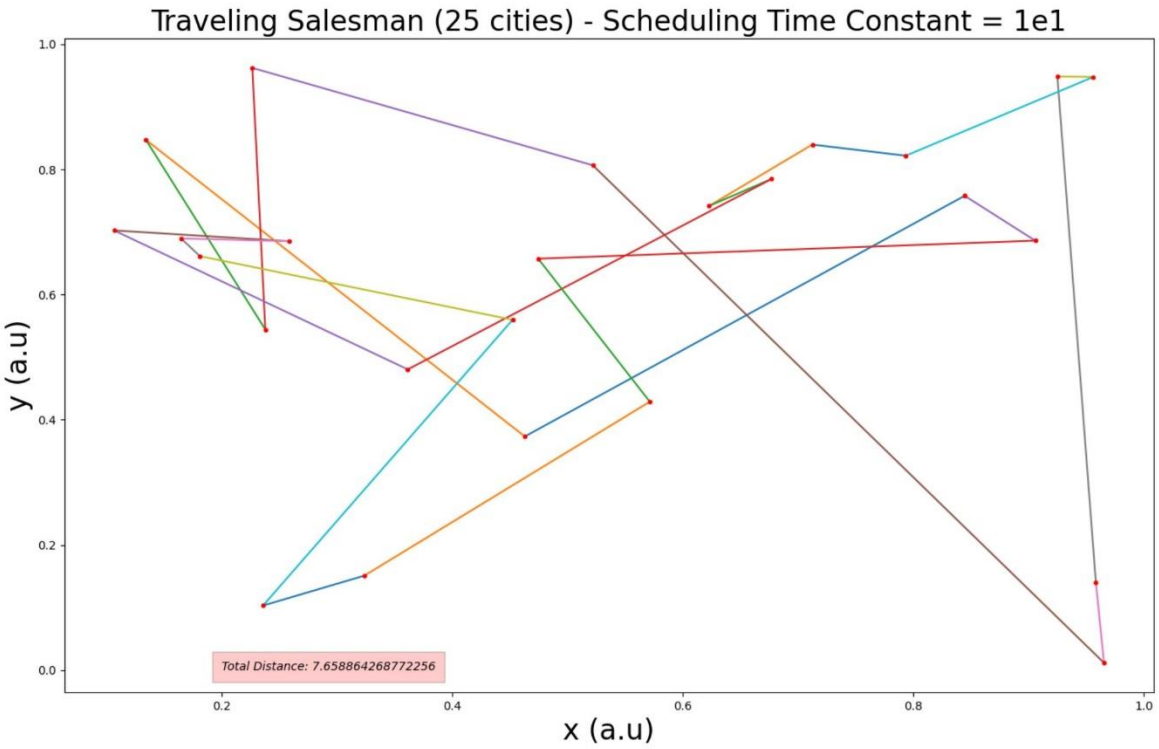

Figure 1.6: The path of travel taken by the salesman with the scheduling time constant being 10^1. Note that the total distance is approximately 7.66 (three sig fig).

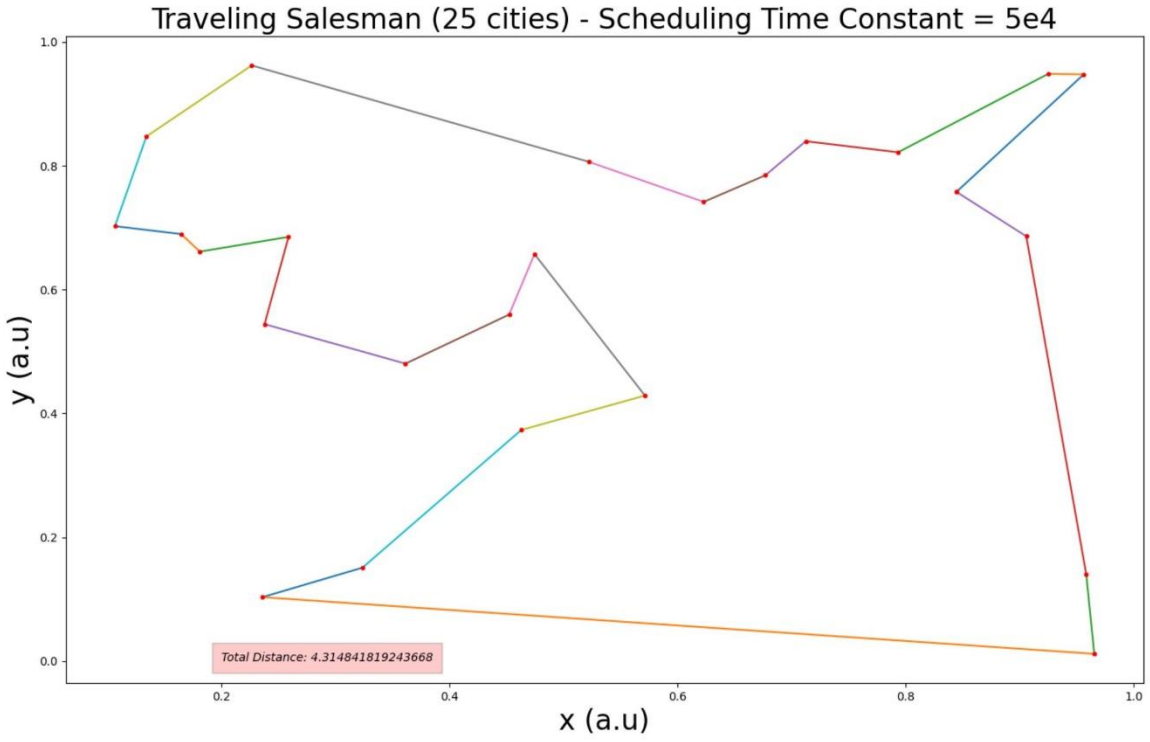

Figure 1.7: The path of travel taken by the salesman with the scheduling time constant being $5*10^4$. Note that the total distance is approximately 4.31 (three sig fig).

The total traveled distance D did not change siginificantly when different paths were taken at the same scheduling time constant. However, the total traveled distances increased as the scheduling time constant decreased from the default value of 10^4, but decreased as τ increased. In other words, the distance D decreases when the system cools more slowly.

Part b.i)

The global minimum of $f(x, y) = x^2 - \cos(4\pi x) + (y-1)^2$ was confirmed to occur at (x,y) = (0,1) by using simulated annealing starting at (x,y)=(2,2), with Montel Carlo moves. Figure 1.8 and 1.9 show the value of x and y as the time progressed, respectively. Note that the value of 'x' converges to 0 and the value of 'y' converges to 1, as expected.

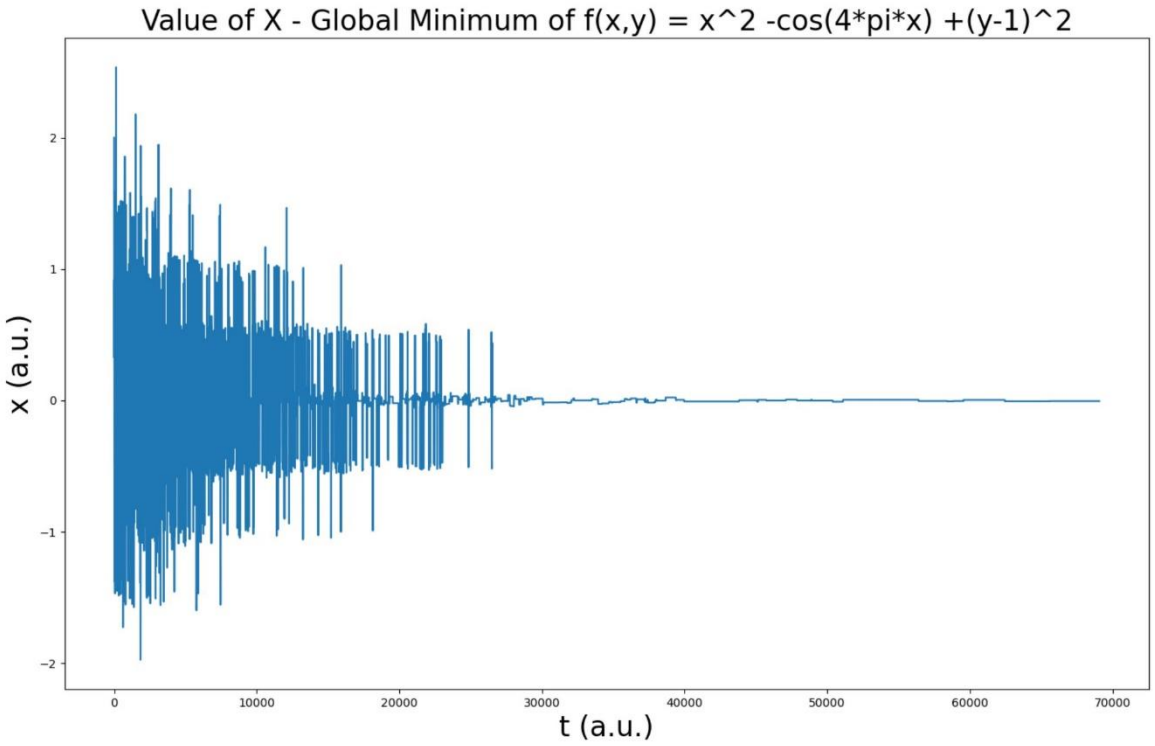

Figure 1.8: The value of 'x' in simulated annealing for function f(x,y).

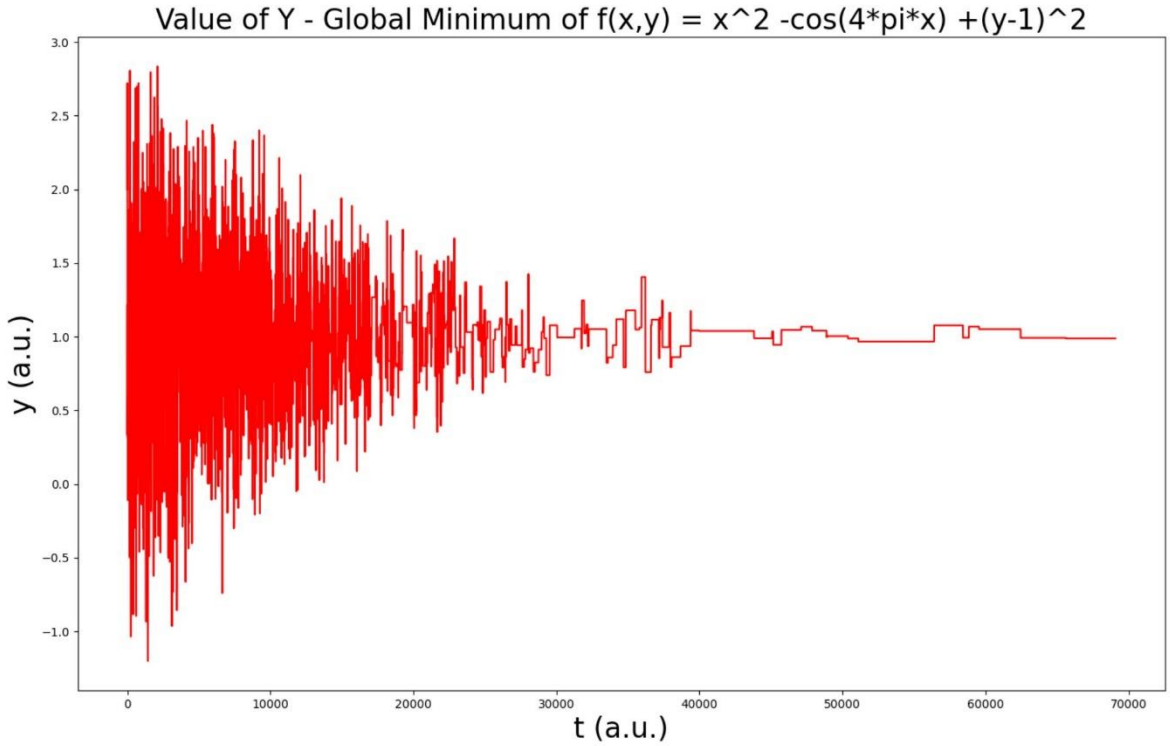

Figure 1.9: The value of 'y' in simulated annealing for function f(x,y).

Part b.ii)

Similar to the previous part, the global minimum of $g(x,y) = \cos(x) + \cos(\sqrt{3}x) + \cos(\sqrt{2}x) + (y-1)^2$ was confirmed to occur at (x,y) = (16,1) with Montel Carlo moves. Figure 1.10 and 1.11 show the value of x and y as the time progressed, respectively. Note that the value of 'x' converges to 16 and the value of 'y' converges to 1, as expected.

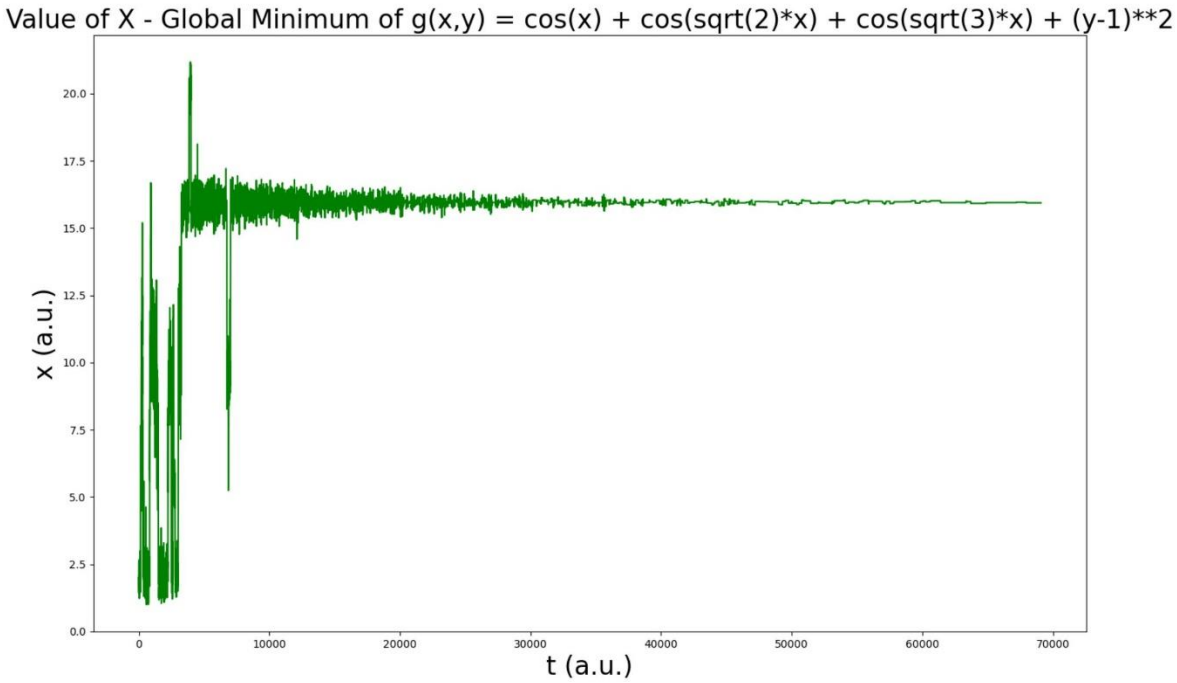

Figure 1.10: The value of 'x' in simulated annealing for function g(x,y).

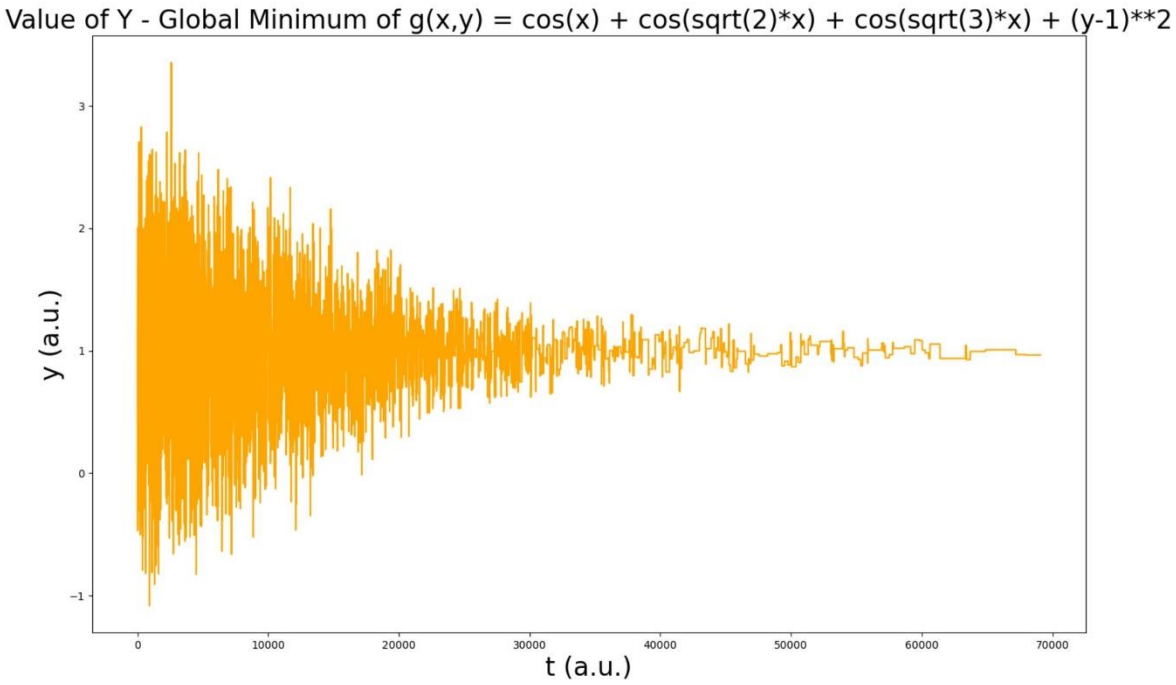

Figure 1.11: The value of 'y' in simulated annealing for function g(x,y).

Question 2

The Ising model, which is a theoretical model of a magnet that explains the magnetization of a material by applying the concept of small magnetic dipoles aligned in the same or opposite directions, was computationally simulated with 20 x 20 grids. In the Ising model, one of the magnetic dipoles is randomly selected and the direction of its spin is flipped. However, such flip is either accepted or refused depending on the probability determined by the Metropolis acceptance formula, which can be found in equation 2.1 below. If the flip is refused, the spin of the magnetic dipole reverts to the original state.

$$P_a = \begin{cases} 1, & if\ E_j \leq E_i \\ e^{-\beta(E_j - E_i)}, & if E_j > E_i \end{cases} \qquad \text{[Eq 2.1]}$$

where $\beta = \frac{1}{k_B T}$, E_j and E_i refers to the energy of the new and original states.

In the simulation, the total energy was computed as the sum of the product of adjacent spins multiplied by the positive interaction constant 'J', as shown in equation 2.2. The Boltzmann constant k_B and the temperature were both set to 1, as specified in Exercise 10.9, which gives $\beta = 1$.

$$E = -J \sum_{<ij>} s_i s_j \quad \text{[Eq 2.2]}$$

where J = 1 and 's' refers to the array of the spins.

The total magnetization was computed as the sum of all spins, as in Equation 2.3

$$M = \sum_i s_i \quad \text{[Eq 2.3]}$$

With the parameters given above, the change of magnetization was investigated and compared as varying the temperature. First, the Ising model was simulated for T = 1 in a total of 1,000,000 Monte Carlo steps and the change of magnetization was plotted and animated, which are Figure 2.1 and *Q2_T1.mp4* in the attachment, respectively. Then, the same procedure was repeated for the case of T=2, which produced the graph and the animation, as found in Figure 2.2 and *Q2_T2.mp4*, respectively. Lastly, the same procedure was also repeated for T=3 case with the graph and animation being Figure 2.3 and *Q2_T3.mp4*, respectively.

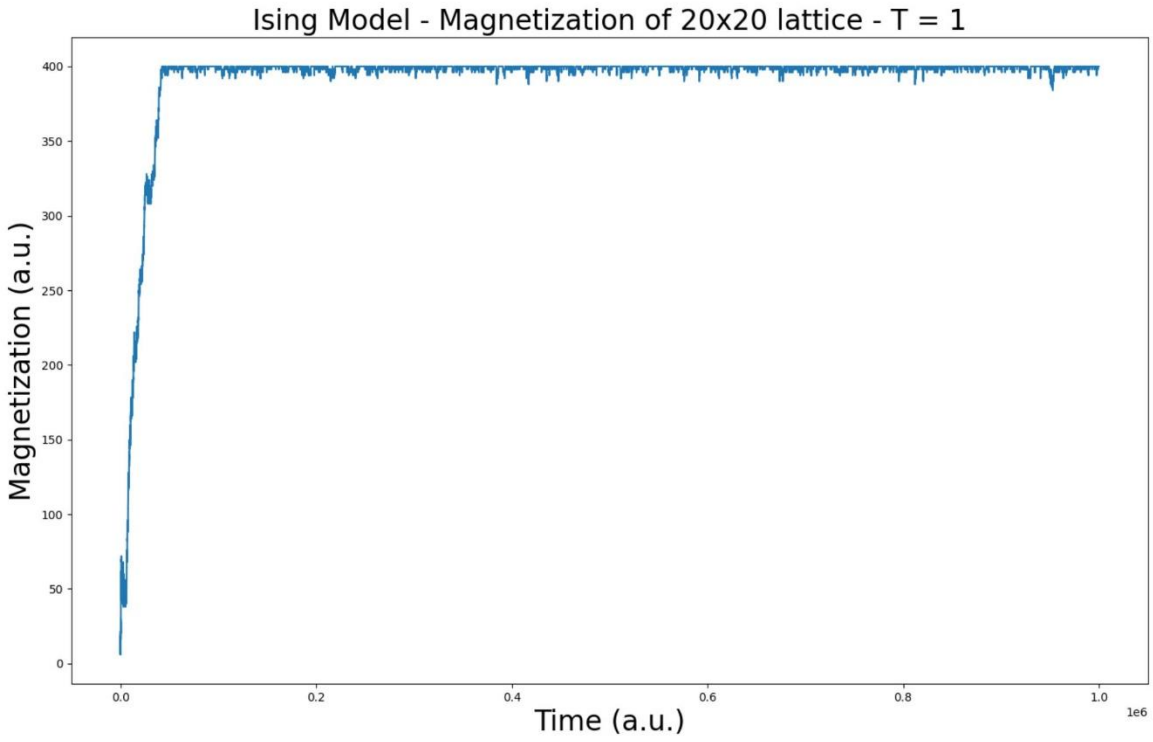

Figure 2.1: The Magnetization of 20x20 lattice at T = 1. Note that the units of time and magnetization are arbitrary.

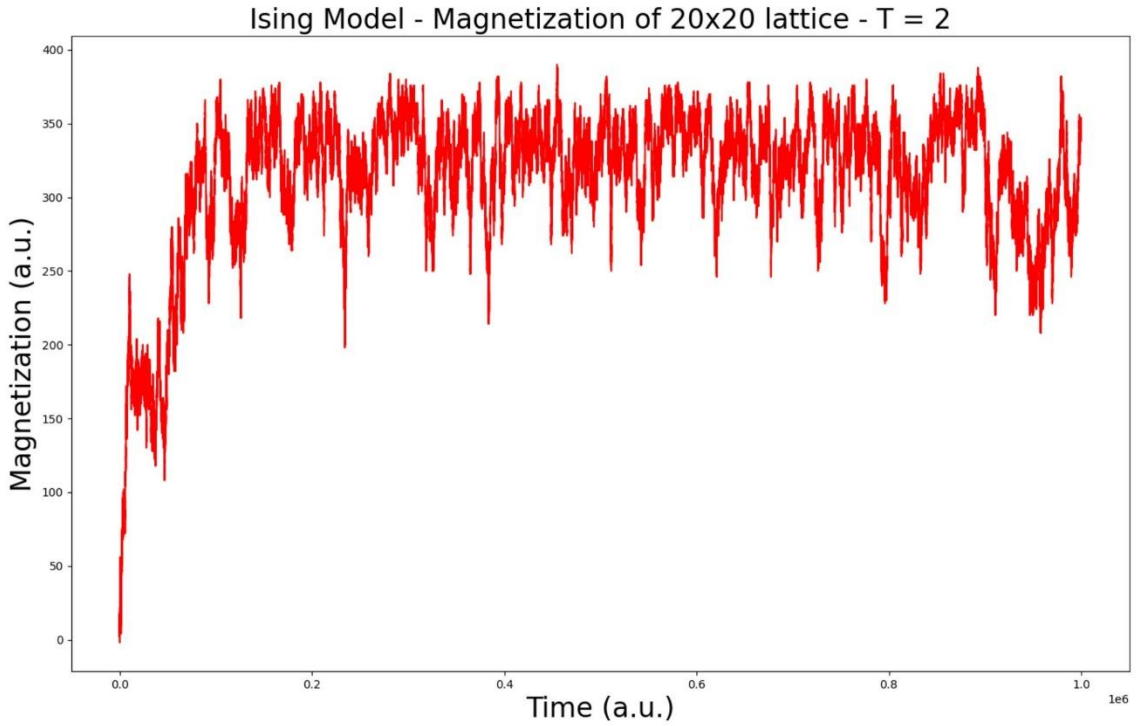

Figure 2.2: The Magnetization of 20x20 lattice at T = 2. Note that the units of time and magnetization are arbitrary.

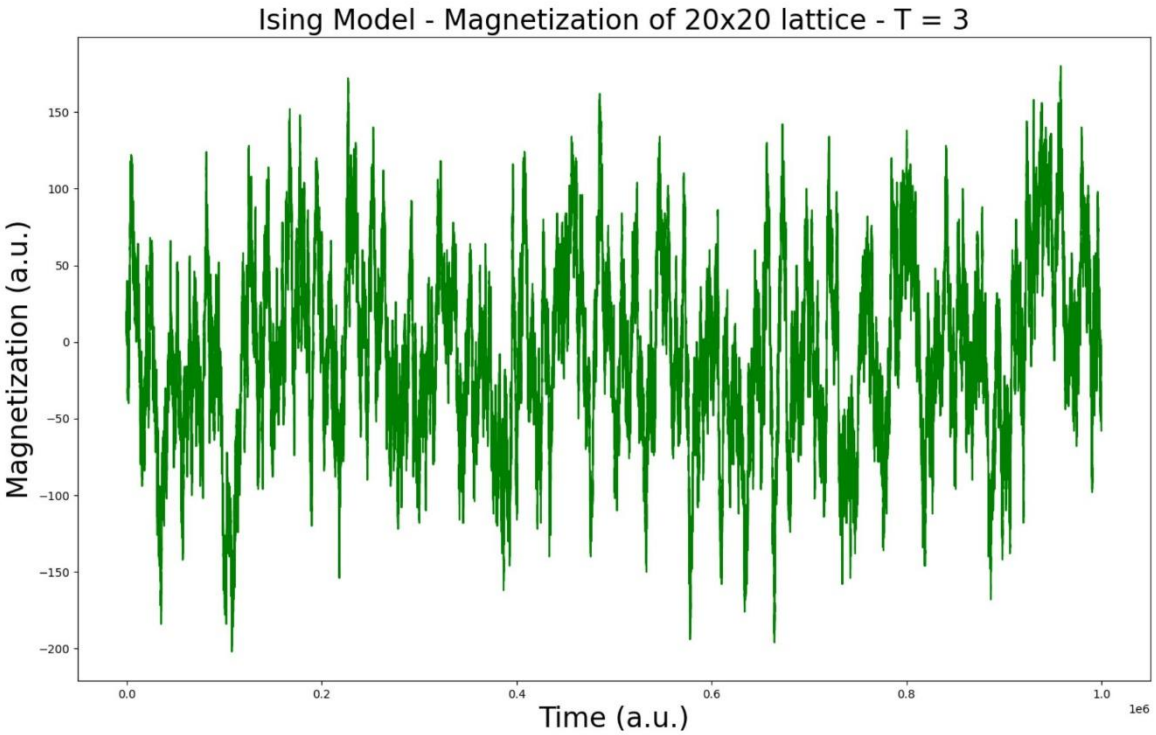

Figure 2.3: The Magnetization of 20x20 lattice at T = 3. Note that the units of time and magnetization are arbitrary.

Figure 2.1 shows that the magnetization reached its maximum value at an early stage of steps, with a tiny fluctuation afterward. A similar pattern is observed in Figure 2.2, but it was not able to reach the maximum value of 400 due to its greater fluctuation. In Figure 2.3, the magnetization seems to be completely unstable, with no clear pattern of reaching either the maximum or minimum value like the previous two figures.

In addition to the figures, the attached animations display the same patterns. Q2_T1.mp4 shows that all spins point to the same up-direction at the end of the animation at T = 1, but Q2_T2.mp4 shows the less organized alignment of the spins at T =2. Lastly, Q2_T3.mp4 shows more chaotic behavior, having no clear pattern of spins aligning in the same direction.

In other words, the system at T = 1 developed a “spontaneous magnetization”, or a nonzero value of the overall magnetization. In this case, the spontaneous magnetization was positive. For the system at T = 2, the spontaneous magnetization was less achieved, as there was more disagreement in directions of spins than T = 1. Lastly, no spontaneous magnetization was reached for the system at T = 3. In conclusion, the system tends to achieve the spontaneous magnetization more easily as the temperature decreases.

Question 3

This question investigates the energy and structure of protein folding. The initial structure of protein will be a straight line, and it will tend to evolve into a structure with lower energy state, it is accomplished by having more ‘fold’. The protein will experience random motions due to thermodynamics, and temperature can be interpreted as ‘juggling’ of molecules. Therefore, the higher the temperature, the protein will have a higher probability of being in a lower energy state.

Part a)

When the temperature is set to be 1.5, length of particle is 30, and number of Monte Carlo steps is 10^5, the structure and energy graphs are shown as following:

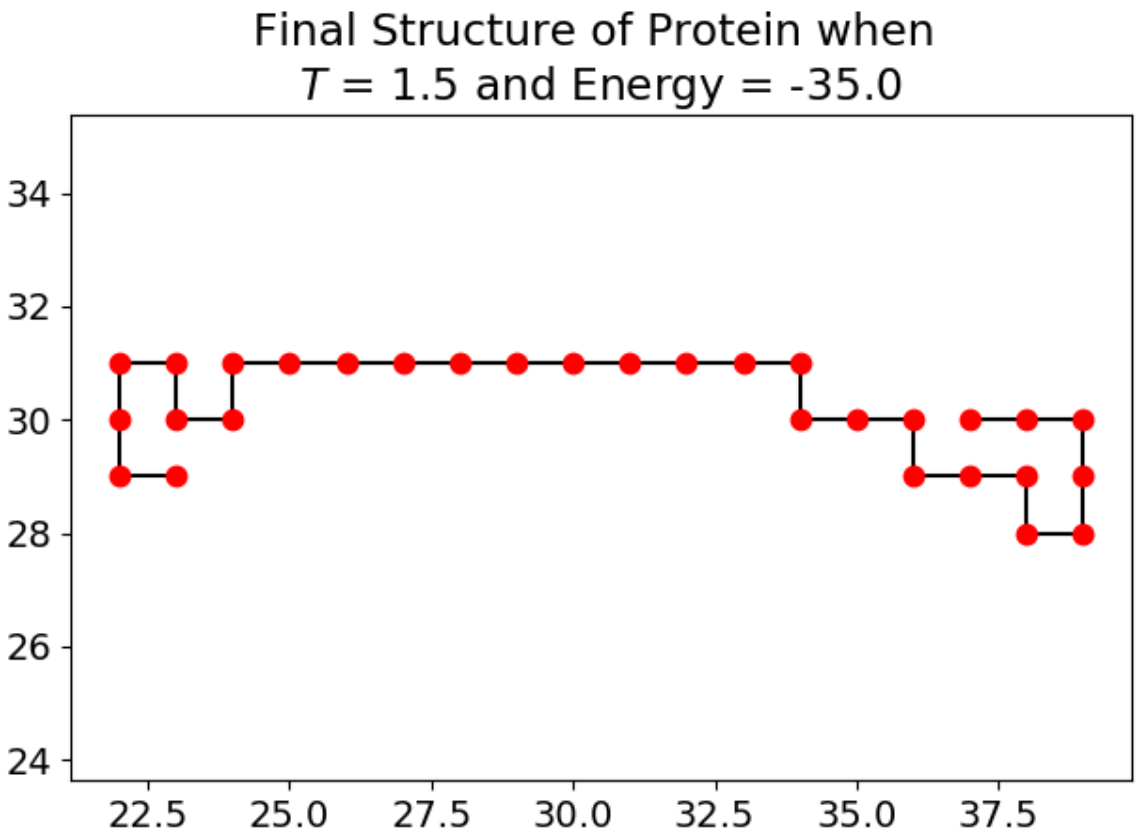

Figure 3.1: Structure of protein with length 30, and temperature 1.5, simulated with Monte Carlo steps of 10^5

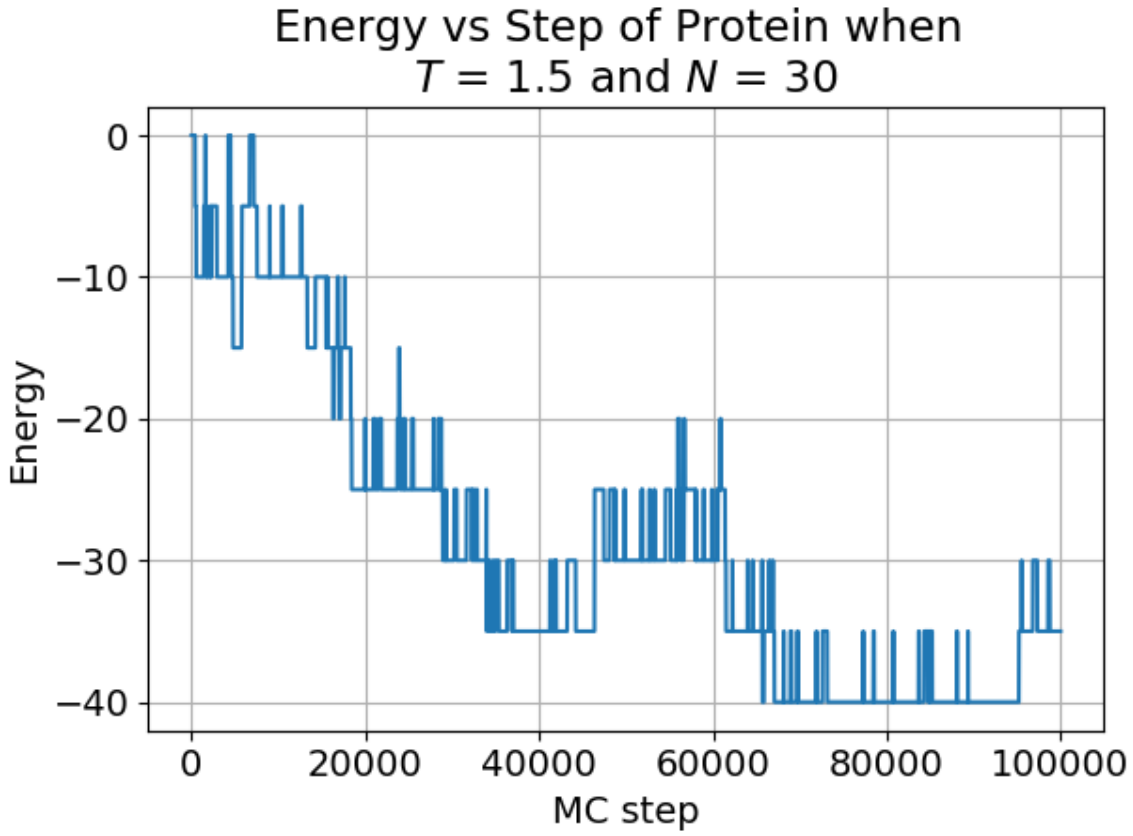

Figure 3.2: Energy of protein vs Monte Carlo steps taken, when temperature = 1.5 amd protein length 30

Figure 3.1 shows that a large portion of protein remains unmoved, they stay as a straight line. Figure 3.2 shows that energy of protein decreases as more Monte Carlo steps are taken, and energy will fluctuate by a small amount. The lowest energy state it reaches is -40. Now, vary the temperature of system to 0.5 and keeping the rest of the variables the same:

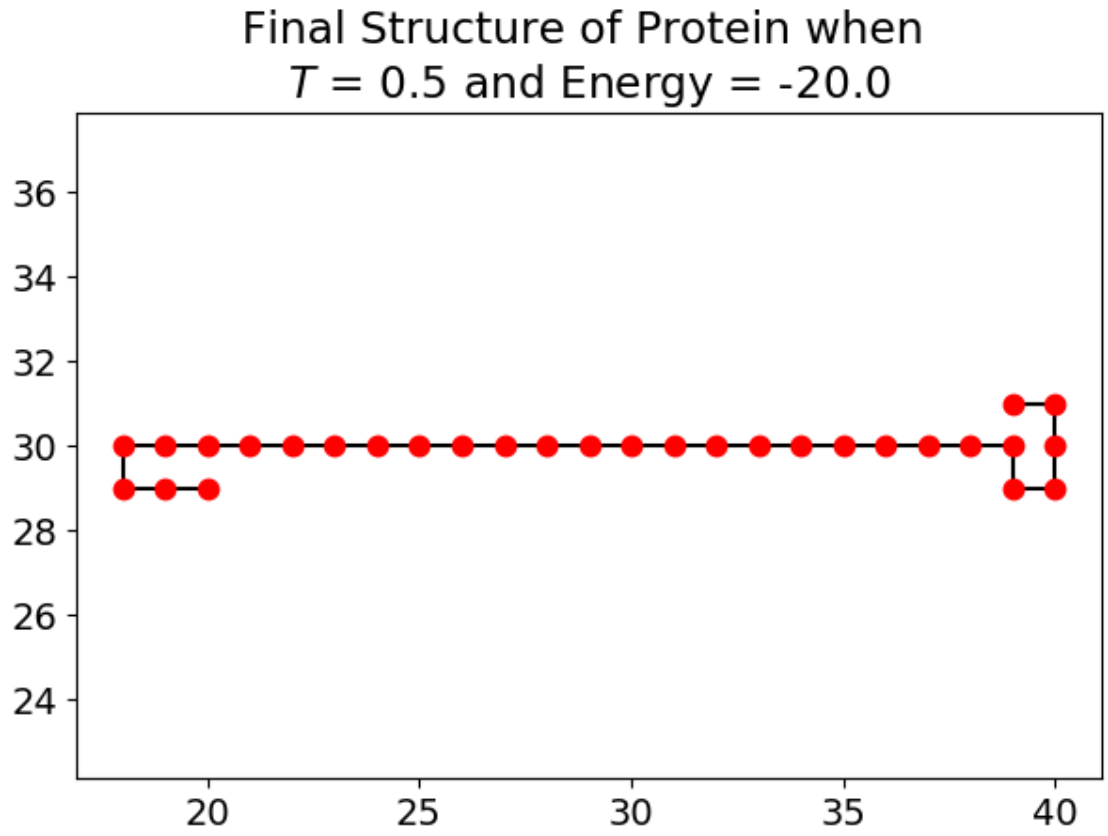

Figure 3.3: Structure of protein with length 30, and temperature = 0.5, simulated with Monte Carlo steps of 10^5

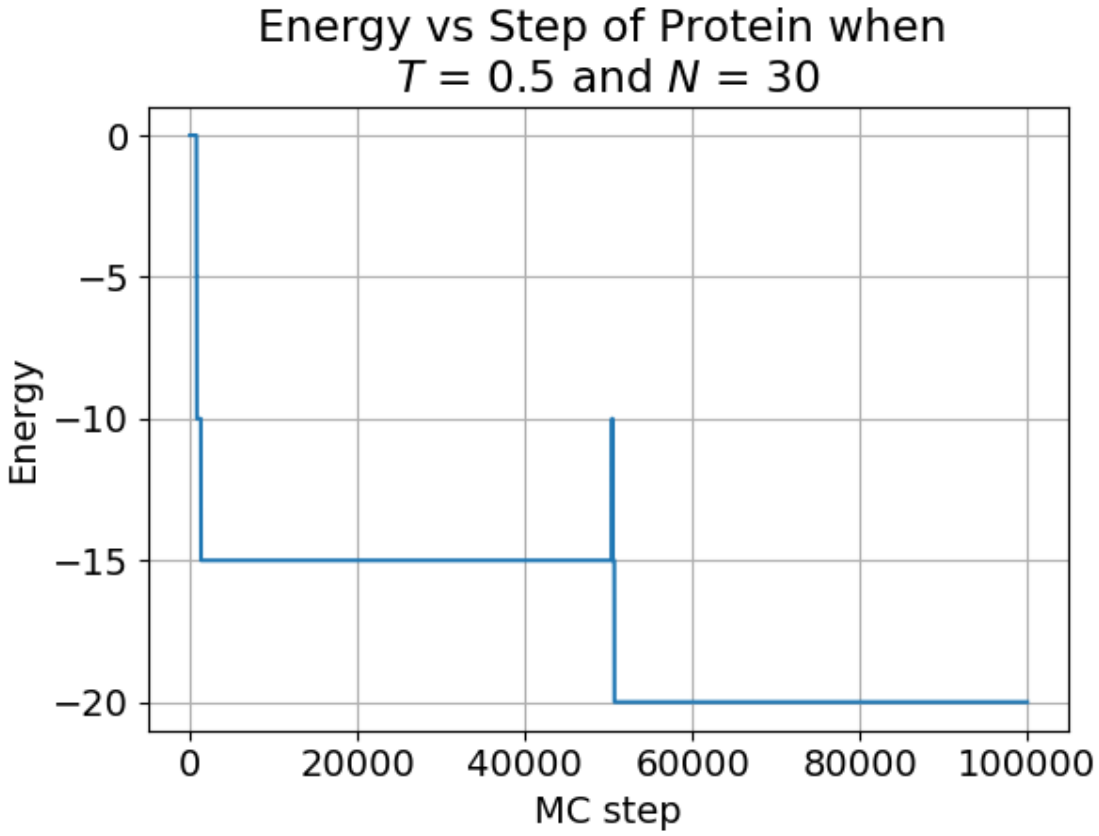

Figure 3.4: Energy of protein vs Monte Carlo steps taken, when temperature = 0.5 and protein length 30

Compared with graphs when T=1.5, this structure consists of a longer straight line. Similar to graph 3.2, energy decreases with more Monte Carlo steps, however, figure 3.4 has less fluctuation, also, the minimum energy is -20 which is larger than minimum energy in figure 3.2. This is as predicted, with lower temperature, the protein will 'juggle' less, thus, the probability of being in a lower energy state is smaller.

When the temperature is increased to 5:

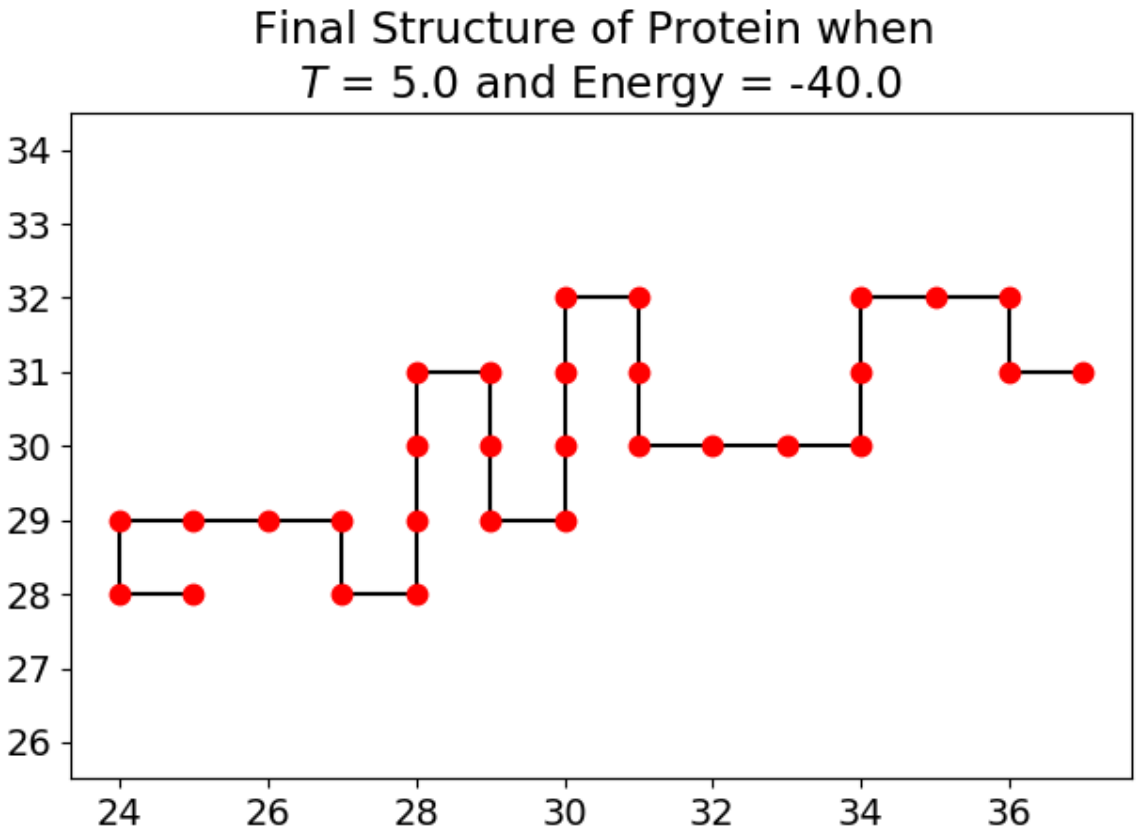

Figure 3.5: Structure of protein with length 30, and temperature = 5, simulated with Monte Carlo steps of 10^5

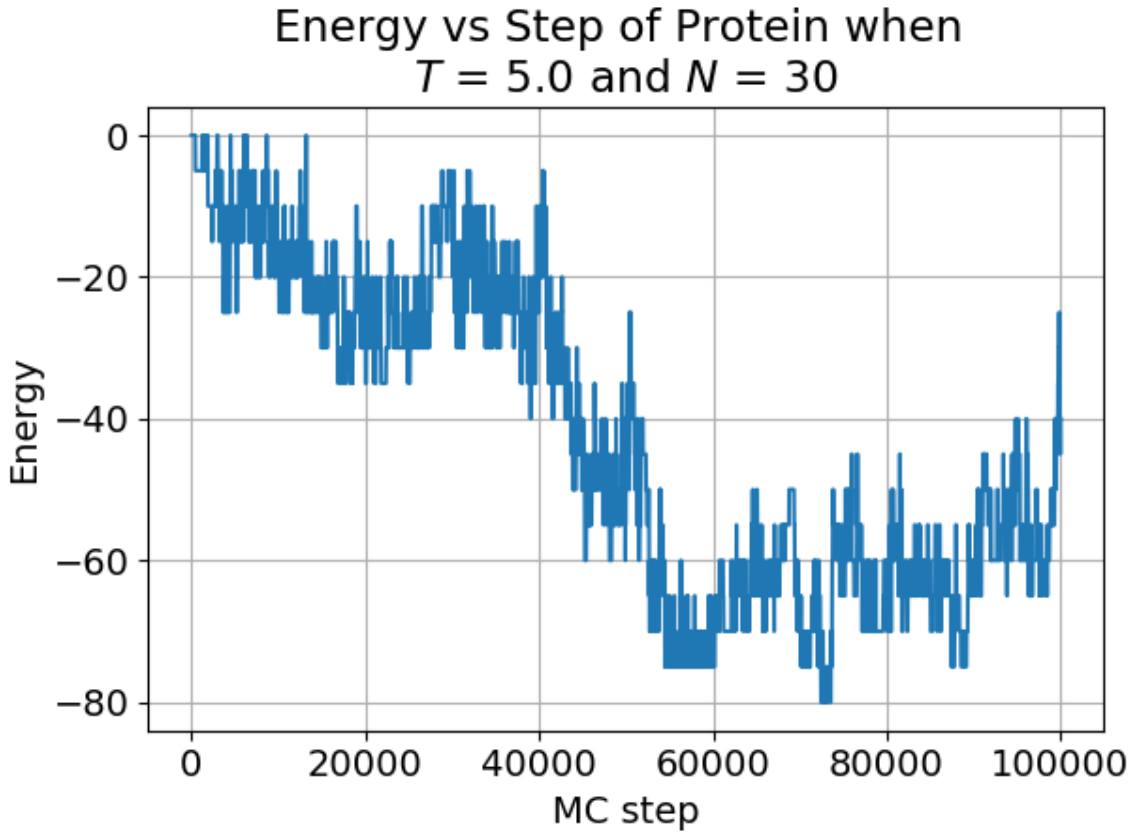

Figure 3.6: Energy of protein vs Monte Carlo steps taken, when temperature = 5 and protein length 30

Compared with figure 3.1 and figure 3.2, this structure has a shorter straight line and more folding. The energy decreases with more Monte Carlo steps, compared with figure 3.2, the fluctuation is larger, also the minimum energy it reaches is -80. Comparing figures 3.1 to 3.6, it becomes obvious that as temperature increases, the protein will tend to make more folding, and the energy of the protein will reach a lower energy state will large Monte Carlo steps, also the energy will fluctuate more violently.

Part b)

Part a changes the temperature of system while keeping Monte Carlo step the same at 10^5, for part b, the Monte Carlo step is changed to 10^6, and when T=1.5:

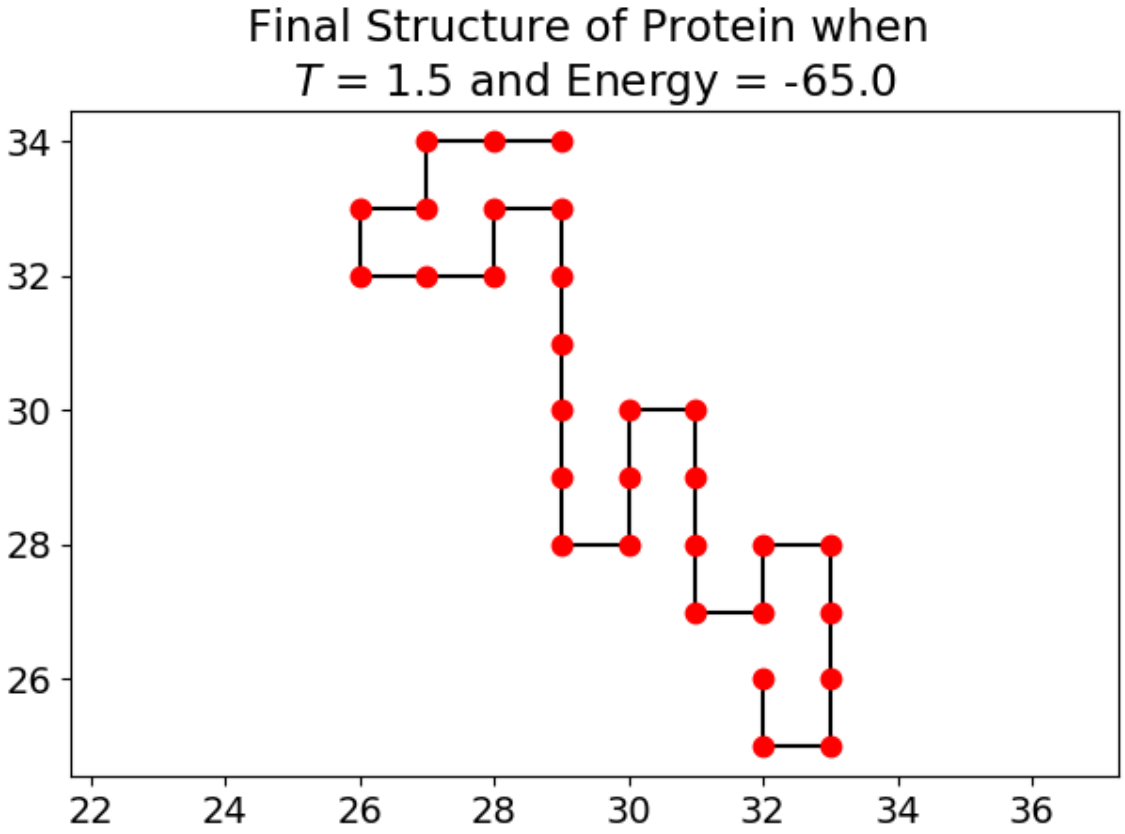

Figure 3.7: Structure of protein with length 30, and temperature = 1.5, simulated with Monte Carlo steps of 10^6

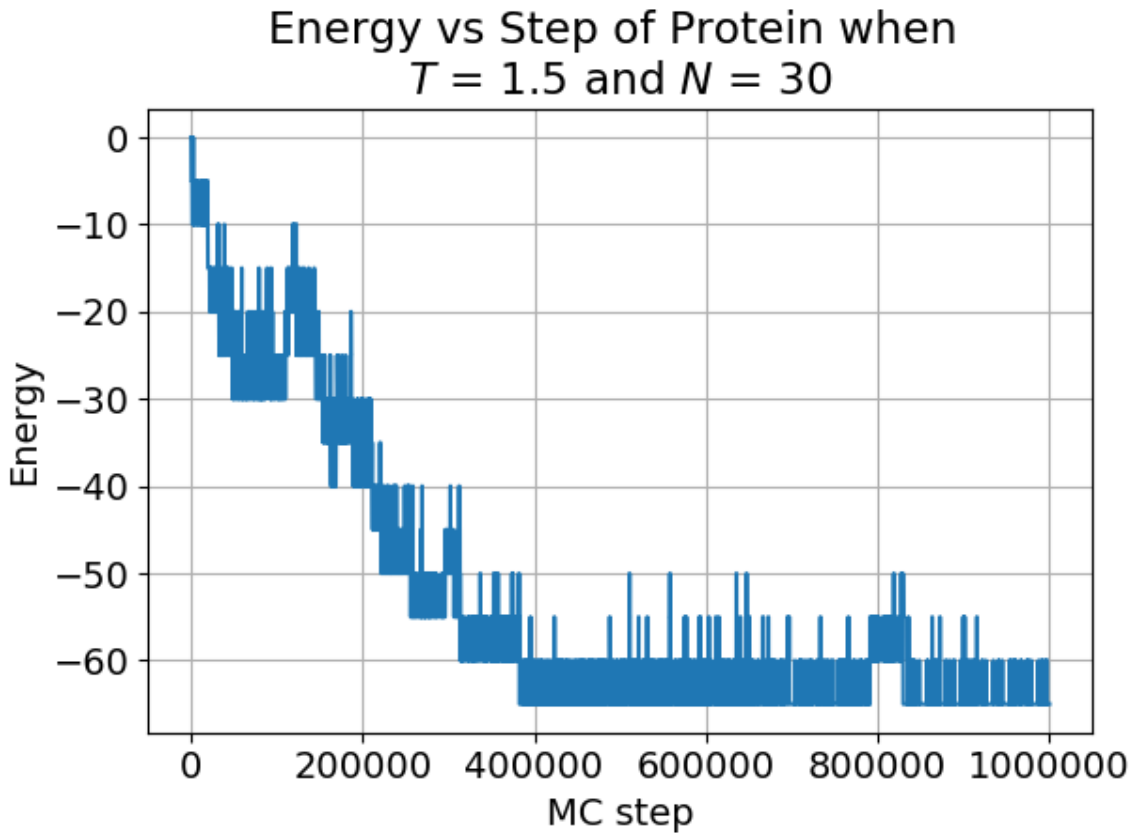

Figure 3.8: Energy of protein vs Monte Carlo steps taken, when temperature = 1.5 and protein length 30

Figure 3.7 shows the resulting folding is a complicated shape, compared with figure 3.1, it has more folding. The Energy graphs have similar shape, size of fluctuation is similar as well. However, the minimum energy is -70, this means with more Monte Carlo steps, the minimum energy will be less. Noticeably, once energy reaches -70, it stays there and does not decrease anymore. If temperature is taken to be 0.5:

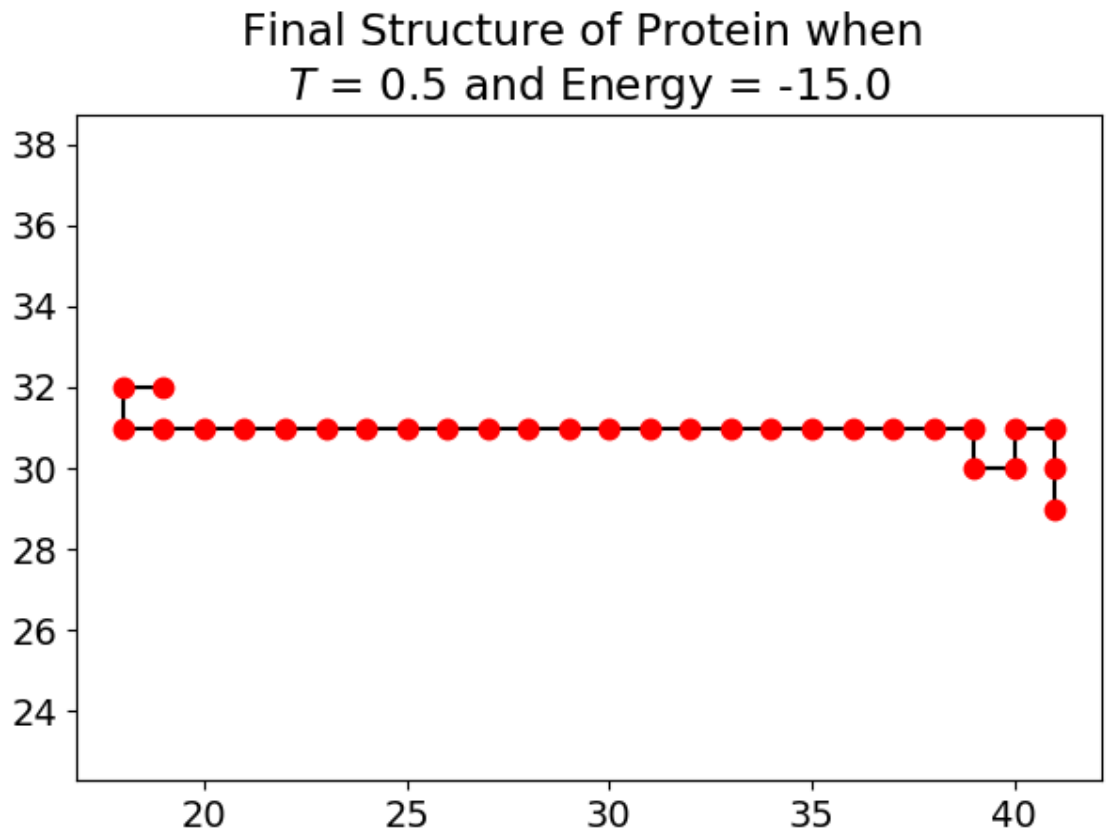

Figure 3.9: Structure of protein with length 30, and temperature = 0.5, simulated with Monte Carlo steps of 10^6

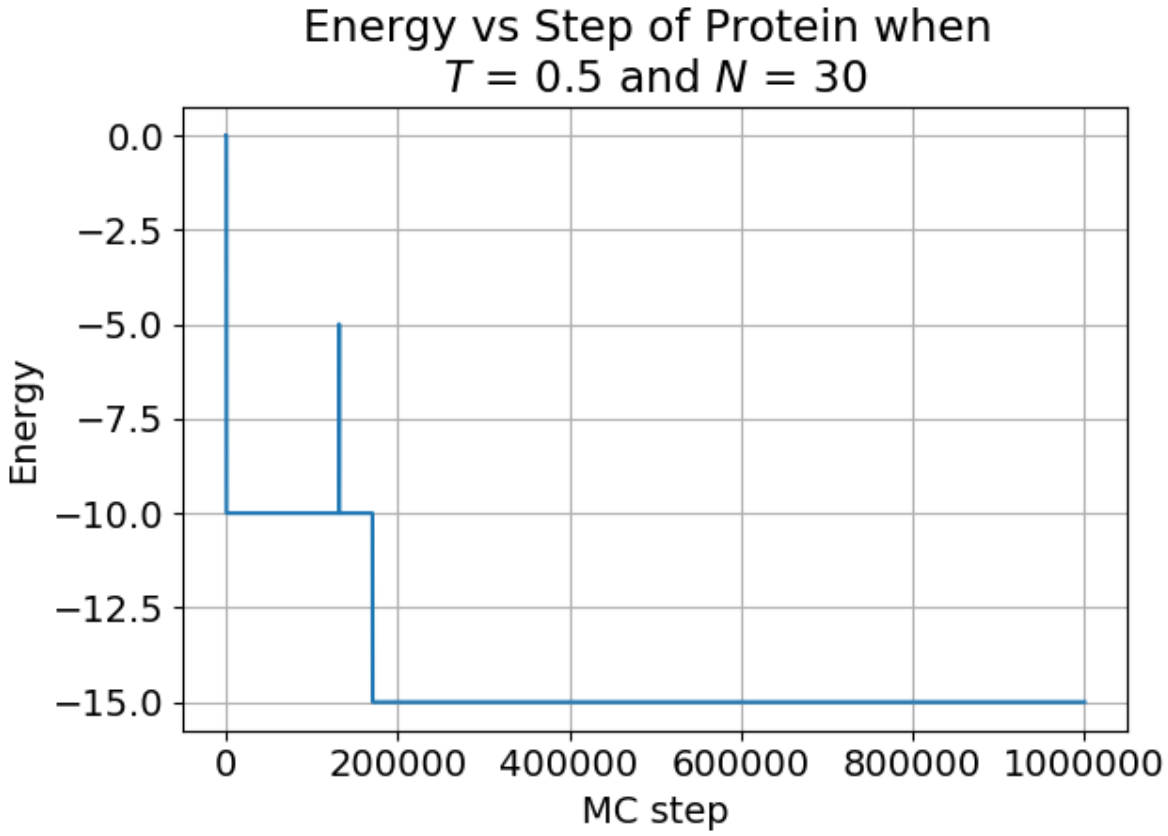

Figure 3.10: Energy of protein vs Monte Carlo steps taken, when temperature = 0.5 and protein length 30

Compared with graphs with 10^5 steps, their structures are similar. Their energy graphs are very similar as well, both have straight lines with no fluctuation. And their minimum energy is very close.

Part c)

Part a and b kept temperature constant for each simulation, and this part will vary the temperature within a simulation. With a starting temperature of 3.5, then it decreases by 1 for every 500,000 steps, until the temperature reaches 0.5. The result is shown as following:

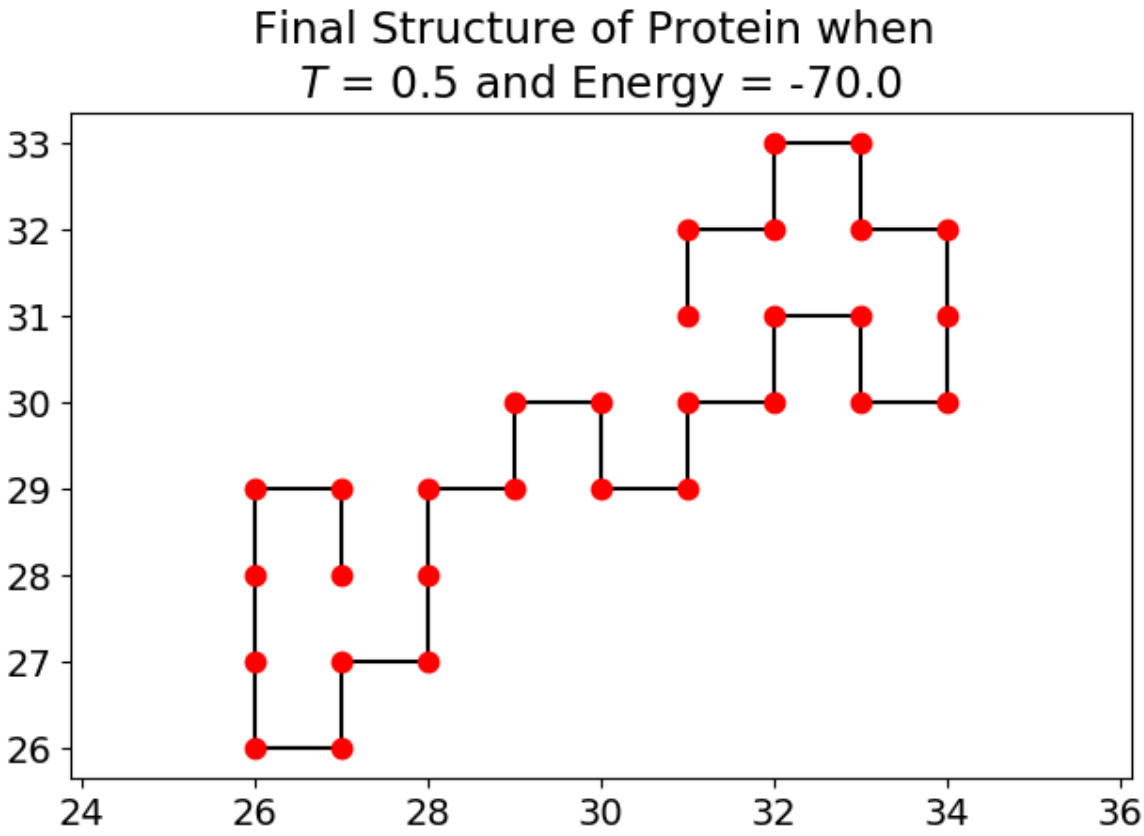

*Figure 3.11: Structure of protein with length 30, and temperature = 1.5, simulated with Monte Carlo steps of 2*10^6 and has simulated annealing.*

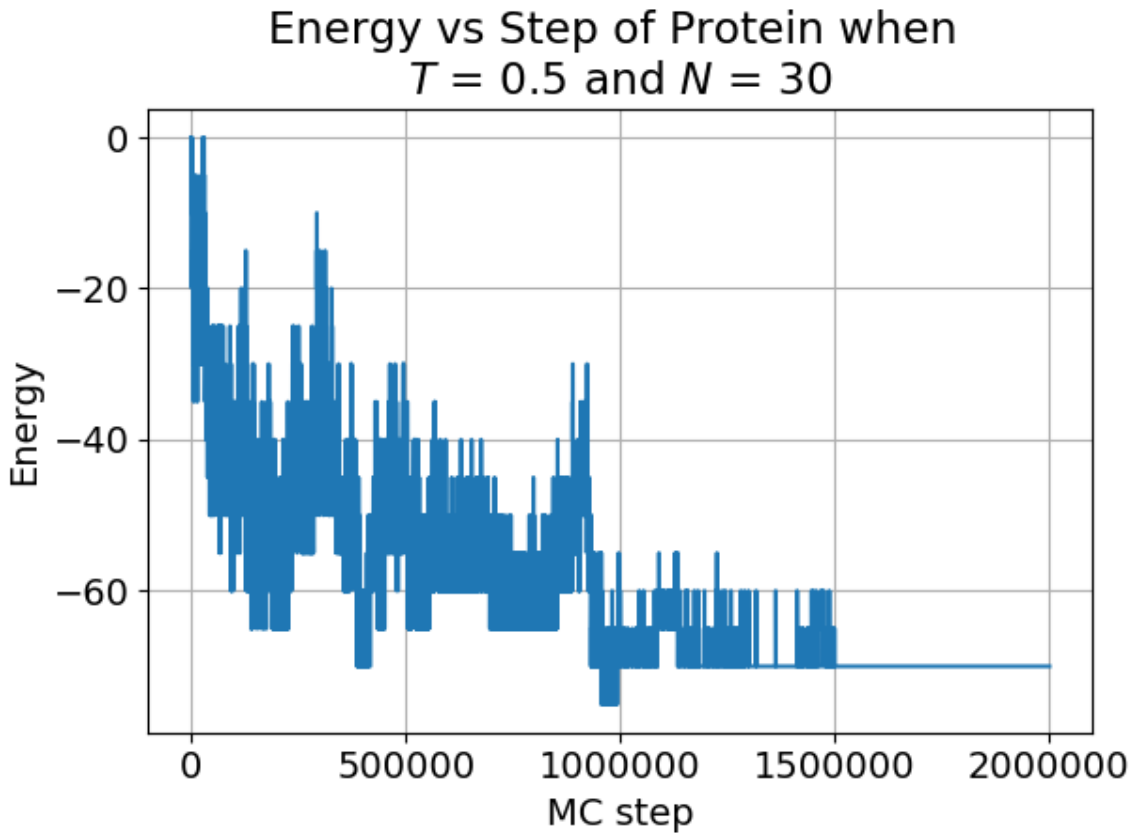

Figure 3.12: Energy of protein vs Monte Carlo steps taken, when temperature = 0.5 and protein length 30 and has simulated annealing.

The final temperature is the same as the one in figure 3.3, but their structures differ a lot, this figure shows a very complicated shape, and the energy is low. In comparison figure 3.3 is still mostly a straight line, and the energy is higher. Energy of protein starts with large fluctuation, but as the Monte Carlo step increases, the energy approaches -70 and becomes stable, with little to no fluctuation.

Part d)

For the last part, multiple simulations are run, with different temperatures. Temperature starts with 10, and decreases by 0.5 for each simulation, until it reaches 0.5. And for each simulation, 500,000 Monte Carlo steps are taken:

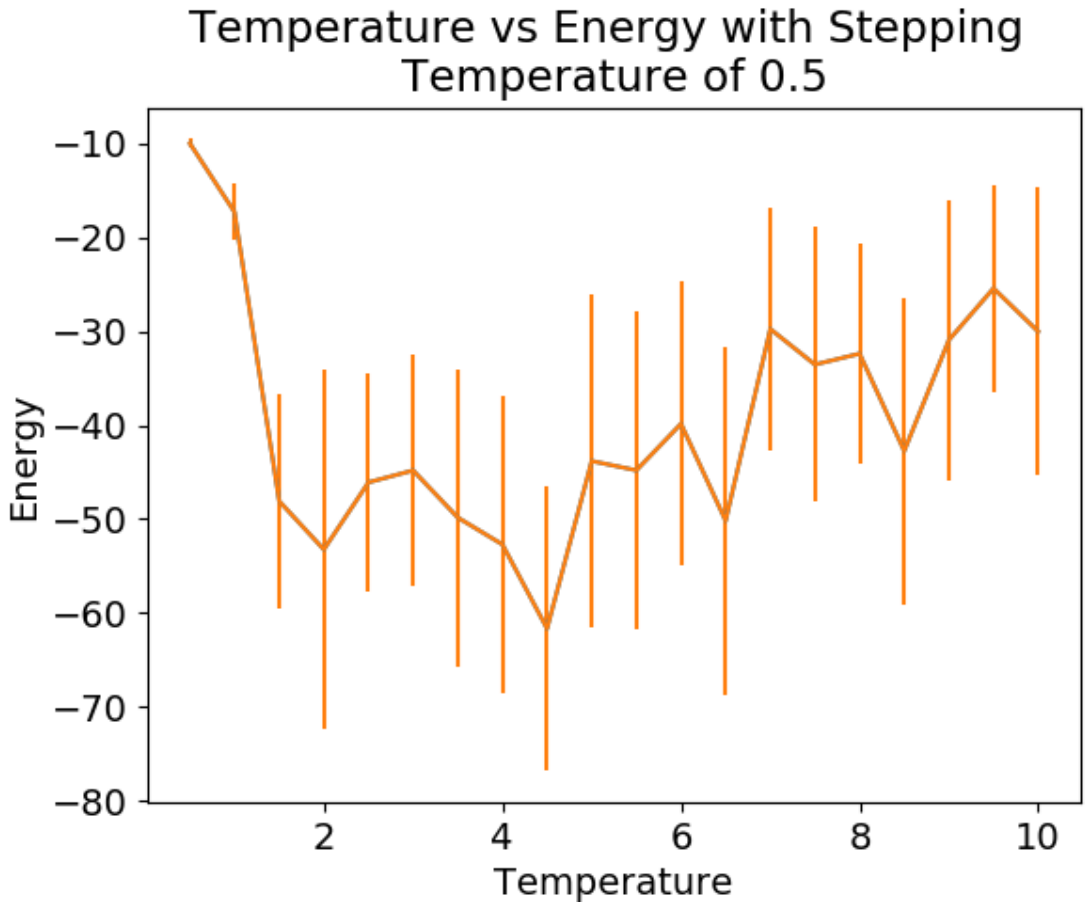

Figure 3.13: Energy of protein vs temperature, with 500,000 steps for each simulation and protein length 30.

This graph shows that the energy ranges from -10 to -75, and it is the least when temperature is less than 1.5. The energy is almost the same for temperature higher than 1.5, this is due to the length of protein, length gives limitation to what energy the protein can have. Noticeably, there is a shape jump between temperature 1 and 1.5, this suggests that there exists a phase transition.