Lab Report 11

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Question 1 done by Juann Jeon
Question 2 done by Seunghyun Park
Lab Report done by Seunghyun Park & Juann Jeon

Q1 a)

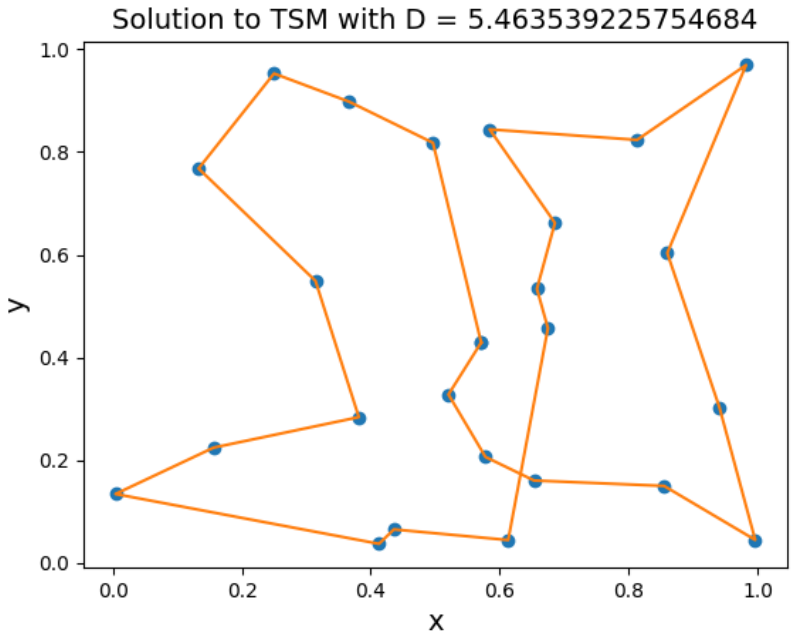

Figure 1: Solution to Traveling Salesman Problem with seed 11 and $\tau = 10^4$

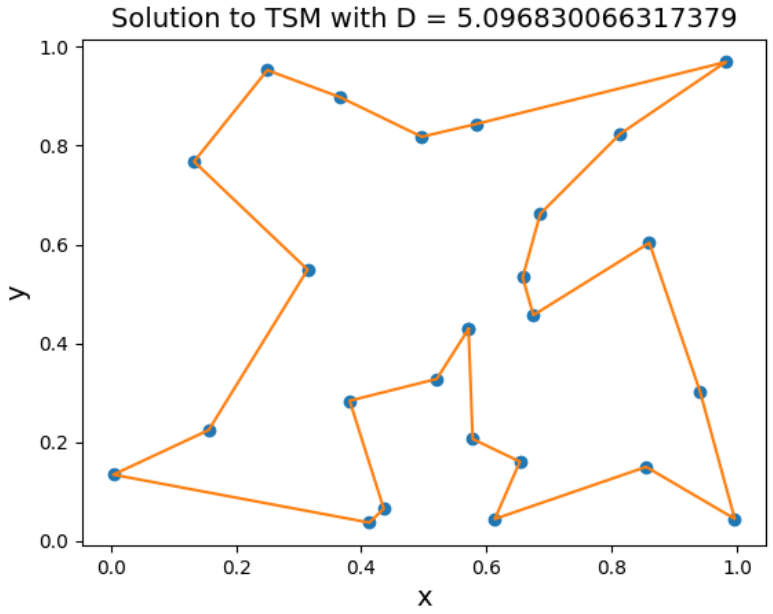

Figure 2: Solution to Traveling Salesman Problem with seed 12 and $\tau = 10^4$

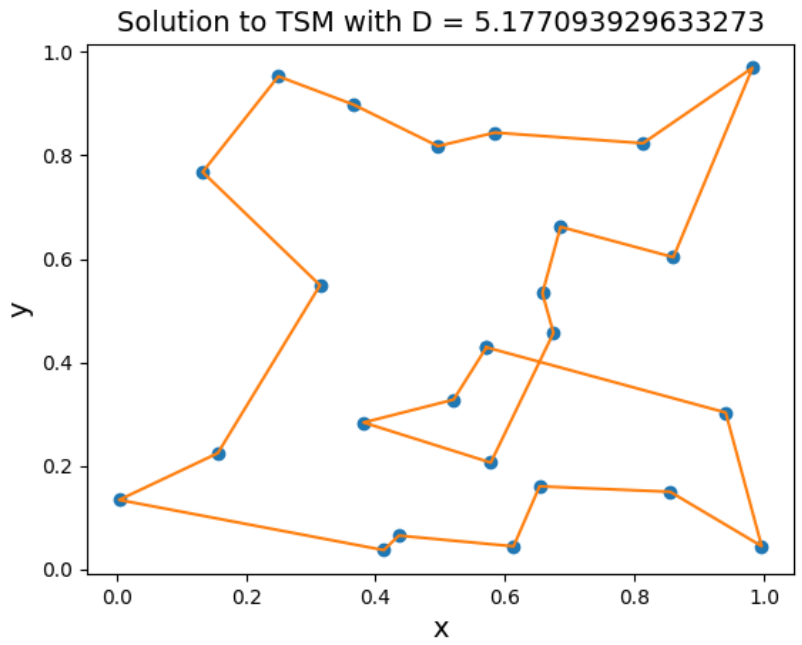

Figure 3: Solution to Traveling Salesman Problem with seed 13 and $\tau = 10^4$

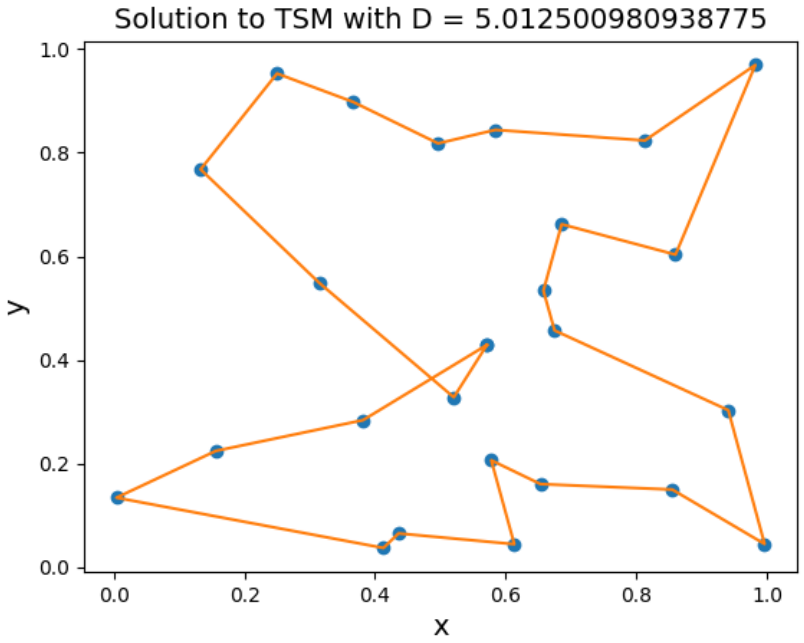

Figure 4: Solution to Traveling Salesman Problem with random seed and $\tau = 10^5$

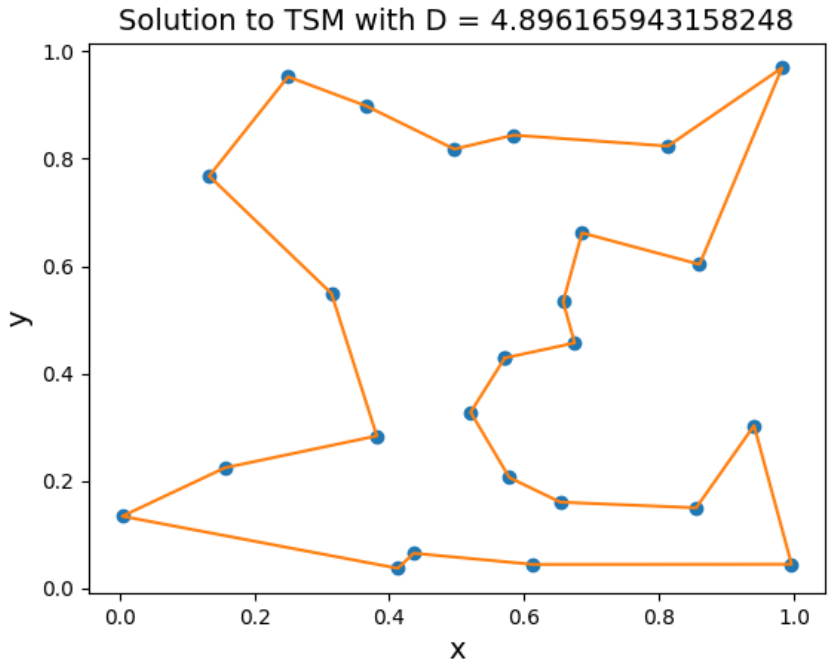

Figure 5: Solution to Traveling Salesman Problem with random seed and $\tau = 10^5$

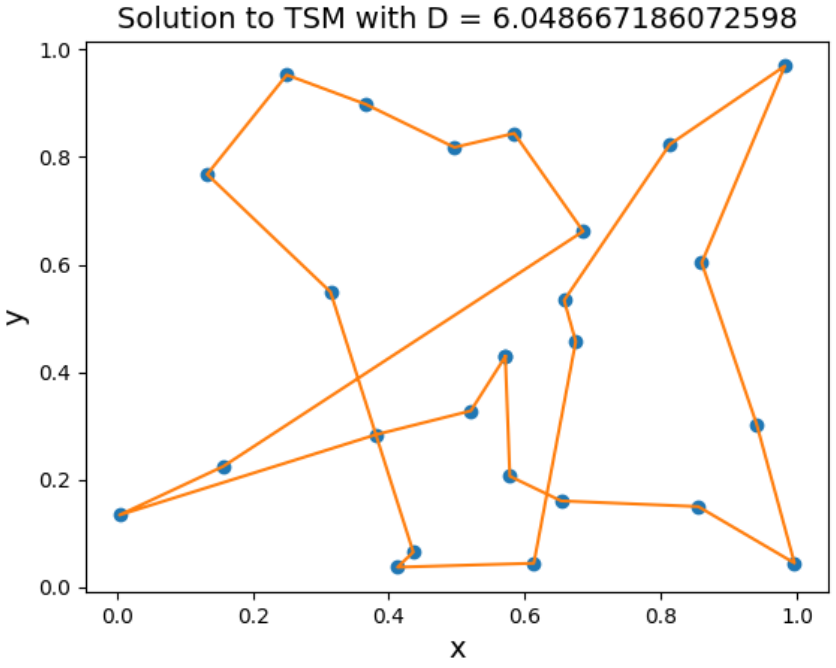

Figure 6: Solution to Traveling Salesman Problem with random seed and $\tau = 10^3$

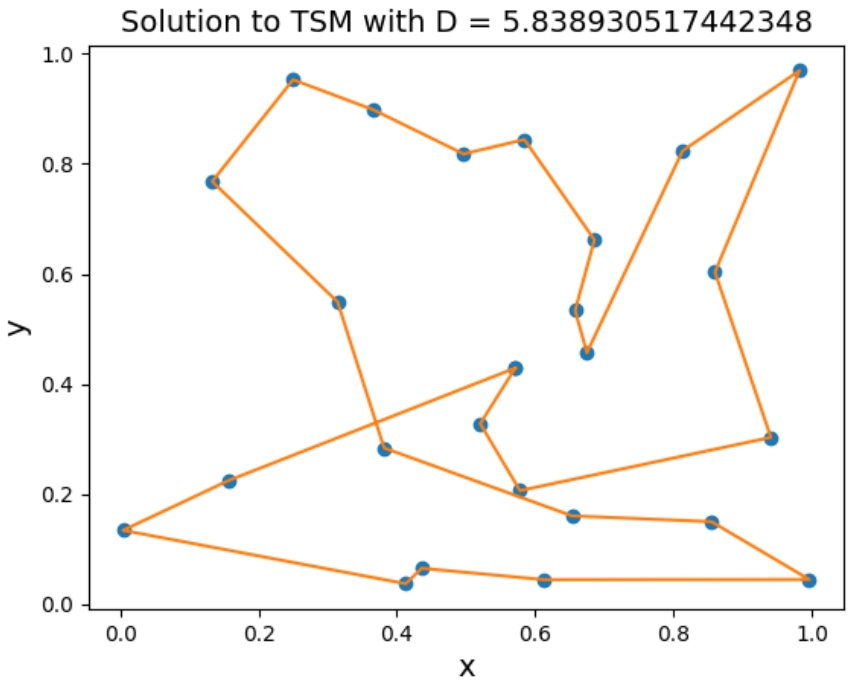

Figure 7: Solution to Traveling Salesman Problem with random seed and $\tau = 10^3$

Figure 1 to 7 coordinates are based on fixed seed 10. Figure 1 to 3 have fixed seed of 11, 12 and 13 in respective order with cooling schedule time constant $\tau = 10^4$ for annealing optimization. As seen from Figure 1 to 3, the distance D tends to vary between approximately 5.1 to 5.5. Figure 4 to 7 used random seed for annealing optimization, with Figure 4 and 5 using $\tau = 10^5$ and Figure 6 and 7 using $\tau = 10^3$. Notice that as system cools more slowly (i.e. τ is greater), the annealing optimization tends to find shorter distance D, and vice versa for when the system cools faster. However, having a bigger τ increases the time it takes for annealing optimization exponentially, which increases the time it takes for better annealing optimization very quickly.

Q1 b)

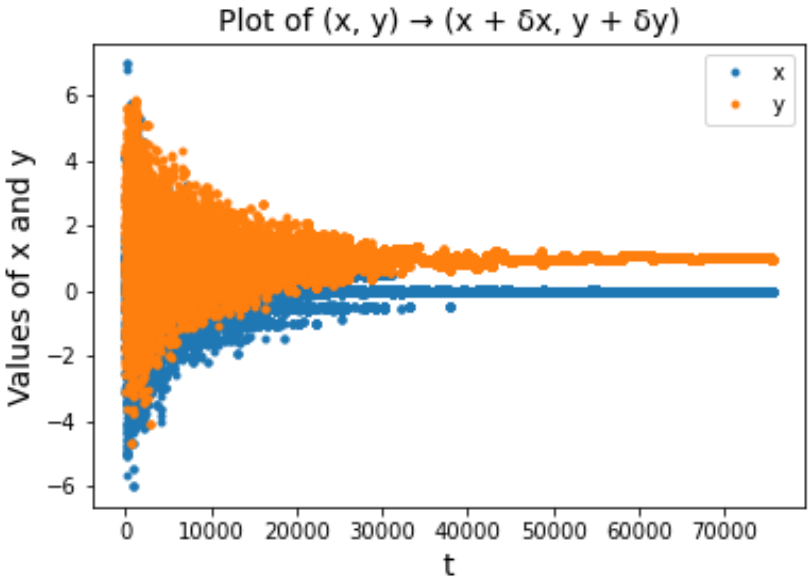

Figure 8: Plot of $(x,\ y) \rightarrow (x\ +\ \delta x,\ y\ +\ \delta y)$ vs time t, the number of runs

```
The global min happens at x = -0.003570078655925562
The global min happens at y = 0.9579826810606805
The global min of f(x, y) is -0.9972156269113981
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Figure 9: Final value of $(x,\ y)$ and $f(x,\ y)$

Q1 c)

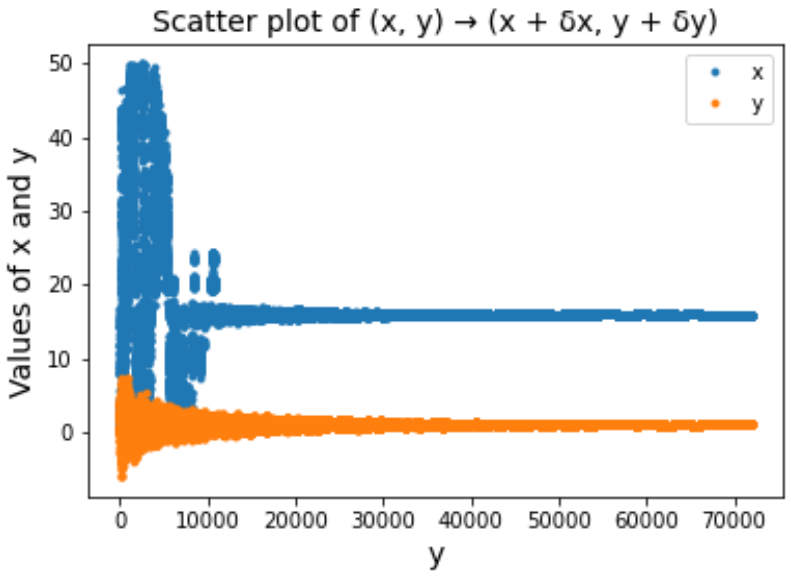

Figure 10: Plot of $(x,\ y) \rightarrow (x\ +\ \delta x,\ y\ +\ \delta y)$ vs time t, the number of runs

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The global min happens at x = 15.931827379863844
The global min happens at y = 0.9958218340484265
The global min of f(x, y) is -2.6106357876096267
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Figure 11: Final value of $(x,\ y)$ and $f(x,\ y)$

Q2 a)

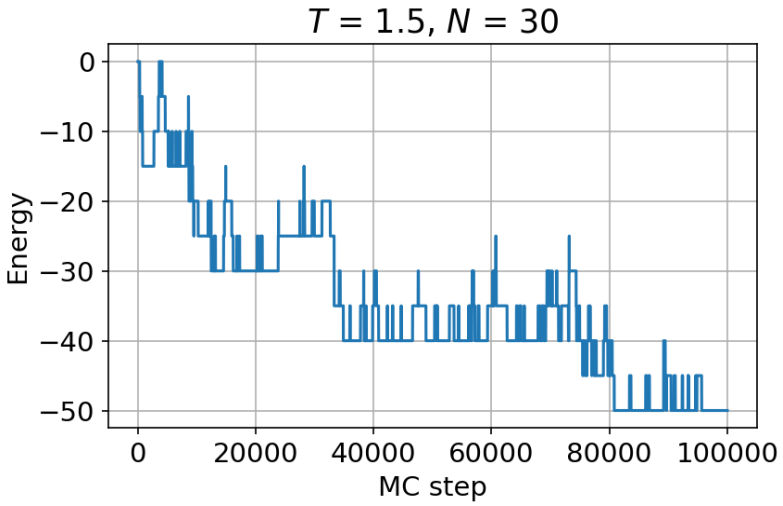

Figure 12: Energy as a function of the Monte Carlo step with T = 1.5

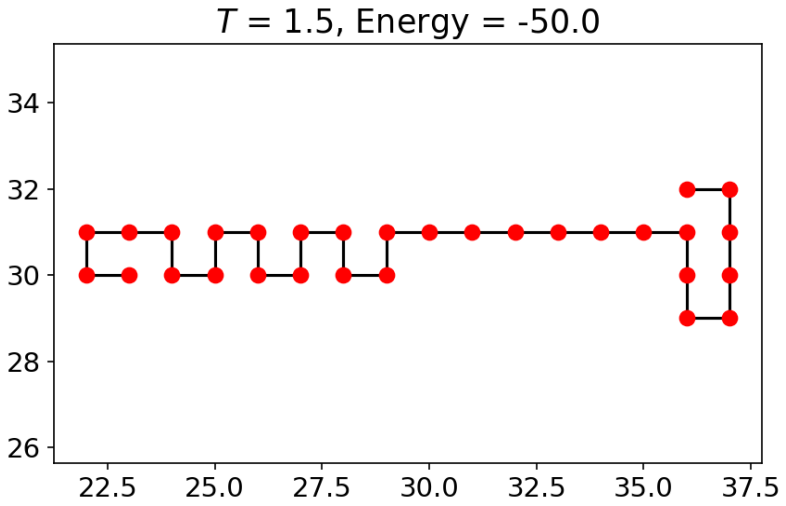

Figure 13: Final Structure of the Protein with T = 1.5

In the figure 12, the overall trend of the energy of the protein is decreasing and slightly fluctuates over the run. However, the energy of the protein never becomes stable and keeps changing until the simulation ends.

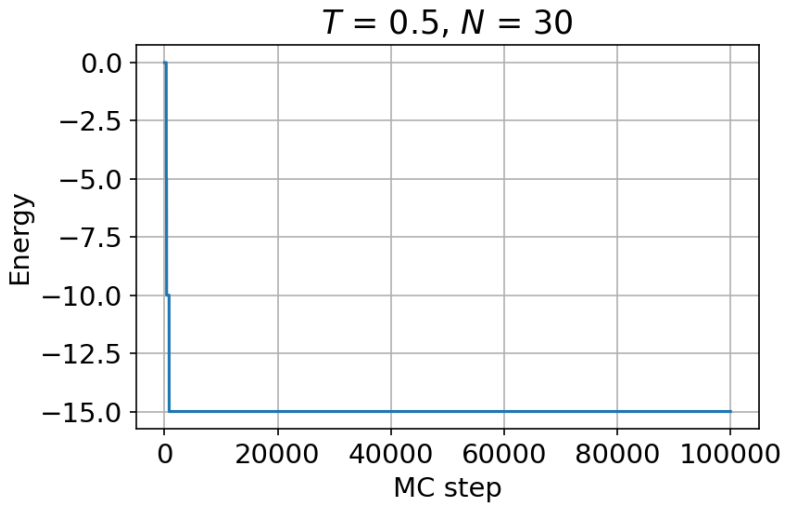

Figure 14: Energy as a function of the Monte Carlo step with T = 0.5

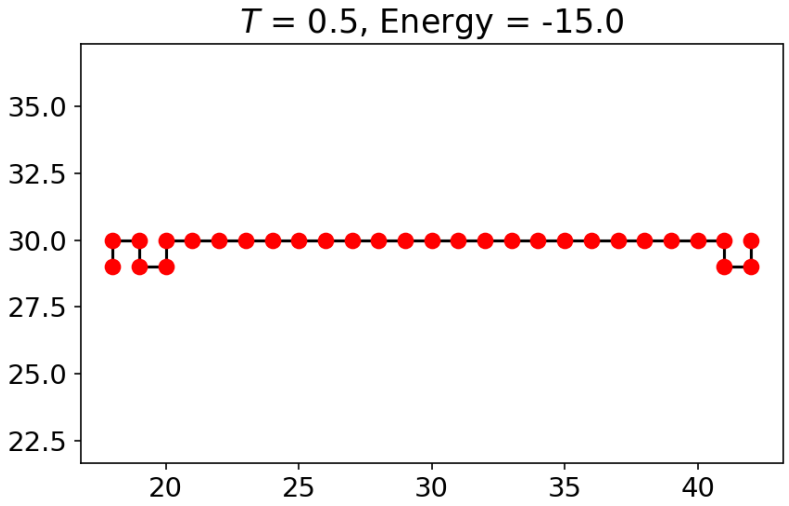

Figure 15: Final Structure of the Protein with T = 0.5

When temperature is 0.5, the energy of the system drops sharply from 0 to -15 at the very beginning of the simulation. After the sharp drop at the beginning, the energy plot of the system is a straight horizontal line and the energy stays at -15 until the simulation ends.

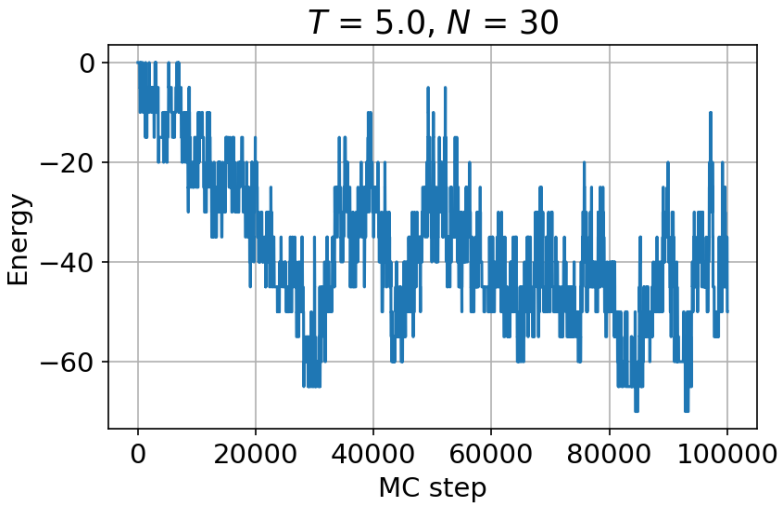

Figure 16: Energy as a function of the Monte Carlo step with T = 5.0

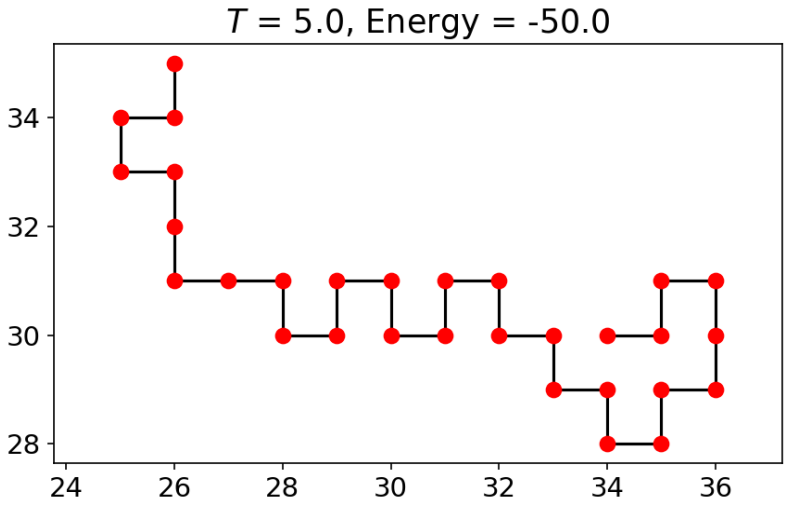

Figure 17: Final Structure of the Protein with T = 5.0

When T = 5.0, the energy plot fluctuates between 0 to -60 and never becomes stable. When the temperature is higher, we can see that the energy of the protein is lower than the energy with lower temperature.

Q2 b)

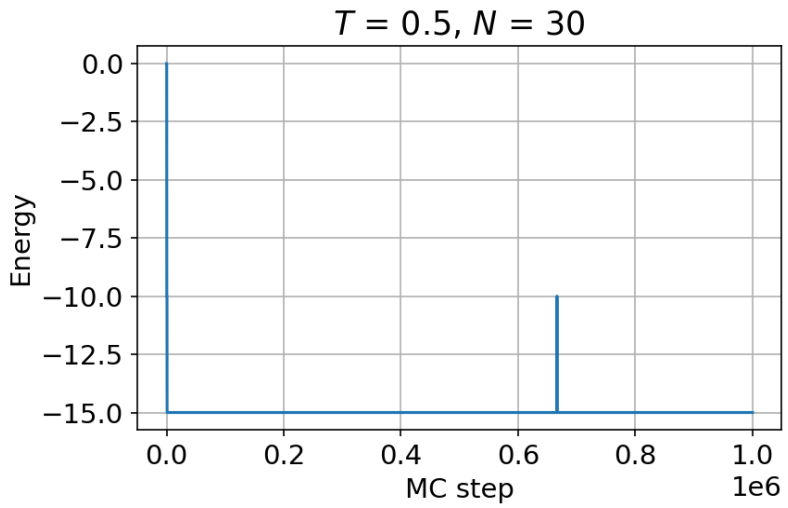

Figure 18: Energy as a function of the Monte Carlo step with T = 0.5 with 1,000,000 steps

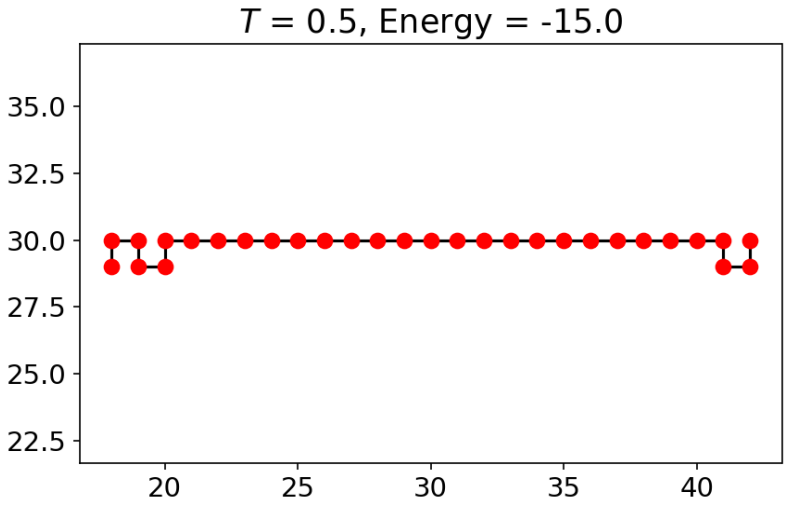

Figure 19: Final Structure of the Protein with T = 0.5 with 1,000,000 steps

When n = 1,000,000 steps, the energy of the protein of the second half of the simulation with T = 0.5 is -15, which is the same as the energy of the protein when the number of steps is 100,000. Also, the final structure of the protein with 1,000,000 steps is the same as the structure of the protein with 100,000 steps. This implies that when the temperature is equal to 0.5, the system is trapped in its local minimum and unable to escape from there. Therefore, there is no change even if we increase the number of simulation steps.

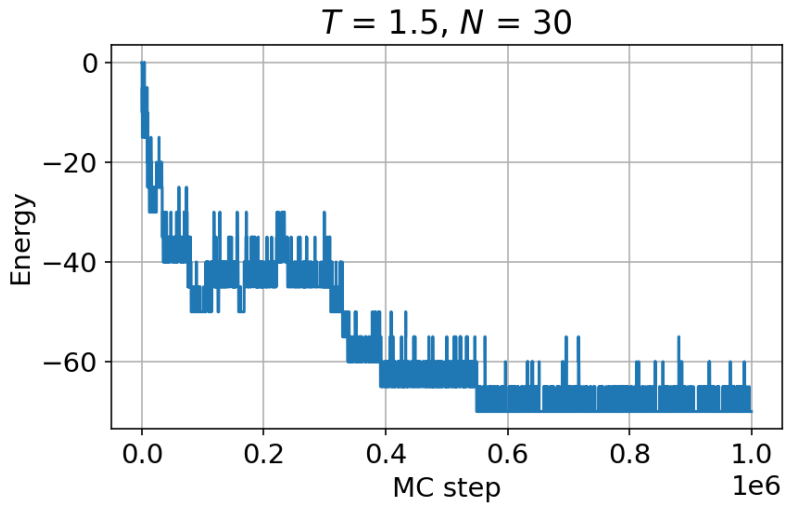

Figure 20: Energy as a function of the Monte Carlo step with T = 1.5 with 1,000,000 steps

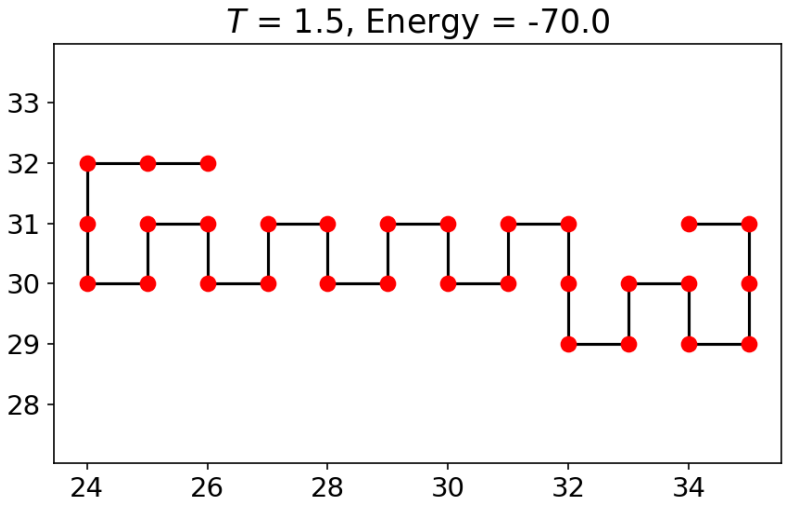

Figure 21: Final Structure of the Protein with T = 1.5 with 1,000,000 steps

With 1,000,000 Monte Carlo steps, the energy of the second half of the simulation with T = 1.5 is -70, which is lower than the energy obtained with 100,000 Monte Carlo steps. Unlike the energy plot of T=1.5 from part (a), the energy plot with larger Monte Carlo steps becomes stable over the last quarter of the simulation.

Q2 d)

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Energy averaged over last quarter of simulations is: -80.00
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Figure 22: Energy averaged over last quarter of the simulation with $T_f = 0.5$ & $n = 2 \times 10^6$

The approximate energy of the protein over last quarter of the simulation is -80.00. The energy obtained by using temperature steps is much lower than the energy from part (b). While the system from part (b) was stuck in the local minimum and was never able to escape from its local minimum, the system with steadily decreasing temperature was able to find global minimum energy of the system.

Q2 e)

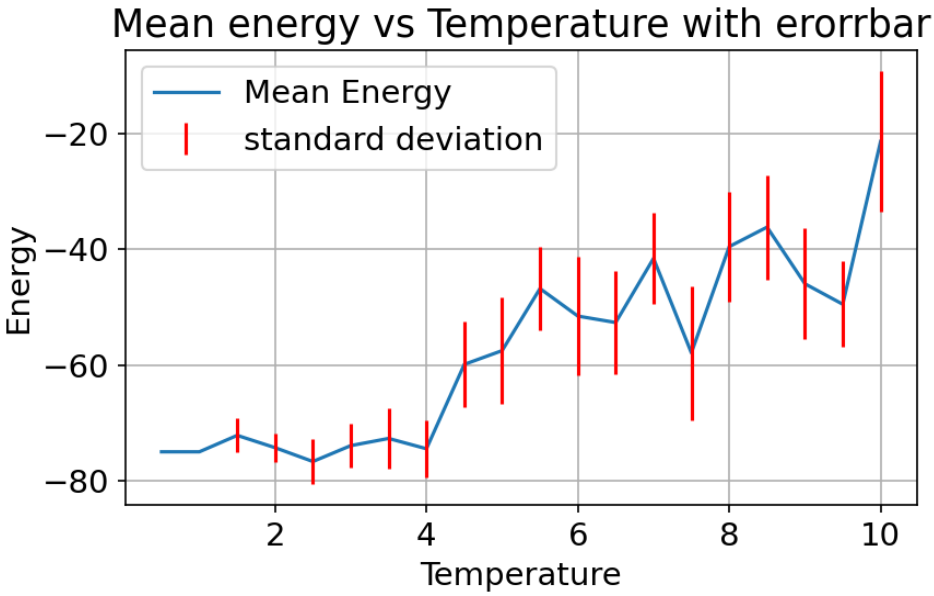

Figure 23: Mean energy versus temperature with standard deviation

The mean energy of the protein moves almost horizontally until the temperature becomes 4. Once the temperature reaches 4, the energy sharply increases to -60 and gradually increases with some fluctuations. From the plot, we can conclude that the phase transition of the protein occurs when the temperature is approximately between 4 and 5.