Lab Assignment 11: Monte Carlo simulations

Q1. Energy of system of free gas particles

a) Plots of system with T = 10 KbT

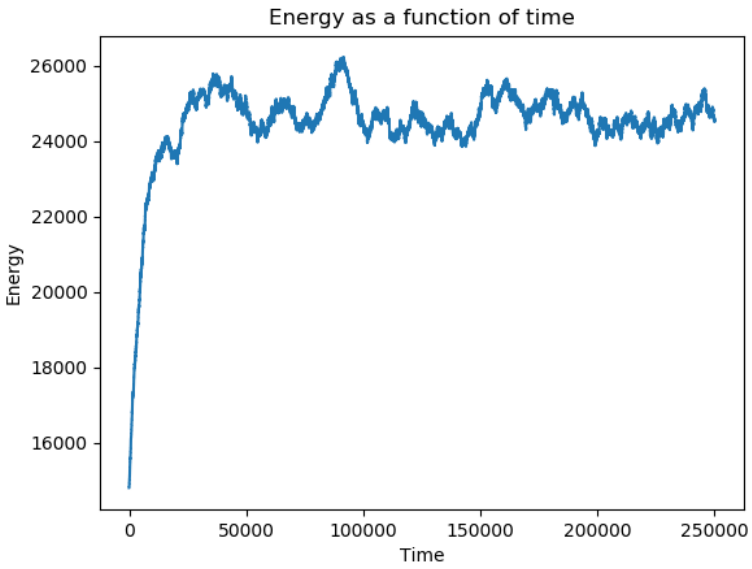


Figure 1. Plot of the system's energy as a function of time, for T = 10 KbT.

b)

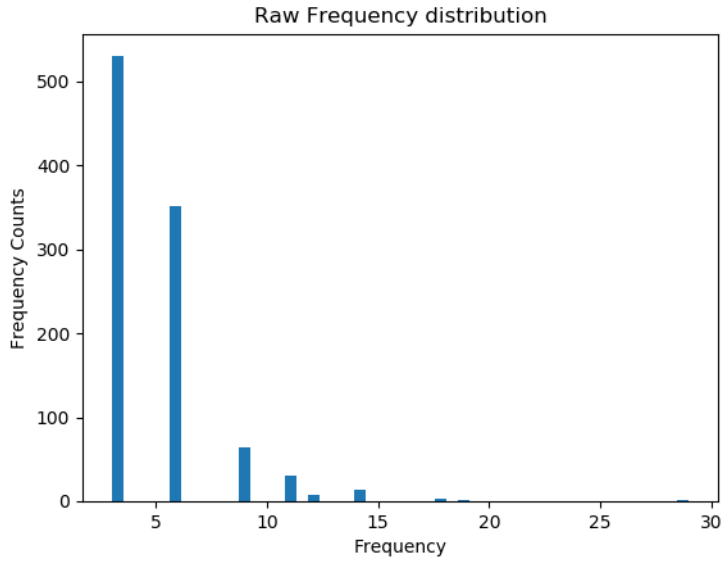
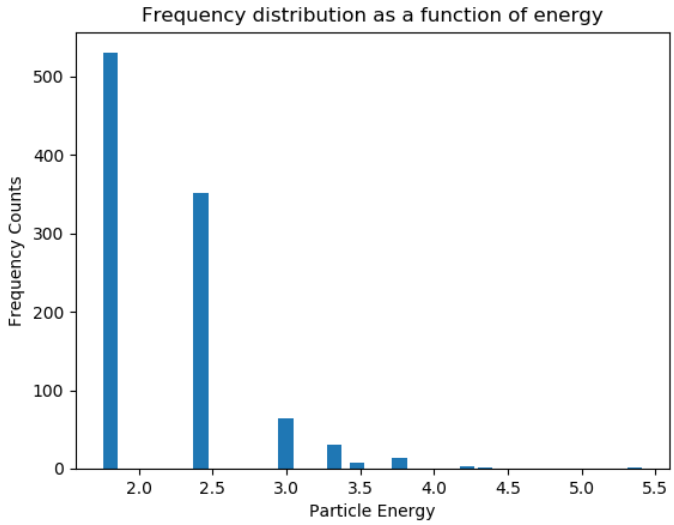


Figure 2. Histogram of the frequency distribution within the system.



c)

Figure 3. Histogram of the frequency distribution as a function of energy.

d) Plots of system with range of T = [10, 40, 100, 400, 1200, 1600] KbT

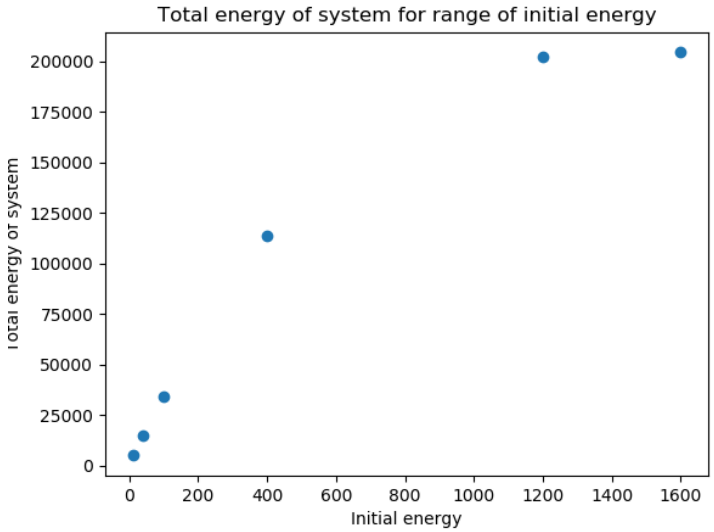


Figure 4. Plot of the final energy of the system as a function of its initial energy.

The heat capacity of the system was estimated to be 125.3849 Kb (Boltzmann constant).

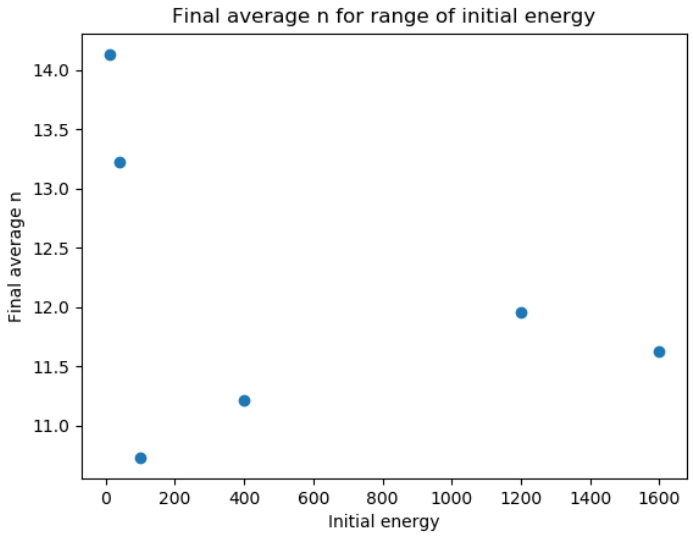


Figure 5. Plot of the final average quantum number of the system as a function of its initial energy.

Varying the initial energy of the system, we find that the final energy that is reached follows a parabolic curve, as shown in Figure 4 – the plot appears to plateau after a value of T = 1200 KbT. For the plot of the final average quantum number (n) of the system, it has a more complicated relationship with the system's initial energy – the average n undergoes a steep decrease between T = [0, 100] KbT, then a gentle increase between T = [100, 1200] KbT, and finally a gentle decrease between T = [1200, 1600] KbT.

To determine whether or not equilibrium was reached in each case, a "while loop" was implemented instead of the "for loop" that was given in Newman's original version of the Monte Carlo simulation. When comparing two non-interacting quantum ideal gas systems, we expected that the system with the greater initial energy would take more time steps to reach equilibrium. Given that T=10Kb was the lowest energy of the range, and based on the results of part a) where we found that this particular system reaches equilibrium by 250 000 time steps, all other systems were allowed to run for at least 250 000 time steps. After reaching 250 000 iterations, for every 500 steps thereafter the program will compare the minimum and maximum values of the last 1000 energy outputs of the program. If the absolute difference between the minimum and maximum values is smaller than 2000 KbT, it is assumed that equilibrium has been reached and the program exits the "while loop". The threshold value of 2000 KbT was determined based on the plateau region observed in the Energy vs Time plot shown in part a).

Below, we have added 3 of the 6 histograms that were outputted by the program; they display the frequency distribution within the system for T = 40, 400 and 1600 KbT. These plots are shown below to demonstrate the trend that was observed when the initial energy of the system (T) was gradually increased – the distribution gradually becomes less discretized, with more frequency values being reached in the system.

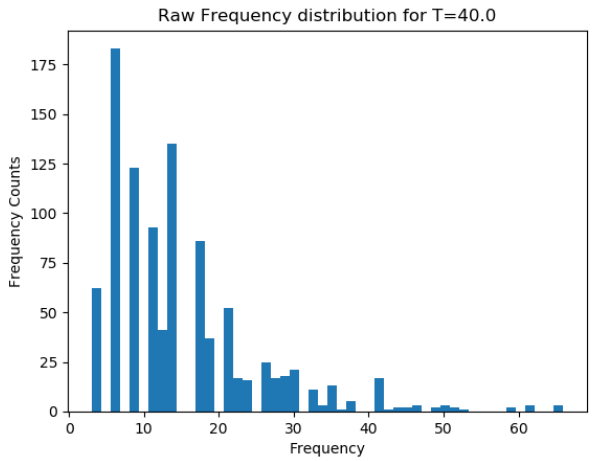


Figure 6. Histogram of the frequency distribution for T = 40 KbT.

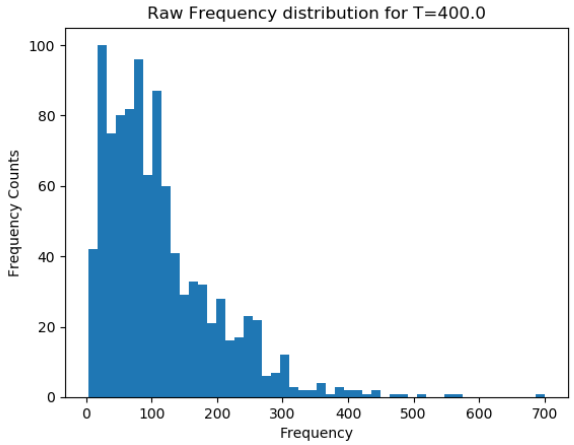


Figure 7. Histogram of the frequency distribution for T = 400 KbT.

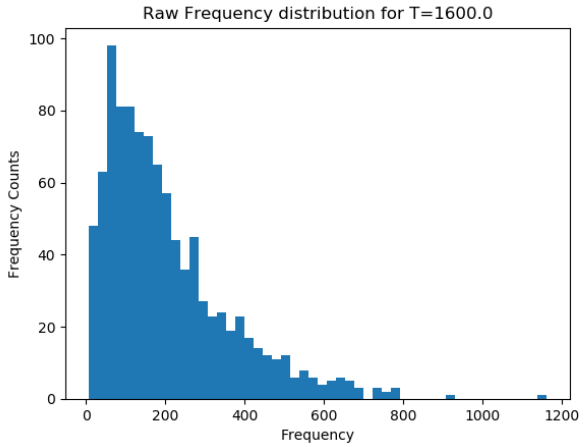


Figure 8. Histogram of the frequency distribution for T = 1600 KbT.

Q2. Ising model

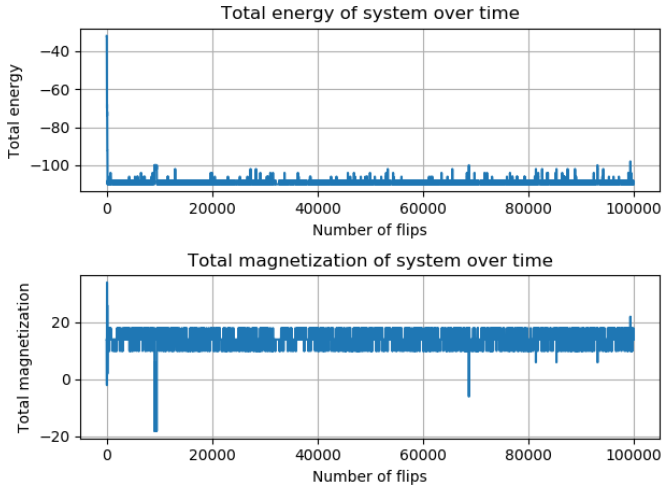


Figure 9. The top plot shows the total energy of the system over time, while the bottom plot shows the total magnetization of the system over time for T = 1.0 KbT.

Final magnetization for T=1.0 KbT was 14 units.

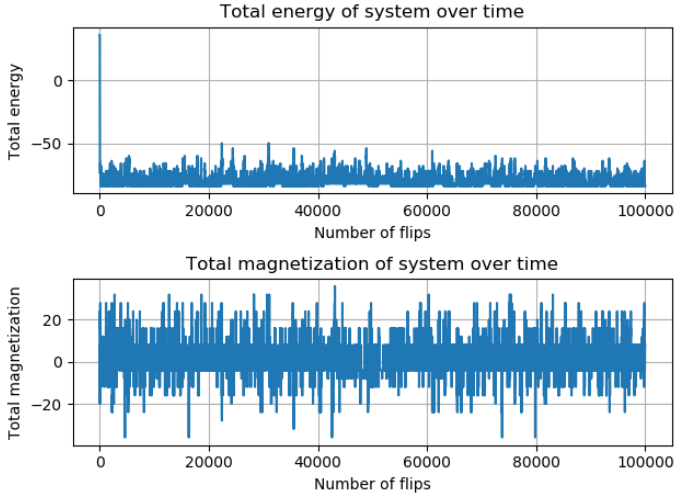


Figure 10. The top plot shows the total energy of the system over time, while the bottom plot shows the total magnetization of the system over time for T = 2.0 KbT.

Final magnetization for T=2.0 KbT was 8 units.

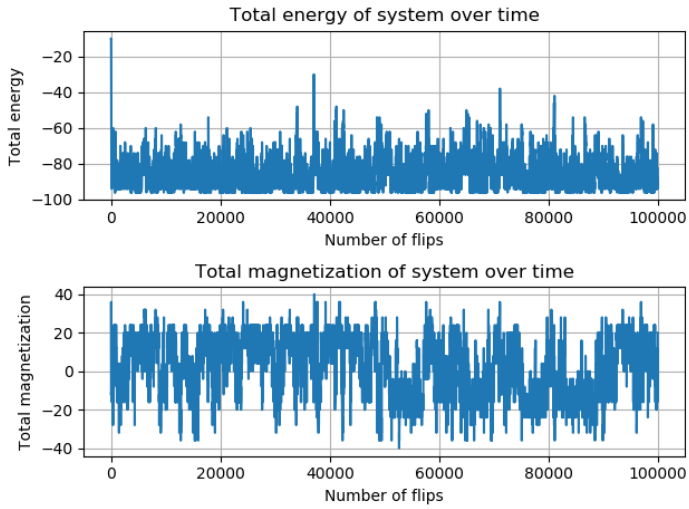


Figure 11. The top plot shows the total energy of the system over time, while the bottom plot shows the total magnetization of the system over time for T = 3.0 KbT.

Final magnetization for T=3.0 KbT was -8 units.

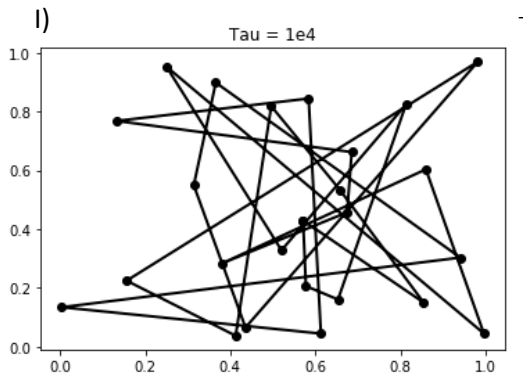
First, we ran the program several times for the system with T = 1.0 KbT alone and observed that the magnitude of the magnetization was usually on the order of 10 – 20 units. There was no apparent bias for the value to either be positive or negative.

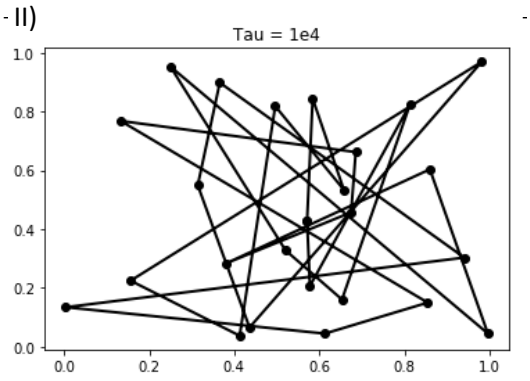
Next, we ran the simulation for T = 1.0, 2.0, and 3.0 KbT and animated the process of the system acquiring a net magnetization. We observed that as the initial energy of the system increased, the frequency of dipole flips also increased. While the animation for T = 1.0 KbT was relatively stagnant, the animation for 3.0 KbT was filled with dipoles flips during almost every frame that was shown.

The Ising model was created to simulate a ferromagnetic material, in which energy is lowered when the dipoles within the material are aligned. For lower values of initial energy (T), this suggests that the outputted magnetization of the system will likely have a large magnitude, with no preference regarding its sign (positive/negative). This is because at lower energy we would expect a more uniform distribution of the dipoles over time and thus a larger overall magnetization. This prediction was confirmed in Figures 9, 10, and 11: as the initial energy of the system increased, so did the variance of the system's magnetization, leading to a decrease in the magnitude of the outputted magnetization.

Q3. Simulated annealing

The following problem asked for modifications to the tau value in the salesman_start.py program. The idea behind the program is to use Monte Carlo to determine the shortest distance connecting randomly generated points. Annealing was incorporated to reach the global minimum of the system's energy by slowly cooling the system. The energy is minimized when the shortest distance between points is used. To do so, city points are randomly generated. The distances between points as well as changes in these distances are calculated. The program decides whether a certain path should be chosen based on the Boltzmann probability model, using changes in distance as an analogy for changes in energy. As expected, the final value of the distance (D) changes each time the city positions are randomly generated. There does not seem to be a major impact on D as the system is cooled down more or less quickly.





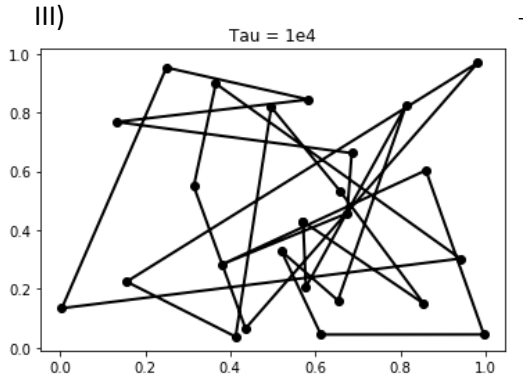
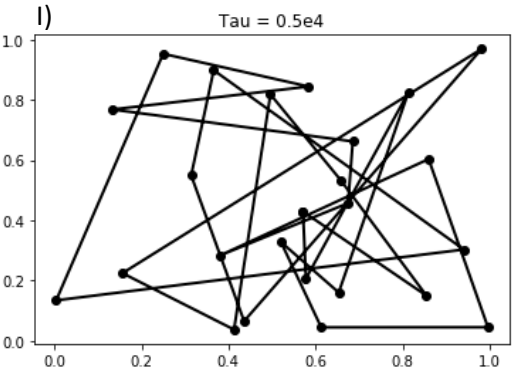


Figure 11. The pictures above show the path travelled by the travelling man with different seed values put into place.

I) Uses seed(2) into place and the D value was measured to be 14.620091025614725. II) Uses seed(5) and the D value was calculated to be 14.691707557421747. Lastly, III) uses seed(8) and had a calculated D value of 13.445934091978504. For all instances, tau was left to be 1e4. The different seed value means that different city positions were chosen.



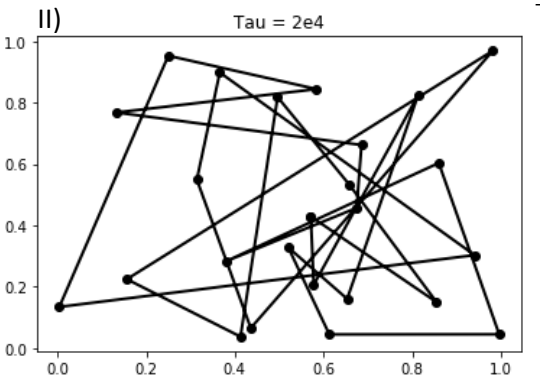


Figure 12. Here we compare the effect of different tau values on the value of D. For both I and II, seed(8) was used. I) had a tau value of 0.5e4 and II) had a tau value of 2e4. Both instances returned a D value of 13.445934091978504

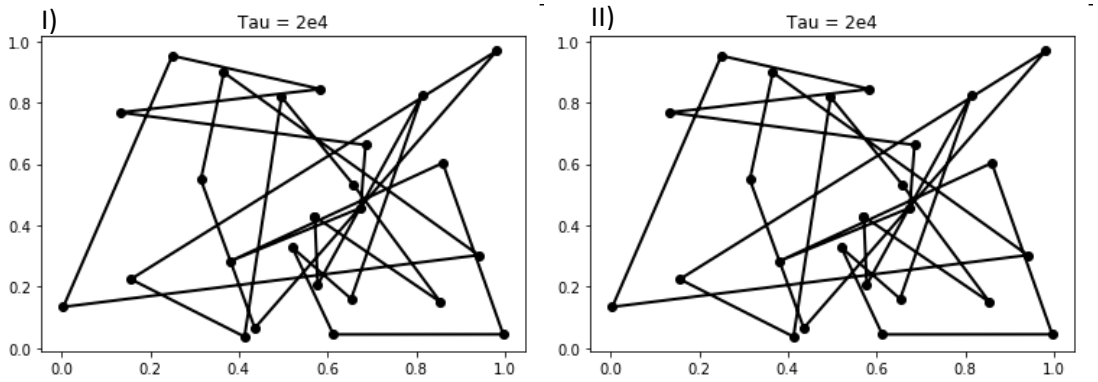


Figure 13. Here we compare the effect of different seed values on the value of D. For both I and II, tau = 2e4 was used. I) used seed(8) and returned D = 13.445934091978504 and II) used seed(2) and returned D = 14.620091025614725

Q4. Dimer covering problem

This program simulates dimers falling onto a lattice. These dimers cannot overlap oe another. As expected, when tau is lowered (faster cooling schedule), less dimers are able to fit on the grid. This is the result of the system not fully reaching the global minimum which is defined as when the whole lattice is filled with dimers.

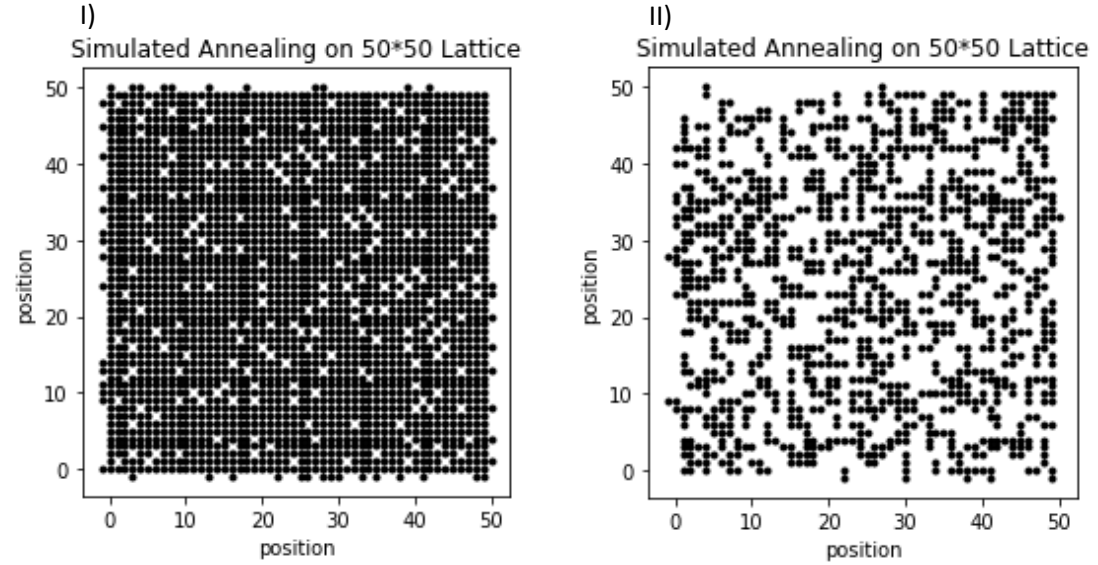


Figure 14. I and II both show simulated annealing on a 50 by 50 lattice. I) uses a tau = 10,000 and II) uses tau = 100.