Albert Wiryawan
avw2@illinois.edu
673431511
PHYS 466: Atomic Scale Simulation

Homework #2

Problem #1

A)

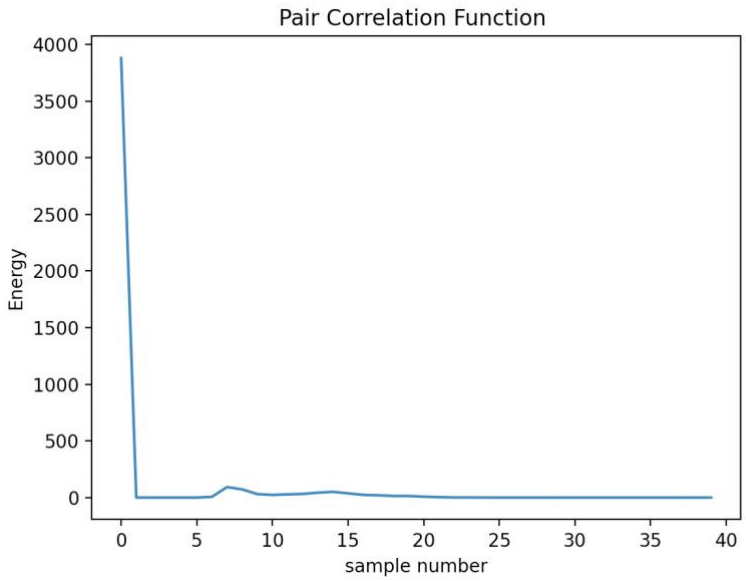


Figure 1. Pair correlation function for Lennard Jones simulation

B)

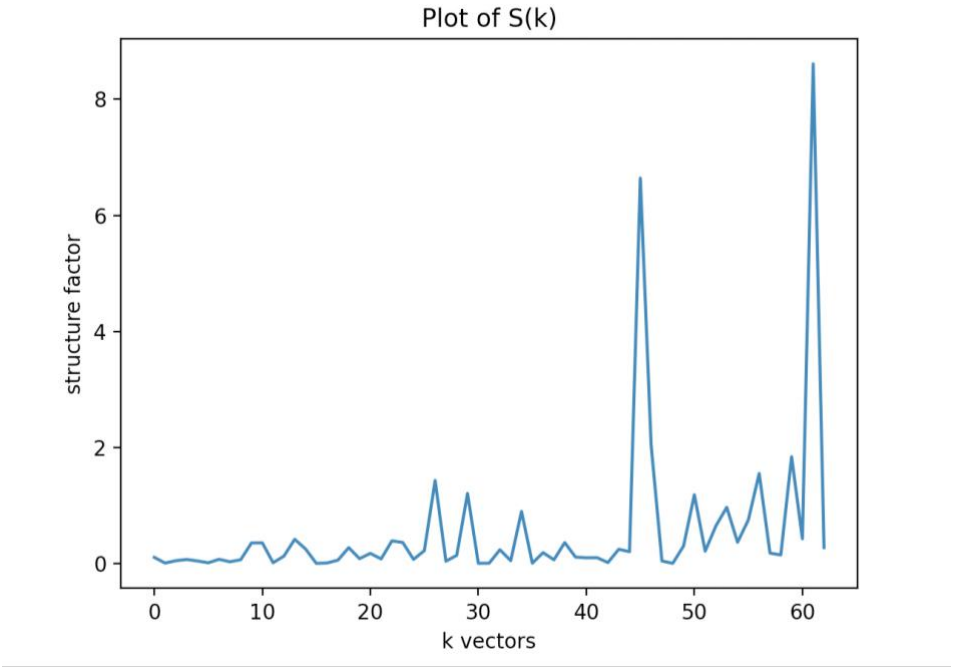


Figure 2. S(k) vs k vectors

In liquids, g(r) will have a smoother peak with the order of 1 and the structure factors will only have small peaks. For solids, g(r) will have more peaks compared to that of g(r) for liquids. In addition, the structure factor of a solid will have steeper peaks similar to that seen by the image above.

C)

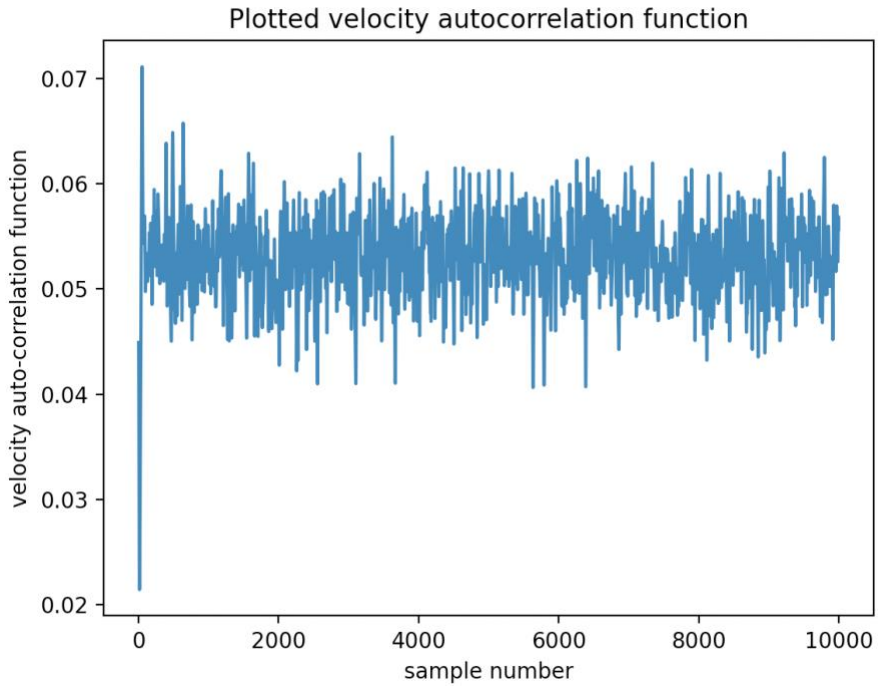


Figure 3. Plotted Velocity autocorrelation function

D) After filtering out the noise by utilizing the first 300 points, the diffusion constant is approximately 0.1676.

Problem #2

A)

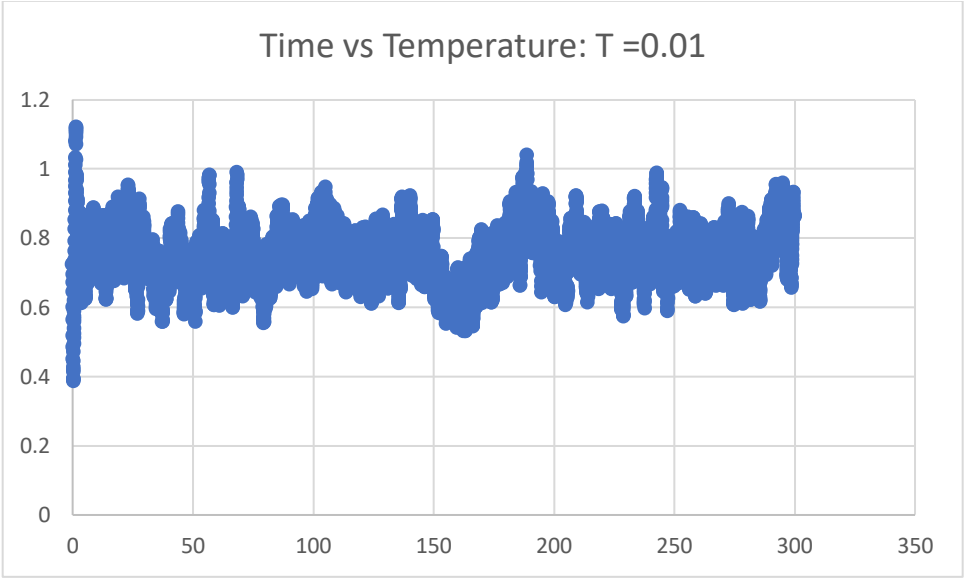


Figure 4. Time vs Temperature with thermostat T = 0.01

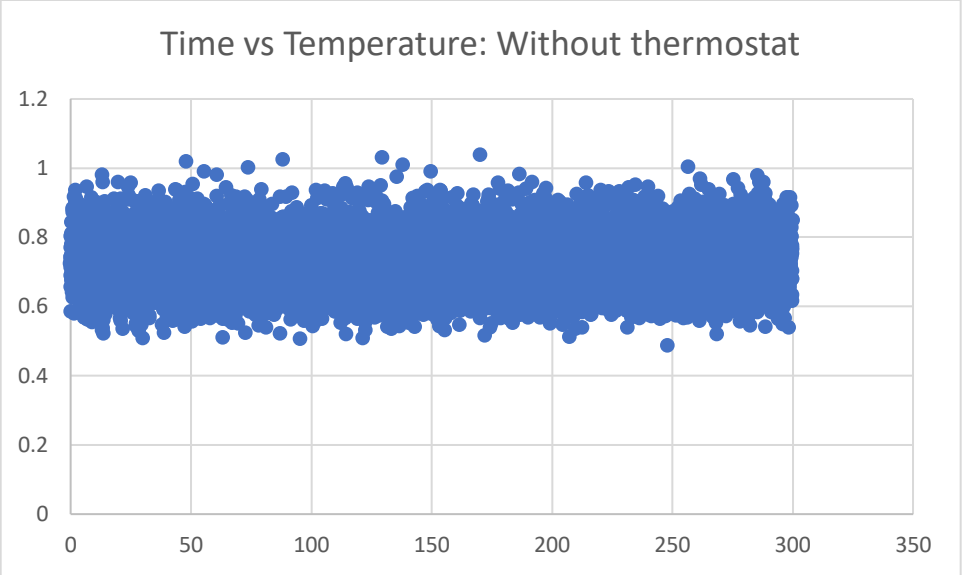


Figure 5. Time vs Temperature without Andersen Thermostat

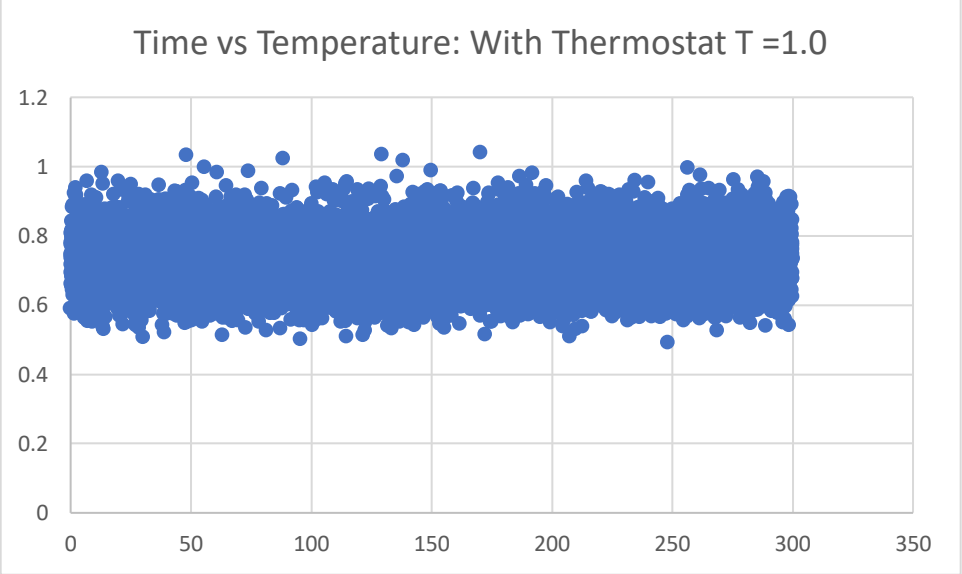
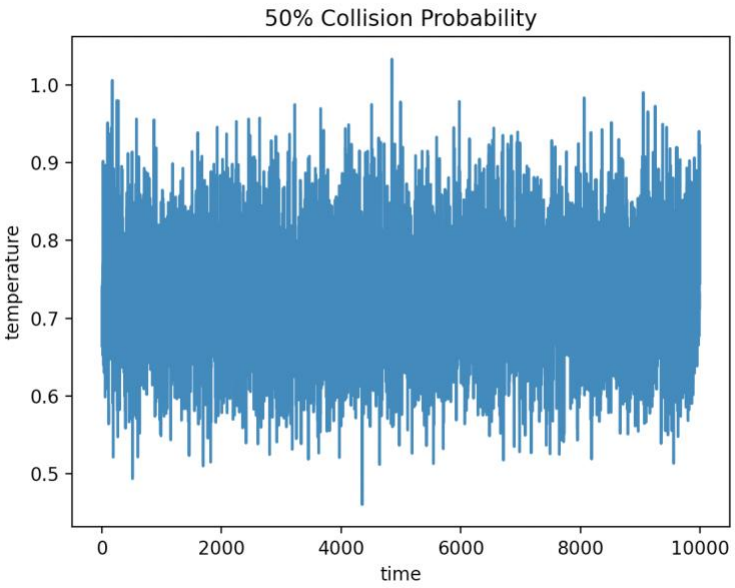
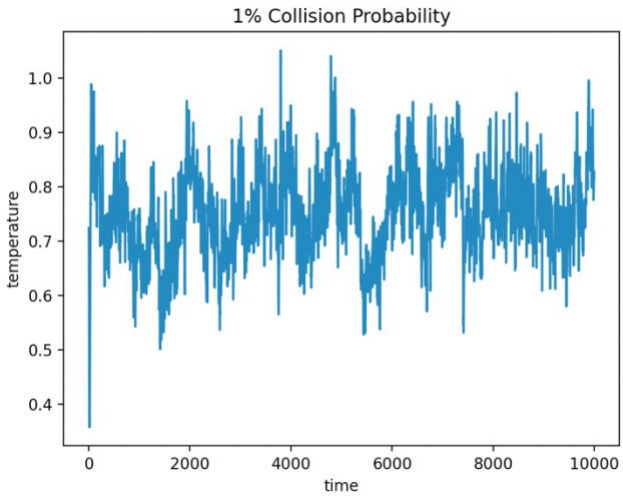


Figure 6. Time vs Temperature with Thermostat T= 1.0

B)

The diffusion constant when the thermostat probability of collision = 0.01 is 0. 1075 while the diffusion constant when probability of collision = 0.5 is 0.2013.





C) The use of Anderson thermostat allows temperature to be held at a constant during simulation. As a result of this, there is a reduction in the noise obtained through the graph and the points convergence pattern becomes more recognizable.

Problem #3

In order to determine the phase of the system S(k) plots need to be produced for various temperatures between 0.5 and 3.5. However, the graphs that I have been producing for s(K) us mostly incorrect.