PHYS-E0412 Computational Physics

# Homework 5

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## a

In figure 1 we can see different energies of a two particle system where the particles were set at the origin and at point [0, 0, 1.2]. From the total energy we can see that the energy is conserved as the particles oscillate.

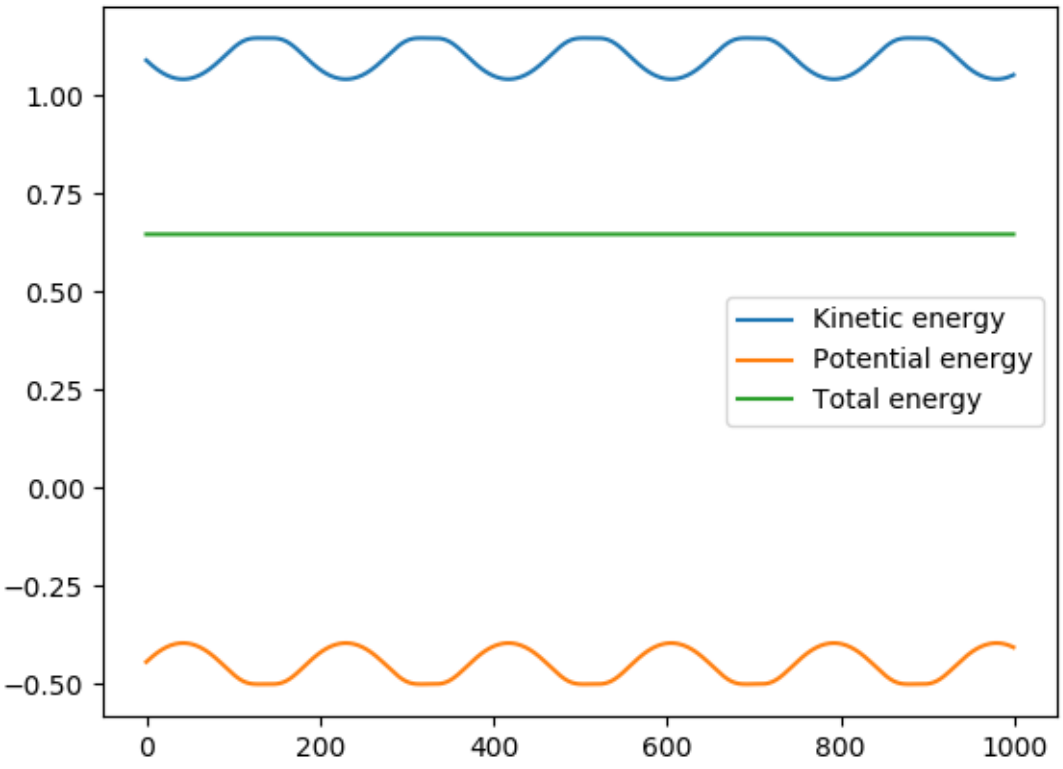


**Figure 1:** The kinetic, potential and total energy of a two particle system

## b

In figure 2 we can see radial distribution function of the system with 108 particles, $\rho = 0.884$ and initial temperature $T = 0.728$. The first peak is located around the Lennard-Jones potential

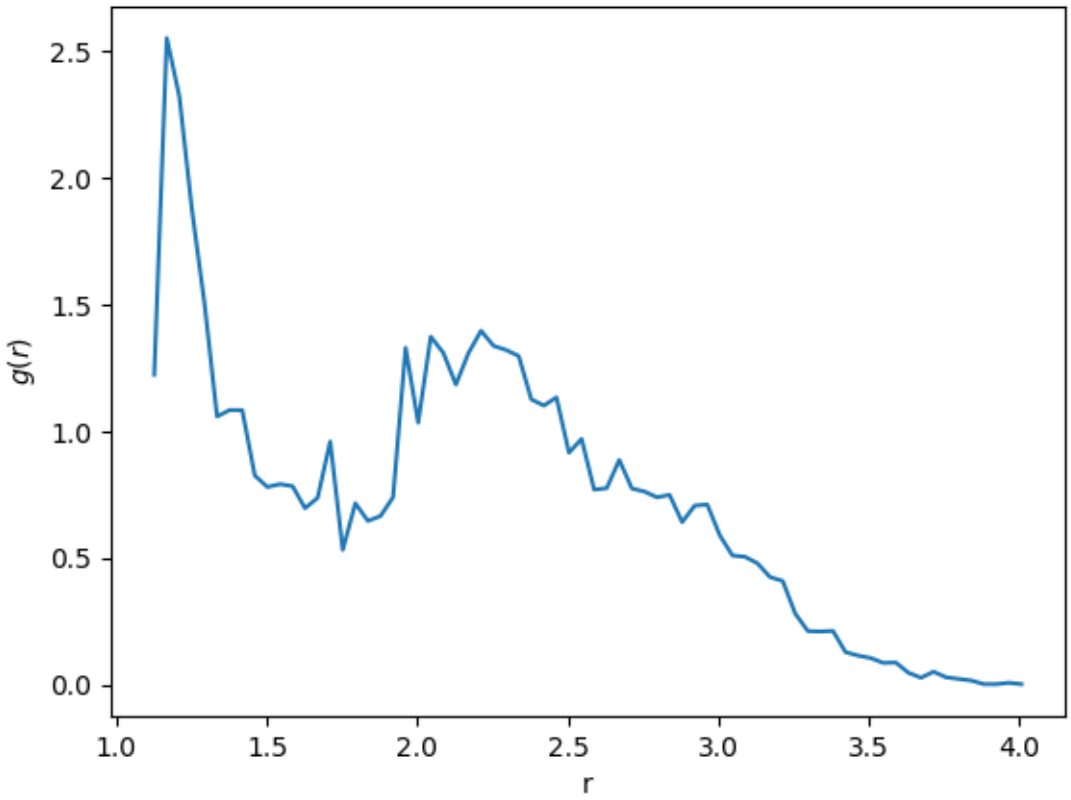


**Figure 2:** Radial distribution function with 108 particles, $\rho = 0.884$ and $T = 0.728$.

minimum of the system since that is where the force acting on the particle is minimized hence we are most likely to find a particle at that distance from another particle.

## c

In figure 3 there is the radial distribution function of a system with initial value $T = 2$. The system should probably be in a gaseous state but based on the radial distribution does not seem right. For a Lennard-Jones gas the RDF should still have a peak at around 1.1 that would fade out to 1 when $r$ approaches infinity. However, my result seems to result some kind of a Gaussian distribution.

I did not try to implement face centered cubic initial state since I battled so long with even the liquid state and based on the gas experiment even my implementation for simple cubic system does not seem to work.

## d

I used about 11 hours for this exercise.

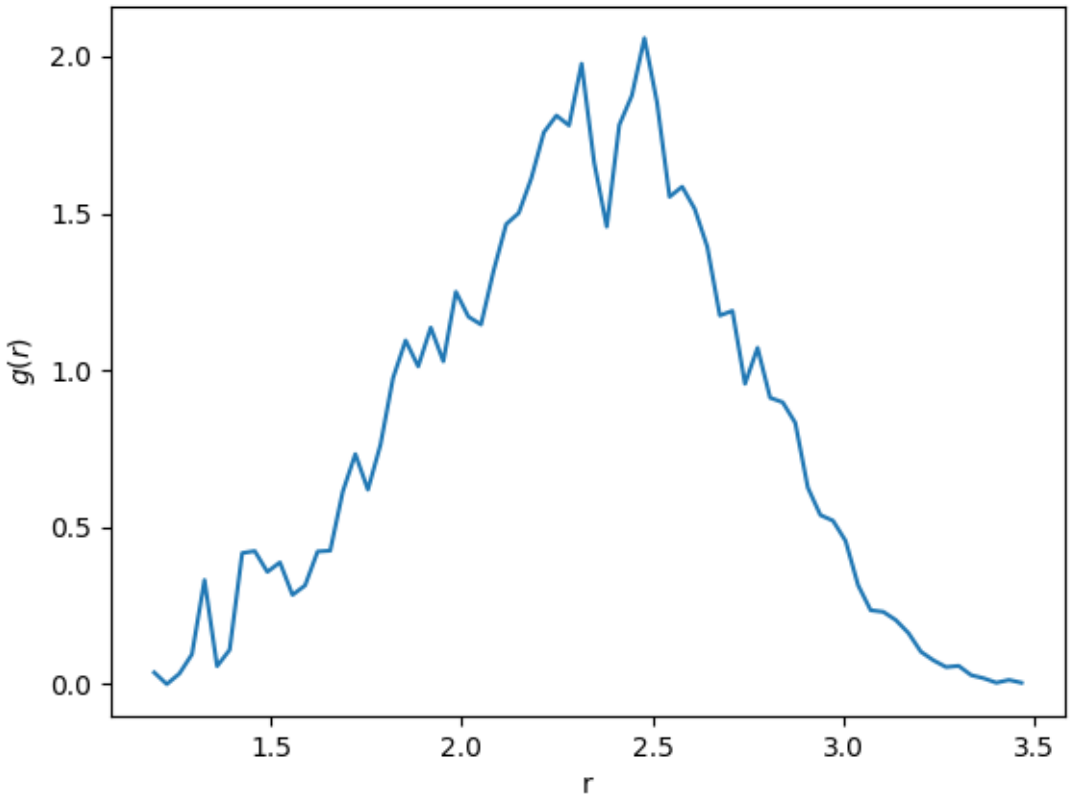


**Figure 3:** My radial distribution function with $T = 2$