Physics of Soft Condensed Matter

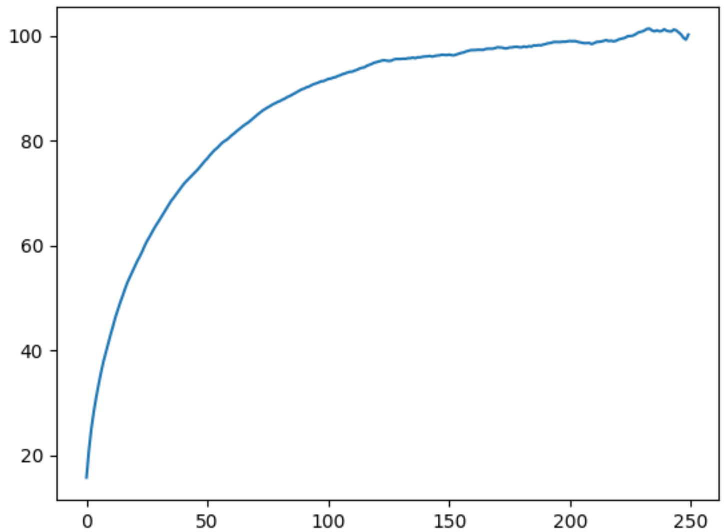
Created By	Ⓝ Nishant Sachdeva
Roll Number	2018111040

There are 4 parts of the assignment :

1. **Mean Square Distribution / Diffusion Coefficient**
2. **Van Hoe Function**
3. **Velocity Correlation Function**
4. **Dipole Dipole Time Correlation Function**

Following are the write ups and observations on each:

MEAN SQUARE DISTRIBUTION



This is a measure of the displacement of the particle over different time periods with respect to a given reference position and time.

Here , in the graph, we see how with time, on an average ,the displacement of a particle is increasing.

$$MSD(t) = \frac{1}{TN} \sum_{t_0=0}^{T} \sum_{i=1}^{N} (r_i(t_0 + t) - r_i(t_0))^2$$

The diffusion coefficient (accounting for some multiplier factors) comes out to be proportional to 0.004 A^2/ps . This is proportional to the slope of the curve at higher values of t.

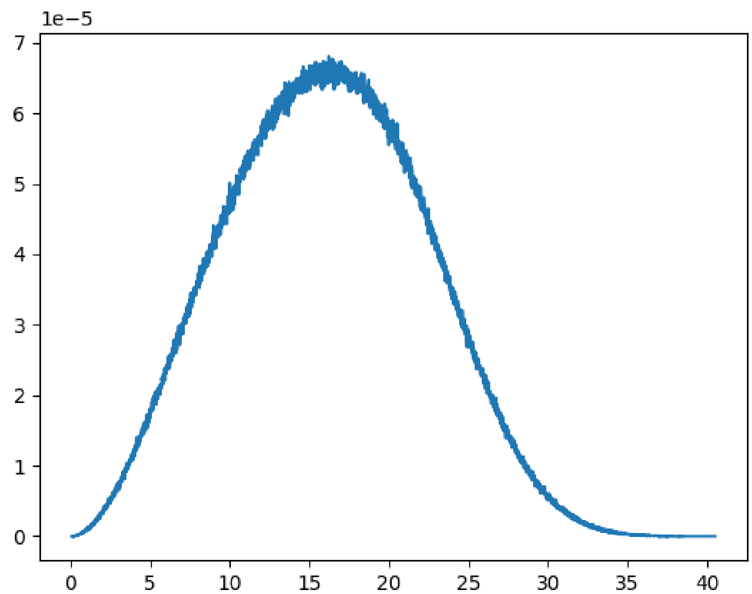
CODE ::

python3 run.py

⇒ data.txt (path to input file)

⇒ enter the value as '1' to run the msd function and display the diffusion coefficient

VAN HOVE FUNCTION



Van Hove function signifies the chances of spotting a particle i in the region of radius r at a given time t . This is calculated knowing that a particle j is in the vicinity of the origin at time t = 0

$$G(r,t) = \frac{1}{N}\sum_{i=0}^{N}\sum_{j=0}^{N}\delta(r-(r_j(t)-r_i(0)))$$

This particular curve represents Van Hove at a time t = 200 . We see, even for other values (although their calculation is really slow, so, we don't plot the graph here), the curve is a Gaussian curve. This shows how the distribution varies for various distances.

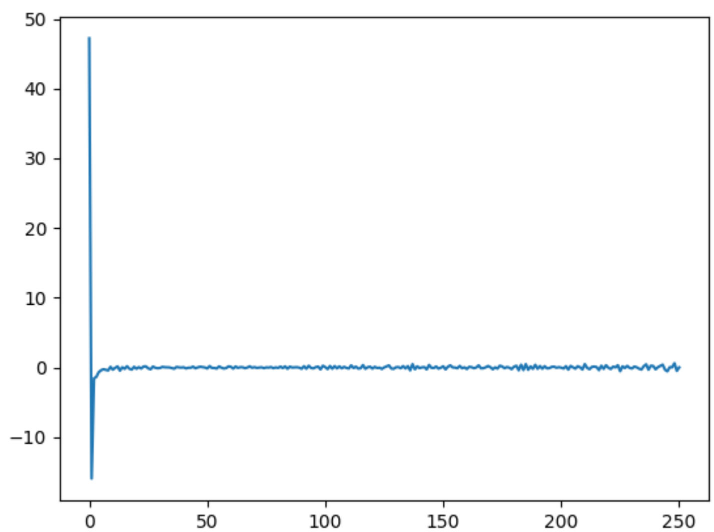
CODE ::

python3 run.py

⇒ data.txt (path to input file)

⇒ enter the value as '2' to run the Van hove function

VELOCITY CORRELATION FUNCTION



This curve displays the correlation between the velocity vectors at various times in the given intervals

$$v(t) = \frac{1}{T} \sum_{t_0=0}^{T} < v_i(t_0 + t) \; v_i(t_0) >$$

Here we see, how in the starting, when all the velocities are mostly same, the correlation is high, and how it goes towards a negative spike as all molecules turn together.

We also see how with time, when velocities become random, the correlation reduces and hovers around the 0 mark, sometimes being positive and sometimes negative.

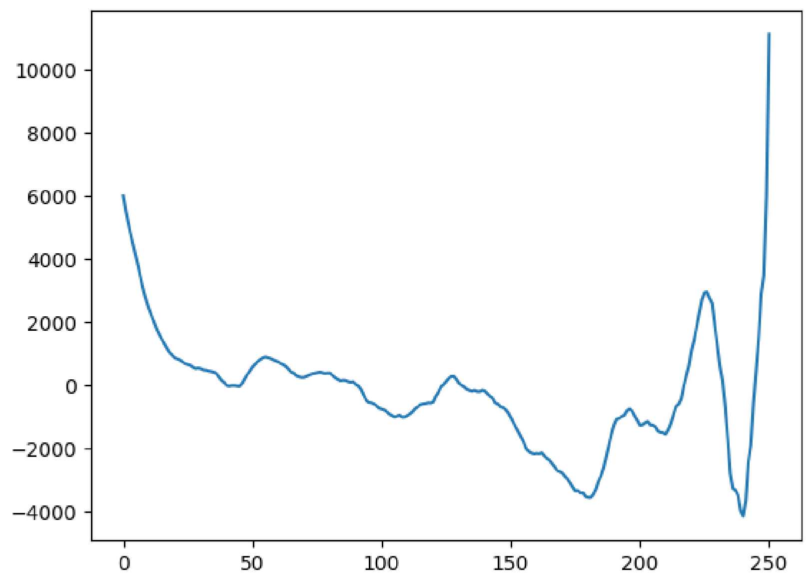
CODE ::

python3 run.py

⇒ data.txt (path to input file)

⇒ enter the value as '3' to run the Velocity Correlation function

DIPOLE - DIPOLE TIME CORRELATION FUNCTION



This curve represents the Total Dipole-Dipole time Correlation function for the given molecular structure.

$$V(t) = \frac{1}{T} \sum_{t_0=0}^{T} < V(t_0 + t)\ V(t_0) >$$

We see here, how with time , the dipole varies in time and how it decreases over time

CODE ::

python3 run.py

⇒ data.txt (path to input file)

⇒ enter the value as '4' to run the Dipole Dipole time correlation function