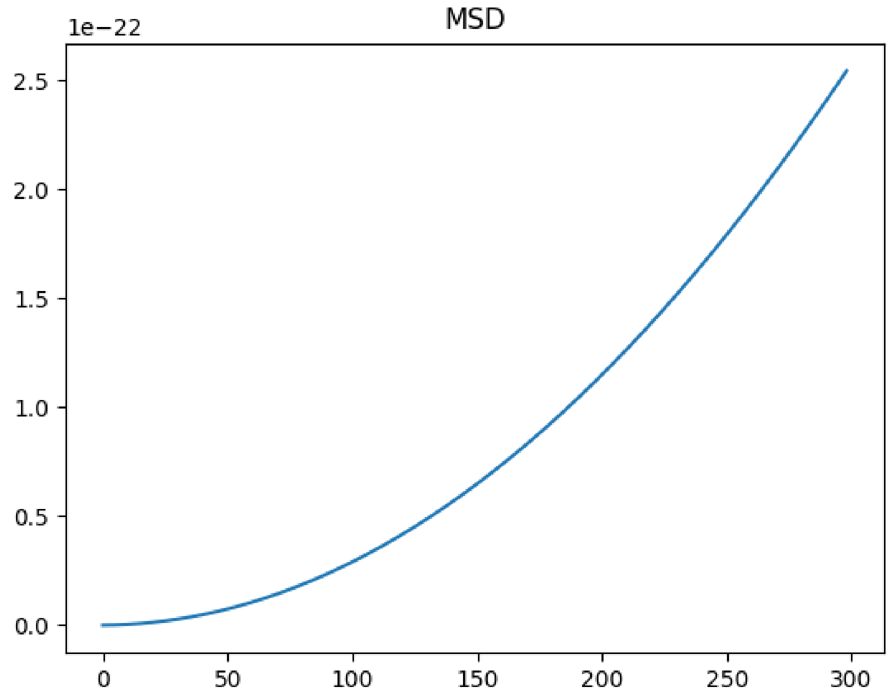
REPORT

There are 4 parts of the assignment :

- **Taking an Initial Configuration**
- **Finding out the Total Potential Energy**
- **Finding out the configuration with min Potential Energy using Gradient Descent**
- **Finding out forces, new velocities and generating the requisite number of frames**
- **Once the Frames have been generated, the following four functions are implemented**
    1. **Mean Square Distribution / Diffusion Coefficient**
    2. **Van Hoe Function**
    3. **Velocity Correlation Function**
    4. **Dynamic Structure Factor**

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.

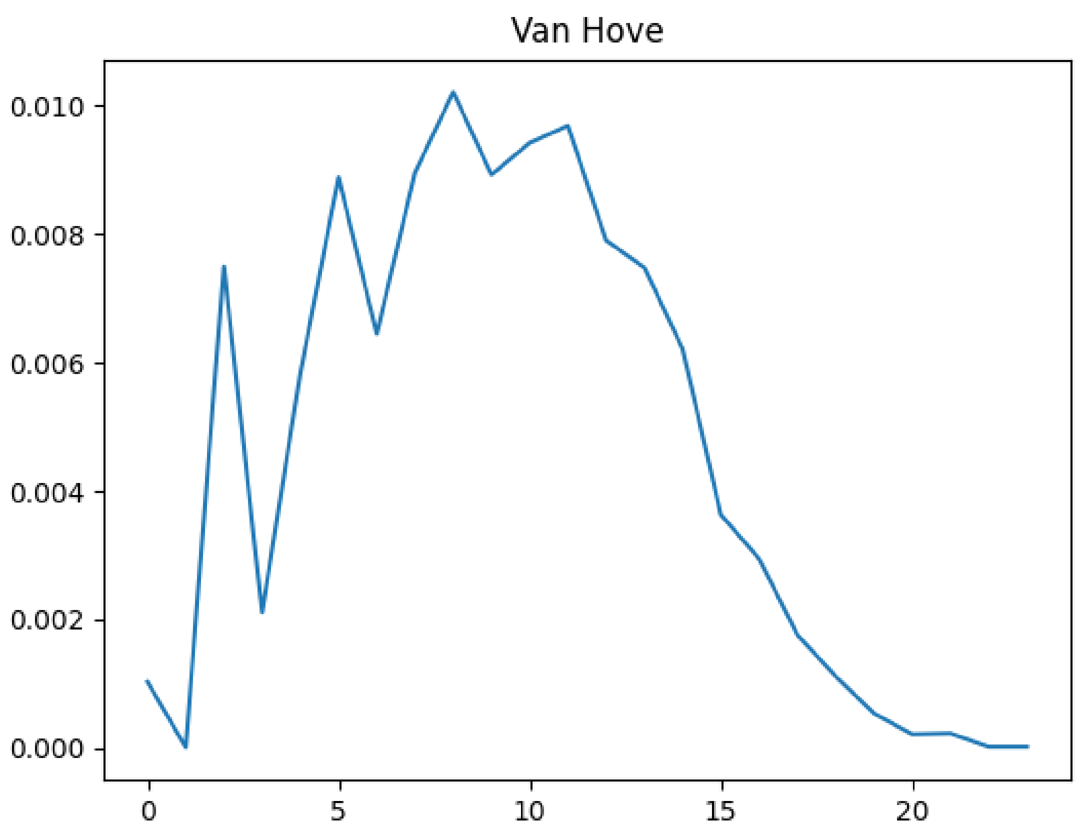
CODE ::

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

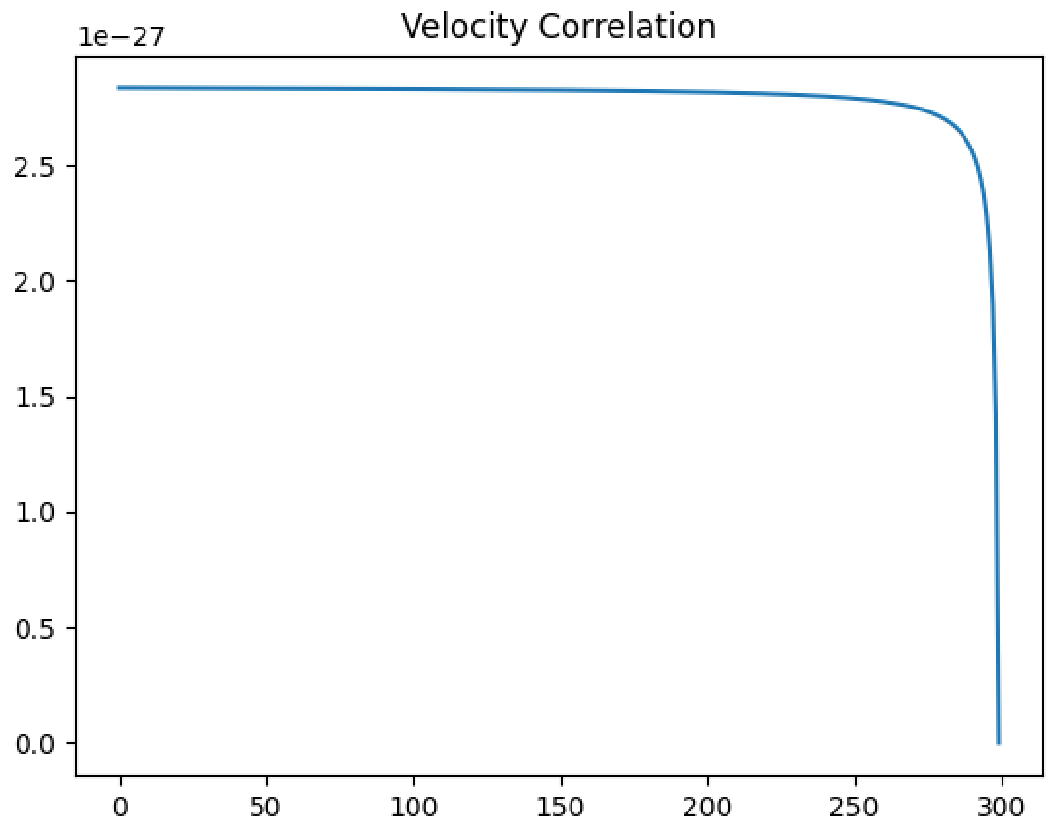


Van Hove function signifies the chances of spotting a particle i in the region of radius r at a given time t . This is calculated knowing that a particle j is in the vicinity of the origin at time t = 0

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

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.

VELOCITY CORRELATION FUNCTION



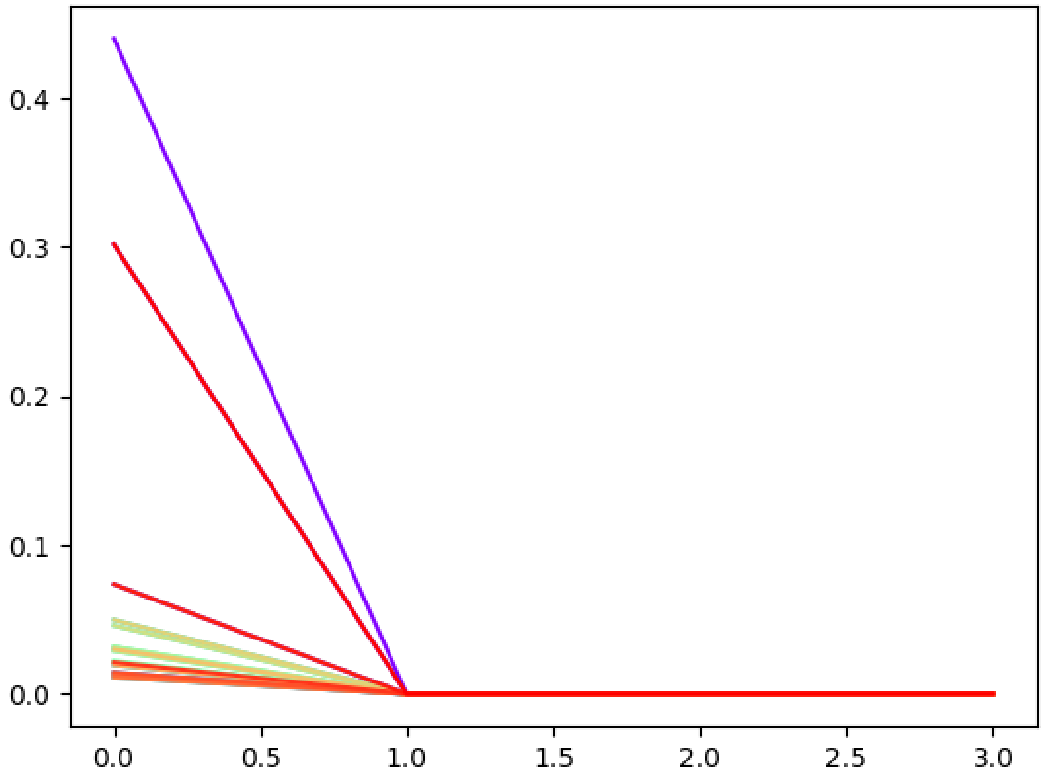
This curve displays the correlation between the velocity vectors at various times in the given intervals

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

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.

DYNAMIC STRUCTURE FACTOR



Here, we get the inference that The Dynamic structure factor quickly approaches to 0 near the value of 1.

The details of the algorithm have been taken from WikiPedia :

The dynamic structure factor is most often denoted $S(\vec{k},\omega)$, where $\vec{k}$ (sometimes $\vec{q}$) is a wave vector (or wave number for isotropic materials), and ω a frequency (sometimes stated as energy, $\hbar\omega$). It is defined as:[1]

$$S(\vec{k},\omega) \equiv \frac{1}{2\pi}\int_{-\infty}^{\infty} F(\vec{k},t)\exp(i\omega t)\,dt$$

Here $F(\vec{k},t)$, is called the **intermediate scattering function** and can be measured by neutron spin echo spectroscopy. The intermediate scattering function is the spatial Fourier transform of the **van Hove function** $G(\vec{r},t)$:[2][3]

$$F(\vec{k},t) \equiv \int G(\vec{r},t)\exp(-i\vec{k}\cdot\vec{r})\,d\vec{r}$$

Thus we see that the dynamical structure factor is the spatial *and* temporal Fourier transform of van Hove's time-dependent pair correlation function. It can be shown (see below), that the intermediate scattering function is the correlation function of the Fourier components of the density ρ:

$$F(\vec{k},t) = \frac{1}{N}\langle\rho_{\vec{k}}(t)\rho_{-\vec{k}}(0)\rangle$$

The dynamic structure is exactly what is probed in coherent inelastic neutron scattering. The differential cross section is :

$$\frac{d^2\sigma}{d\Omega d\omega} = a^2\left(\frac{E_f}{E_i}\right)^{1/2} S(\vec{k},\omega)$$

where a is the scattering length.

We replace the first integral, with another Fourier Transform