PROJECT
SCIENCE - II

Question 1:

The process for creating a random configuration satisfying PBC conditions was rather simple. I basically ran a loop which adds points in the array only if the point satisfies PBC conditions checked with the points already present in the array. If it satisfies, it is pushed in an array else it is discarded.

Question 2:

The total interaction energy of the configuration is the sum of pairwise interaction energy, and each pair of interaction energies is calculated using the formula described in the question PDF. On running the code, the total interaction energy for the configuration made is equal to -122.63092381976412 kcal/mol

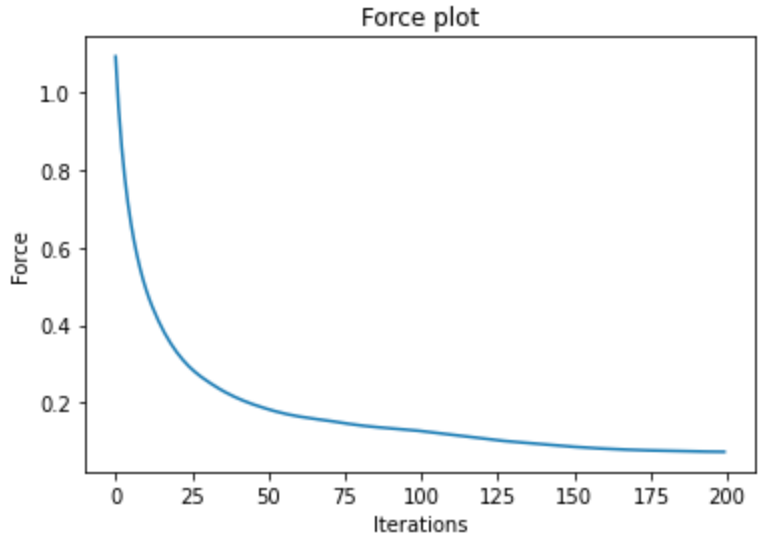
Question 3:

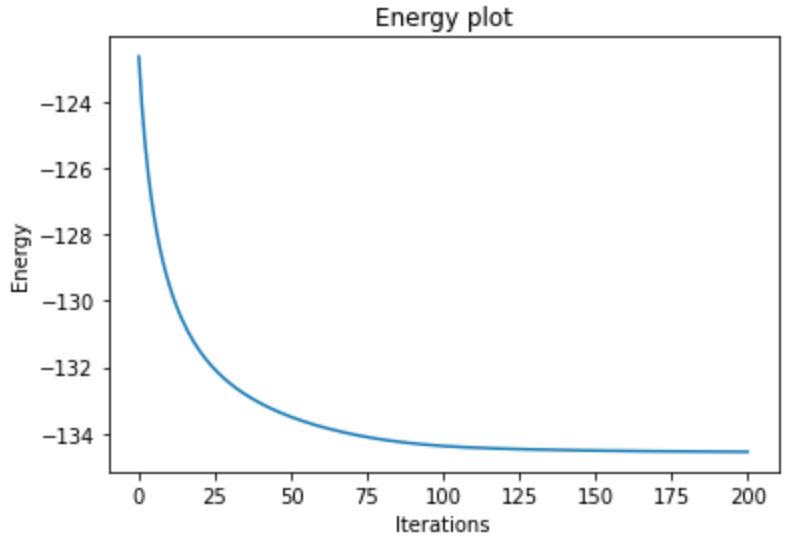
The force was analytically calculated by taking the negative of the derivative of interaction energy obtained with respect to r. The formula obtained is

$$F_{ij} = 4 \in \frac{\left((-12) \left(\frac{\sigma}{r_{ij}} \right)^{12} + 6 \left(\frac{\sigma}{r_{ij}} \right)^{6} \right)}{r_{ij}}$$

To obtain the minimum potential energy, each particle was applied a small amount of force to pull the particles away from each other and hence decreasing the distance between them. This was simulated until either 200 iterations were completed or the net force acting on the system was less than 0.01 kcal/mol A°.

The minimum potential energy reached was nearly equal to -134 kcal/mol





Question 4:

$$f_{xy}(x,y) \approx \frac{f(x+h,y+k) - f(x+h,y) - f(x,y+k) + 2f(x,y) - f(x-h,y) - f(x,y-k) + f(x-h,y-k)}{2hk},$$

The above stated equation is used to calculate the approximate value of second order partial derivatives for the Hessian matrix. Since the time complexity of code to calculate all the derivatives was quite high, multithreading was incorporated to reduce the effective time taken by the program. All the values were stored in a dictionary and written in a file. These values were then used to calculate the Hessian matrix as shown in the equation.

The energies were calculated by shifting the particles by small displacements which are written in the equations as h and k and then calculating the total potential energy of the whole system as described in Q2. After obtaining the Hessian matrix, the eigen values and eigen vectors were calculated using numpy's linear algebra library.

Question 5:

The vibrational frequency histogram is basically making a histogram of eigen values obtained from the Hessian matrix. So the eigen values calculated previously were directly used to create the histogram shown below.