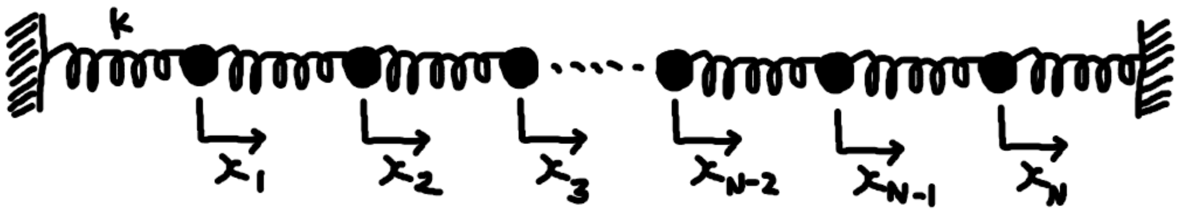
Numerical Assignment III

Question Consider a **1D horizontal chain** of **N identical atoms** on a horizontal frictionless floor, each of mass m, connected by bonding forces modeled by identical **springs** having spring constants k, the first and last springs are fixed to the wall. Let x_j be the **displacement of the j-th atom from its equilibrium (unstretched) position**.



a. Find the Lagrangian of this system for N atoms.

b. Show that **the equations of motion** for the end atoms and j-th atom can be written in the following form:

$$\ddot{x}_1 + 2\omega_0^2 x_1 - \omega_0^2 x_2 = 0$$

$$\ddot{x}_N + 2\omega_0^2 x_N - \omega_0^2 x_{N-1} = 0$$

$$\ddot{x}_j + 2\omega_0^2 x_j - \omega_0^2 x_{j-1} - \omega_0^2 x_{j+1} = 0, \qquad j = 2, 3, 4, \ldots\ N-1$$

$$\omega_0^2 = \frac{k}{m}$$

c. Show that the **eigenvalues** associated with the eigenmodes of this system are given by the **zeroes of the determinant** of the following matrix called D_N for a fixed value of N.

$$D_N(\omega) = \begin{pmatrix}
2\omega_0^2-\omega^2 & -\omega_0^2 & 0 & & 0\;0\;0 & & & 0\;0\;0 & \\
-\omega_0^2 & 2\omega_0^2-\omega^2 & -\omega_0^2 & & 0\;0\;0 & \cdots & & 0\;0\;0 & \\
0 & -\omega_0^2 & 2\omega_0^2-\omega^2 & & 0\;0\;0 & & & 0\;0\;0 & \\
 & & & \ddots & & & & & \\
 & 0\;0\;0 & & 2\omega_0^2-\omega^2 & -\omega_0^2 & 0 & & 0\;0\;0 & \\
 & 0\;0\;0 & & -\omega_0^2 & 2\omega_0^2-\omega^2 & -\omega_0^2 & & 0\;0\;0 & \\
 & 0\;0\;0 & & 0 & -\omega_0^2 & 2\omega_0^2-\omega^2 & & 0\;0\;0 & \\
 & \vdots & & & & & & & \\
 & 0\;0\;0 & & & 0\;0\;0 & & 2\omega_0^2-\omega^2 & -\omega_0^2 & 0 \\
 & 0\;0\;0 & & & 0\;0\;0 & & -\omega_0^2 & 2\omega_0^2-\omega^2 & -\omega_0^2 \\
 & 0\;0\;0 & & & 0\;0\;0 & & 0 & -\omega_0^2 & 2\omega_0^2-\omega^2
\end{pmatrix}$$

d. Now we would like to investigate an important property of the energy spectrum, the so called **density of states**. For this purpose we start by defining the number of eigenvalues less than ω, we call it $N(\omega)$, mathematically we can write $N(\omega) = \{\text{number of eigenvalues } \lambda \text{ of } \mathrm{D_N} \text{ such } \lambda < \omega\}$. Then we compute numerically the density of states defined mathematically by

$$\rho(\omega) = \frac{dN}{d\omega}$$

or **numerically** through

$$\rho(\omega) = \frac{N(\omega + d\omega) - N(\omega)}{d\omega}$$

where $d\omega$ is small energy step to be fixed. Then Plot $\rho(\omega)$ i.e. ρ versus ω. All above computations should be done for $\omega_0^2 = 1$ and increasing values of N until the plot of $\rho(\omega)$ is smooth enough. Try few values of N above 1000 at least.

e. Try to explain what happen to the edges of the density of states and identify the values of these edges.