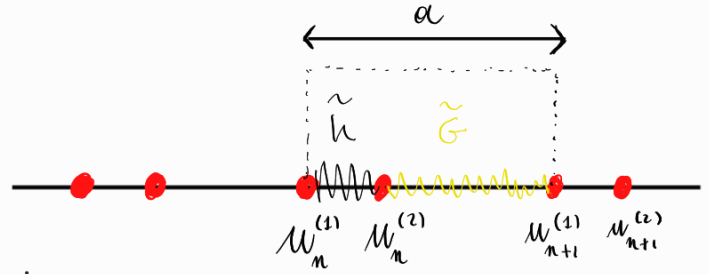


Biatomic linear chain - Force calculation

We begin by building the total potential energy in the framework of the harmonic approximation

$$U = U_0 + \frac{\tilde{K}}{2} \sum_{n=1}^N (u_n^{(1)} - u_n^{(2)})^2 + \frac{\tilde{G}}{2} \sum_{n=1}^N (u_{n+1}^{(1)} - u_n^{(2)})^2$$



Now we evaluate directly the forces by the expressions:

$$M \ddot{u}_m^{(1)} = - \frac{\partial U}{\partial u_m^{(1)}} \quad \textcircled{I}$$

$$M \ddot{u}_m^{(2)} = - \frac{\partial U}{\partial u_m^{(2)}} \quad \textcircled{II}$$

$$\textcircled{I} \quad M \ddot{u}_m^{(1)} = - \frac{\tilde{K}}{2} \sum_{n=1}^N 2 (u_n^{(1)} - u_n^{(2)}) (-\delta_{m,n}) - \frac{\tilde{G}}{2} \sum_{n=1}^N 2 (u_{n+1}^{(1)} - u_n^{(2)}) \delta_{n+1,m} \quad \left| \quad \frac{\partial u_m^{(2)}}{\partial u_n^{(1)}} = 0 \quad \forall n, m \right.$$

$$M \ddot{u}_m^{(1)} = - \frac{\tilde{K}}{2} \sum_{n=1}^N 2 (u_n^{(1)} - u_n^{(2)}) (-\delta_{m,n}) - \frac{\tilde{G}}{2} \sum_{n=1}^N 2 (u_{n+1}^{(1)} - u_n^{(2)}) \delta_{n,m-1}$$

$$M \ddot{u}_m^{(1)} = \tilde{K} (u_m^{(1)} - u_m^{(2)}) - \tilde{G} (u_m^{(1)} - u_{m-1}^{(2)})$$

$$M \ddot{u}_m^{(1)} = - \tilde{K} (u_m^{(1)} - u_m^{(2)}) - \tilde{G} (u_m^{(1)} - u_{m-1}^{(2)})$$

$$\textcircled{II} \quad M \ddot{u}_m^{(2)} = - \frac{\tilde{K}}{2} \sum_{n=1}^N 2 (u_n^{(1)} - u_n^{(2)}) (\delta_{m,n}) - \frac{\tilde{G}}{2} \sum_{n=1}^N 2 (u_{n+1}^{(1)} - u_n^{(2)}) (-\delta_{n,m}) \quad \left| \quad \frac{\partial u_m^{(1)}}{\partial u_n^{(2)}} = 0 \quad \forall n, m \right.$$

$$M \ddot{u}_m^{(2)} = - \tilde{K} (u_m^{(1)} - u_m^{(2)}) + \tilde{G} (u_{m+1}^{(1)} - u_m^{(2)})$$

$$M \ddot{u}_m^{(2)} = - \tilde{K} (u_m^{(1)} - u_m^{(2)}) - \tilde{G} (u_m^{(2)} - u_{m+1}^{(1)})$$

So that, in the end:

$$\begin{cases} M \ddot{u}_m^{(1)} = - \tilde{K} (u_m^{(1)} - u_m^{(2)}) - \tilde{G} (u_m^{(1)} - u_{m-1}^{(2)}) \\ M \ddot{u}_m^{(2)} = - \tilde{K} (u_m^{(1)} - u_m^{(2)}) - \tilde{G} (u_m^{(2)} - u_{m+1}^{(1)}) \end{cases}$$