

# Linear monoatomic chain with mass defect - calculations

We start by the equations of motion

$$\begin{cases} m \ddot{u}_n = \tilde{\kappa} [u_{n+1} + u_{n-1} - 2u_n] & n \neq 0 \\ M \ddot{u}_0 = \tilde{\kappa} [u_1 + u_{-1} - 2u_0] & n = 0 \end{cases}$$

We want to show that the solution is:

$$u_n = A e^{-\kappa |n|a - i\omega t} \quad \kappa \in \mathbb{C}, \forall n.$$

We obtain by substitution

$$\begin{cases} -\omega^2 m A e^{-\kappa |n|a - i\omega t} = \tilde{\kappa} A e^{i\omega t} [e^{-\kappa(n+1)a} + e^{-\kappa(n-1)a} - 2e^{-\kappa |n|a}] & n \neq 0 \\ -\omega^2 M A e^{-i\omega t} = \tilde{\kappa} A e^{i\omega t} [e^{-\kappa a} + e^{-\kappa a} - 2] & n = 0 \end{cases}$$

$$\begin{cases} \omega^2 m e^{-\kappa |n|a} = \tilde{\kappa} [2e^{-\kappa |n|a} - e^{-\kappa(n+1)a} - e^{-\kappa(n-1)a}] & n \neq 0 \\ \omega^2 M = 2\tilde{\kappa} [1 - e^{-\kappa a}] & n = 0 \end{cases} \quad \textcircled{I}$$

$$\textcircled{I} \bullet n \geq 1$$

$$\omega^2 m e^{-\kappa n a} = \tilde{\kappa} [2e^{-\kappa n a} - e^{-\kappa(n+1)a} - e^{-\kappa(n-1)a}]$$

$$\omega^2 m = \tilde{\kappa} [2 - e^{-\kappa a} - e^{\kappa a}]$$

$$\bullet n \geq -1$$

$$\omega^2 m e^{\kappa n a} = \tilde{\kappa} [2e^{\kappa n a} - e^{\kappa(n+1)a} - e^{\kappa(n-1)a}]$$

$$\omega^2 m = \tilde{\kappa} [2 - e^{\kappa a} - e^{-\kappa a}]$$

So, in the end

$$\begin{cases} \omega^2 m = \tilde{\kappa} [2 - e^{\kappa a} - e^{-\kappa a}] & n \neq 0 \\ \omega^2 M = 2\tilde{\kappa} [1 - e^{-\kappa a}] & n = 0 \end{cases}$$