Normal modes of CO_2

Philippe W. Courteille, 05/02/2021

Solution: *The differential equations are*

$$\begin{aligned} m_O\ddot{x}_1 &= -k(x_1 - x_2) \\ m_C\ddot{x}_2 &= -k(x_2 - x_1) - k(x_2 - x_3) \\ m_O\ddot{x}_3 &= -k(x_3 - x_2) \ . \end{aligned}$$

With the ansatz $x_n = A_n e^{i\omega t}$ *and the abbreviations* $\omega_O \equiv \sqrt{\frac{k}{m_O}}$ *and* $\omega_C \equiv \sqrt{\frac{k}{m_C}}$ *we get the characteristic equations,*

$$\begin{aligned} \omega^2 A_1 &= \omega_O^2(A_1 - A_2) \\ \omega^2 A_2 &= \omega_C^2(A_2 - A_1) + \omega_C^2(A_2 - A_3) \\ \omega^2 A_3 &= \omega_O^2(A_3 - A_2) \ . \end{aligned}$$

Introducing the matrix and the vector,

$$M \equiv \begin{pmatrix} \omega_O^2 & -\omega_O^2 & 0 \\ -\omega_C^2 & 2\omega_C^2 & -\omega_C^2 \\ 0 & -\omega_O^2 & \omega_O^2 \end{pmatrix} \qquad \text{and} \qquad \vec{A} \equiv \begin{pmatrix} A_1 \\ A_2 \\ A_3 \end{pmatrix} \ ,$$

the equation takes the form of an eigenvalue equation,

$$M\vec{A} = \omega^2 \vec{A} \ .$$

The frequencies of the normal modes are the eigenvalues of the matrix,

$$\begin{aligned} 0 = \det[M - \omega^2 E_3] &= -2\omega_O^2\omega_C^2\omega^2 - \omega_O^4\omega^2 + 2\omega_O^2\omega^4 + 2\omega^4\omega_C^2 - \omega^6 \\ &= -\omega^2(\omega^2 - \omega_O^2 - 2\omega_C^2)(\omega^2 - \omega_O^2) \ . \end{aligned}$$

Entering the eigenvalue $\omega = 0$ *in the eigenvalue equation gives,*

$$A_1 = A_2 = A_3 \qquad \text{and hence} \qquad \vec{A} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \ .$$

Entering the eigenvalue $\omega = \omega_O$ *in the eigenvalue equation we get,*

$$A_2 = 0 \qquad , \qquad A_1 = -A_3 \qquad \text{and hence} \qquad \vec{A} = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \ .$$

Entering the eigenvalue $\omega = \sqrt{\omega_O^2 + 2\omega_C^2}$ *in the eigenvalue equation we get,*

$$2\omega_C^2 A_1 = -\omega_O^2 A_2 = 2\omega_C^2 A_3 \qquad \text{and hence} \qquad \vec{A} = \begin{pmatrix} 1 \\ -2\omega_C^2/\omega_O^2 \\ 1 \end{pmatrix} \ .$$