Next Up Previous

Next: Exercises **Up:** Coupled Oscillations **Previous:** Spring-Coupled Masses

Triatomic Molecule

Consider the simple model of a linear triatomic molecule (*e.g.,* carbon dioxide) illustrated in Figure 38. The molecule consists of a central atom of mass M flanked by two identical atoms of mass m. The atomic bonds are represented as springs of spring constant k. The linear displacements of the flanking atoms are q_1 and q_2, whilst that of the central atom is q_3. Let us investigate the linear modes of oscillation our model molecule.
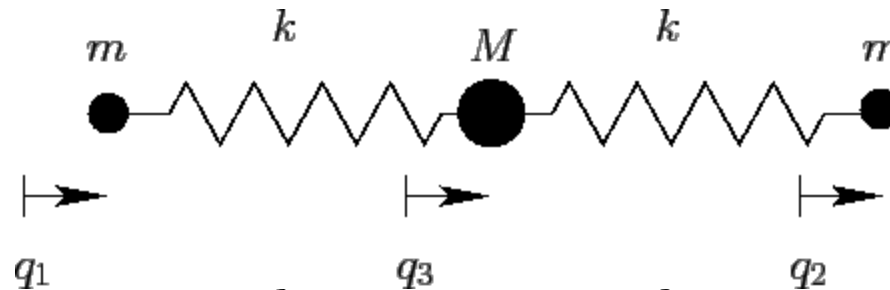

Figure 38: *A model triatomic molecule.*

The kinetic energy of the molecule is written

$$K = \frac{m}{2}\left(\dot{q}_1^2 + \dot{q}_2^2\right) + \frac{M}{2}\,\dot{q}_3^2, \tag{840}$$

whereas the potential energy takes the form

$$U = \frac{k}{2}\left(q_3 - q_1\right)^2 + \frac{k}{2}\left(q_2 - q_3\right)^2. \tag{841}$$

Clearly, we have a three degree of freedom dynamical system. However, we can reduce this to a two degree of freedom system by only considering *oscillatory* modes of motion, and, hence, neglecting *translational* modes. We can achieve this by demanding that the center of mass of the system remains stationary. In other words, we require that

$$m\,(q_1 + q_2) + M\,q_3 = 0. \tag{842}$$

This constraint can be rearranged to give

$$q_3 = -\frac{m}{M}\,(q_1 + q_2). \tag{843}$$

Eliminating q_3 from Equations ([840](#)) and ([841](#)), we obtain

$$K = \frac{m}{2}\left[(1+\alpha)\,\dot{q}_1^2 + 2\,\alpha\,\dot{q}_1\,\dot{q}_2 + (1+\alpha)\,\dot{q}_2^2\right], \tag{844}$$

and

$$U = \frac{k}{2}\left[(1+2\,\alpha+2\,\alpha^2)\,q_1^2 + 4\,\alpha\,(1+\alpha)\,q_1\,q_2 + (1+2\,\alpha+2\,\alpha^2)\,q_2^2\right], \tag{845}$$

respectively, where $\alpha = m/M$.

A comparison of the above expressions with the standard forms ([775](#)) and ([780](#)) yields the following expressions for the mass matrix, $\mathbf{M}$, and the force matrix, $\mathbf{G}$:

$$\mathbf{M} = m\begin{pmatrix} 1+\alpha & \alpha \\ \alpha & 1+\alpha \end{pmatrix}, \tag{846}$$

$$\mathbf{G} = -k\begin{pmatrix} 1+2\,\alpha+2\,\alpha^2 & 2\,\alpha\,(1+\alpha) \\ 2\,\alpha\,(1+\alpha) & 1+2\,\alpha+2\,\alpha^2 \end{pmatrix}. \tag{847}$$

Now, the equation of motion of the system takes the form [see Equation ([786](#))]

$$(\mathbf{G} - \lambda\,\mathbf{M})\,\mathbf{x} = \mathbf{0}, \tag{848}$$

where $\mathbf{x}$ is the column vector of the q_1 and q_2 values. The solubility condition for the above equation is

$$|\mathbf{G} - \lambda\,\mathbf{M}| = 0, \tag{849}$$

which yields the following quadratic equation for the eigenvalue λ:

$$(1 + 2\,\alpha)\left[m^2\lambda^2 + 2\,m\,k\,(1 + \alpha)\,\lambda + k^2\,(1 + 2\alpha)\right] = 0. \tag{850}$$

The two roots of the above equation are

$$\lambda_1 \quad = \quad -\frac{k}{m}, \tag{851}$$

$$\lambda_2 \quad = \quad -\frac{k\,(1 + 2\alpha)}{m}. \tag{852}$$

The fact that the roots are negative implies that both normal modes are indeed *oscillatory* in nature. The characteristic oscillation frequencies are

$$\omega_1 \quad = \quad \sqrt{-\lambda_1} = \sqrt{\frac{k}{m}}, \tag{853}$$

$$\omega_2 \quad = \quad \sqrt{-\lambda_2} = \sqrt{\frac{k\,(1 + 2\,\alpha)}{m}}. \tag{854}$$

Equation ([848](#)) can now be solved, subject to the normalization condition ([799](#)), to give the two eigenvectors:

$$\mathbf{x}_1 = (2\,m)^{-1/2}(1,-1),\tag{855}$$

$$\mathbf{x}_2 = (2\,m)^{-1/2}(1+2\,\alpha)^{-1/2}(1,\ 1).\tag{856}$$

Thus, we conclude from Equations ([843](#)) and ([853](#))-([856](#)) that our model molecule possesses two normal modes of oscillation. The first mode oscillates at the frequency ω_1, and is an *anti-symmetric* mode in which $q_1 = -q_2$ and $q_3 = 0$. In other words, in this mode of oscillation, the two end atoms move in opposite directions whilst the central atom remains stationary. The second mode oscillates at the frequency ω_2, and is a mixed symmetry mode in which $q_1 = q_2$ but $q_3 = -2\,\alpha\,q_1$. In other words, in this mode of oscillation, the two end atoms move in the same direction whilst the central atom moves in the opposite direction.

Finally, it is easily demonstrated that the normal coordinates of the system are

$$\eta_1 = \sqrt{\frac{m}{2}}\,(q_1 - q_2),\tag{857}$$

$$\eta_2 = \sqrt{\frac{m\,(1+2\,\alpha)}{k}}\,(q_1 + q_2).\tag{858}$$

When expressed in terms of these coordinates, K and U reduce to

$$K = \frac{1}{2}\,(\dot{\eta}_1^2 + \dot{\eta}_2^2),\tag{859}$$

$$U = \frac{1}{2}\,(\omega_1^2\,\eta_1^2 + \omega_2^2\,\eta_2^2),\tag{860}$$

respectively.