Vibrations of a linear triatomic molecule:

Here we are describing the linear triatomic molecule, you should go through other problems with two degrees of freedom, you may refer section-9.5 of J.C. Upadhyay's Classical Mechanics where two coppled pendulum has been solved fully.

Let us consider a linear triatomic molecule of the type AB_2(e.g. CO_2) in which A atom is in the middle and B atom are at the ends [See figure below]. The mass of A atom is M and that of each of the B atom is m. The interatomic force between A and B atom is approximated by elastic force of spring force constant k. The motion of the three atoms is constrained along the line joining them. There are three coordinates marking the positions of three atoms on the line. If x_1, x_2 and x_3 are the positions of the three atoms at any instant from some arbitrary origin, then

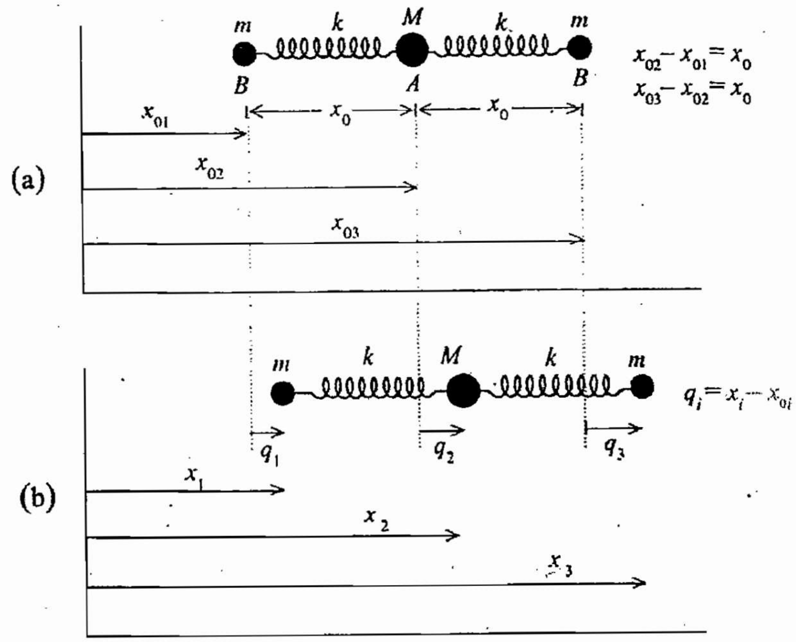


Figure: Longitudinal oscillations of a linear symmetric triatomic molecule
(a) Equilibrium configuration (b) Configuration at any instant t.

Note that q's are same as η's used in our derivation, also note that q_i can be positive or negative depending on x_i.

where, $$x_{02} - x_{01} = x_{03} - x_{02} = x_0$$

Then, $$T = \frac{1}{2}m\left(\dot{q}_1^2 + \dot{q}_3^2\right) + \frac{1}{2}M\dot{q}_2^2 = \frac{1}{2}\begin{pmatrix}\dot{q}_1 & \dot{q}_2 & \dot{q}_3\end{pmatrix}\begin{pmatrix} m & 0 & 0 \\ 0 & M & 0 \\ 0 & 0 & m\end{pmatrix}\begin{pmatrix}\dot{q}_1 \\ \dot{q}_2 \\ \dot{q}_3\end{pmatrix}$$

and $$V = \frac{1}{2}k(q_2 - q_1)^2 + \frac{1}{2}k(q_3 - q_2)^2$$

We can visualize it as follows:

The change in length of spring on the left part is $(q_2 - q_1)$ and on the right part it is $(q_3 - q_2)$. So, the potential energy $V = \frac{1}{2}k(\text{change in length on right part})^2 + \frac{1}{2}k(\text{change in length on left part})^2$.

Now, $$V=\frac{1}{2}k\left(q_1^2+q_2^2-2q_1q_2+q_2^2+q_3^2-2q_2q_3\right)$$

We can write the V matrix by inspection only because

$$V=\frac{1}{2}V_{ij}\eta_i\eta_j\equiv\sum_{i=1}^{3}\sum_{j=1}^{3}\frac{1}{2}V_{ij}q_iq_j$$

$$=\frac{1}{2}\left(V_{11}q_1^2+V_{12}q_1q_2+V_{13}q_1q_3+V_{21}q_2q_1+V_{22}q_2^2+V_{23}q_2q_3+V_{31}q_3q_1+V_{32}q_3q_2+V_{33}q_3^2\right)$$

$$=\frac{1}{2}\left(V_{11}q_1^2+2V_{12}q_1q_2+2V_{13}q_1q_3+V_{22}q_2^2+2V_{23}q_2q_3+V_{33}q_3^2\right)$$

because $V_{ij}=V_{ji}$.

Comparing above expression with our potential energy $\frac{1}{2}k\left(q_1^2-2q_1q_2+0+2q_2^2-2q_2q_3+q_3^2\right)$

We get, $V_{11}=V_{33}=k,\ V_{22}=2k$, $V_{12}=V_{21}=V_{23}=V_{32}=-k$ and $V_{13}=V_{31}=0$

So, $$V=\begin{pmatrix}V_{11}&V_{12}&V_{13}\\V_{21}&V_{22}&V_{23}\\V_{31}&V_{32}&V_{33}\end{pmatrix}=\begin{pmatrix}k&-k&0\\-k&2k&-k\\0&-k&k\end{pmatrix}$$

Also, note that $\left(\frac{\partial^2V}{\partial q_1^2}\right)_{q_1=0}=k=V_{11},\ \left(\frac{\partial^2V}{\partial q_2^2}\right)_{q_2=0}=2k=V_{22},\ \left(\frac{\partial^2V}{\partial q_3^2}\right)_{q_3=0}=k=V_{33}$

$$\left(\frac{\partial^2V}{\partial q_1q_2}\right)_{\substack{q_1=0\\q_2=0}}=-k=V_{12}=V_{21},\ \left(\frac{\partial^2V}{\partial q_1q_3}\right)_{\substack{q_1=0\\q_3=0}}=0=V_{13}=V_{31}$$

and $$\left(\frac{\partial^2V}{\partial q_2q_3}\right)_{\substack{q_2=0\\q_3=0}}=-k=V_{23}=V_{32}$$

Thus the **T** and **V** matrices are

$$\mathbf{T}=\begin{pmatrix}m&0&0\\0&M&0\\0&0&m\end{pmatrix}\text{ and }\mathbf{V}=\begin{pmatrix}k&-k&0\\-k&2k&-k\\0&-k&k\end{pmatrix}\qquad\text{... (11.23)}$$

The secular equation is

$$\left|\mathbf{V}-\omega^2\mathbf{T}\right|=\begin{vmatrix}k-m\omega^2&-k&0\\-k&2k-M\omega^2&-k\\0&-k&k-m\omega^2\end{vmatrix}=0\qquad\text{... (11.24)}$$

Applying the operation, $R_1\to R_1-R_3$

We have, $$\begin{vmatrix}k-m\omega^2&0&-\left(k-m\omega^2\right)\\-k&2k-M\omega^2&-k\\0&-k&k-m\omega^2\end{vmatrix}=0$$

Again applying, $C_3 \to C_3 + C_1$

$$\begin{vmatrix} k - m\omega^2 & 0 & 0 \\ -k & 2k - M\omega^2 & -2k \\ 0 & -k & k - m\omega^2 \end{vmatrix} = 0$$

$$\Rightarrow \quad \left(k - m\omega^2\right)\left[\left(2k - M\omega^2\right)\left(k - m\omega^2\right) - 2k^2\right] = 0$$

$$\Rightarrow \quad \left(k - m\omega^2\right)\left(2k^2 - 2km\omega^2 - M\omega^2 k + mM\omega^4 - 2k^2\right) = 0$$

$$\Rightarrow \quad \left(k - m\omega^2\right)\left[-2km\omega^2 - M\omega^2 k + mM\omega^4\right] = 0$$

$$\Rightarrow \quad \omega^2\left(k - m\omega^2\right)\left[mM\omega^2 - k\left(2m + M\right)\right] = 0$$

We get $\omega_1 = 0,\ \omega_2 = \sqrt{\dfrac{k}{m}}$ and $\omega_3 = \sqrt{\dfrac{k}{m}\left(1 + \dfrac{2m}{M}\right)}$ ... (11.25)

The first eigenvalue $\omega_1 = 0$ corresponds to non-oscillatory motion and refers to translatory motion of the molecule as a whole rigidly.

To determine the eigenvectors, we use the equation,

$$\left(\mathbf{V} - \omega_k^2 \mathbf{T}\right) a_k = 0 \quad \text{or} \quad \begin{pmatrix} k - m\omega_k^2 & k & 0 \\ -k & 2k - M\omega_k^2 & -k \\ 0 & -k & k - m\omega_k^2 \end{pmatrix} \begin{pmatrix} a_{1k} \\ a_{2k} \\ a_{3k} \end{pmatrix} = 0$$

Let us now discuss the eigen vectors for the three modes of vibrations.

(1) For $\omega_1 = 0$,

$$\begin{pmatrix} k & -k & 0 \\ -k & 2k & -k \\ 0 & -k & k \end{pmatrix} \begin{pmatrix} a_{11} \\ a_{21} \\ a_{31} \end{pmatrix} = 0$$

Or, $\quad a_{11} - a_{21} = 0,\ -a_{11} + 2a_{21} - a_{31} = 0,\ -a_{21} + a_{31} = 0$

Or, $\quad a_{11} = a_{21} = a_{31} = \alpha\ (say)$

Thus for $\omega_1 = 0$, the eigen vector is given by

$$\mathbf{a}_1 = \begin{pmatrix} \alpha \\ \alpha \\ \alpha \end{pmatrix}$$

(2) For $\omega_2 = \sqrt{k/m}$,

$$\begin{pmatrix} 0 & -k & 0 \\ -k & 2k - \dfrac{Mk}{m} & -k \\ 0 & -k & 0 \end{pmatrix} \begin{pmatrix} a_{12} \\ a_{22} \\ a_{32} \end{pmatrix} = 0$$

Or, $\quad a_{22}=0,\ -a_{12}-a_{32}=0$

Therefore, $\quad a_{22}=0,\ a_{12}=-a_{32}=\beta\ (say)$

Thus, for $\omega_2=\sqrt{k/m},\ \mathbf{a}_2=\begin{pmatrix}\beta\\0\\-\beta\end{pmatrix}$

(3) For $\quad \omega_3=\sqrt{\dfrac{k}{m}\left(1+\dfrac{2m}{M}\right)},\ \begin{pmatrix}-\dfrac{2mk}{M} & -k & 0\\ -k & -\dfrac{kM}{m} & -k\\ 0 & -k & -\dfrac{2mk}{M}\end{pmatrix}\begin{pmatrix}a_{13}\\a_{23}\\a_{33}\end{pmatrix}=0$

which gives, $\quad \dfrac{2m}{M}a_{13}+a_{23}=0,\ a_{13}+\dfrac{M}{m}a_{23}+a_{33}=0,\ a_{23}+\dfrac{2m}{M}a_{33}=0$

Therefore, $\quad a_{13}=a_{33}=\gamma\,(say)$ and $a_{23}=-(2m/M)\gamma$

Thus for, $\quad \omega_3=\sqrt{\dfrac{k}{m}\left(1+\dfrac{2m}{M}\right)},\ \mathbf{a}_3=\begin{pmatrix}\gamma\\-\dfrac{2m}{M}\gamma\\\gamma\end{pmatrix}$

Now, the **A** matrix is

$$\mathbf{A}=\begin{bmatrix}a_{11} & a_{12} & a_{13}\\a_{21} & a_{22} & a_{23}\\a_{31} & a_{32} & a_{33}\end{bmatrix}=\begin{bmatrix}\alpha & \beta & \gamma\\ \alpha & 0 & -\dfrac{2m}{M}\gamma\\ \alpha & -\beta & \gamma\end{bmatrix}$$

Now, we have to determine α, β and γ

We impose the condition, Given in equation (9.18)

$$\tilde{\mathbf{A}}\mathbf{T}\mathbf{A}=\mathbf{1}$$

i.e.

$$\begin{pmatrix}\alpha & \alpha & \alpha\\ \beta & 0 & -\beta\\ \gamma & -\dfrac{2m}{M}\gamma & \gamma\end{pmatrix}\begin{pmatrix}m & 0 & 0\\0 & M & 0\\0 & 0 & m\end{pmatrix}\begin{pmatrix}\alpha & \beta & \gamma\\ \alpha & 0 & -\dfrac{2m}{M}\gamma\\ \alpha & -\beta & \gamma\end{pmatrix}=\begin{pmatrix}1 & 0 & 0\\0 & 1 & 0\\0 & 0 & 1\end{pmatrix}$$

$$\Rightarrow\quad \begin{bmatrix}\alpha & \alpha & \alpha\\ \beta & 0 & -\beta\\ \gamma & -\dfrac{2m}{M}\gamma & \gamma\end{bmatrix}\begin{bmatrix}m\alpha & m\beta & m\gamma\\ M\alpha & 0 & -2m\gamma\\ m\alpha & -m\beta & m\gamma\end{bmatrix}=\begin{pmatrix}1 & 0 & 0\\0 & 1 & 0\\0 & 0 & 1\end{pmatrix}$$

Or,

$$\begin{pmatrix} \alpha^2(2m+M) & 0 & 0 \\ 0 & 2\beta^2 m & 0 \\ 0 & 0 & 2\gamma^2 m\left(1+ \right. \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Thus,

$$\alpha = \frac{1}{\sqrt{2m+M}}, \quad \beta = \frac{1}{\sqrt{2m}}, \quad \gamma = -\frac{}{\sqrt{\quad M)}}$$

Hence the eigen vectors are

$$\mathbf{a}_1 = \frac{1}{\sqrt{2m+M}}\begin{bmatrix}1\\1\\1\end{bmatrix}, \quad \mathbf{a}_2 = \frac{1}{\sqrt{2m}}\begin{bmatrix}1\\0\\-1\end{bmatrix}, \quad \mathbf{a}_3 = \frac{}{\sqrt{2m\left(\right.}}$$

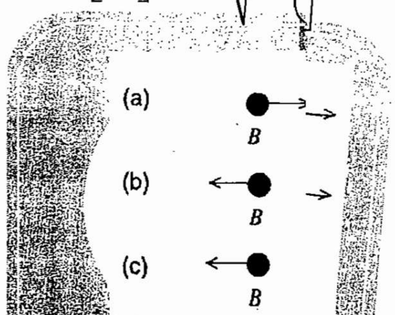


Figure: Longitudinal normal ...ic molecule

(a) Mode 1, all the three atoms are displaced equally in the sam...

(b) Mode 2, A atom does not vibrate and B atoms oscilalte with ... opposite directions.

(c) B atoms vibrate in phase with equal amplitudes and the mid... posite phase with different amplitude.

Thus, in case (1), $a_{11} = a_{21} = a_{31}$ means that the displ... ns are the same in the same direction (see in figure below). This is what expected from tra...

In case (2), $a_{22} = 0$, and $a_{12} = -a_{32}$ implies tha... iddle atom does not vibrate and the end atoms (B) oscillate with equal amplitudes but in ... n case (3),

$$a_{13} = a_{33} = \gamma \text{ and } a_{23} = -\left(\frac{2m}{M}\right)\gamma$$

show that end atoms oscillate in phase with equal am... ral atom vibrates in opposite phase with different amplitude.

The generalized coordinates q_1, q_2 and q_3 are ... coordinates Q_1, Q_2 and Q_3 by the relation

$$q_i = a_{ik}Q_k \qquad \text{where summation}$$

i.e. $$q_1 = q_{11}Q_1 + q_{12}Q_2 + q_{13}Q_3, \quad q_2 = \text{ and } q_3 = q_{31}Q_1 + q_{32}Q_2 + q_{33}Q_3$$

Therefore,

$$\begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix} = \begin{pmatrix} \alpha & \beta & \gamma \\ \beta & 0 & -\frac{2m}{M}\gamma \\ \gamma & -\beta & \gamma \end{pmatrix}\begin{pmatrix} Q_1 \\ Q_2 \\ Q_3 \end{pmatrix}$$

Further the normal coordinate Q_1 oscillates with frequency $\omega_1 = 0,\ Q_2$ with $\omega_2 = \sqrt{\frac{k}{m}}$ and Q_3 with $\omega_3 = \sqrt{\frac{k}{m}\left(1+\frac{2m}{M}\right)}$. So

$$Q_1 = f_1\cos(\omega_1 t+\phi_1),\ Q_2 = f_2\cos(\omega_2 t+\phi_2) \text{ and}$$

$$Q_3 = f_3\cos(\omega_3 t+\phi_3)$$

where f_1, f_2 and f_3 are the amplitudes of the normal coordinates (Q's) and ϕ_1, ϕ_2 and ϕ_3 are the phase factors of Q's.

Thus, $$q_1 = \alpha f_1\cos(\omega_1 t+\phi_1)+\beta f_2\cos(\omega_2 t+\phi_2)+\gamma f_3\cos(\omega_3 t+\phi_3)$$

Since, $$x_1 = q_1 + x_{01}$$

So, $$x_1 = A'\cos(\omega_1 t+\phi_1)+B\cos(\omega_2 t+\phi_2)+C\cos(\omega_3 t+\phi_3)+x_{01}$$

But $\omega_1 = 0$, therefore,

$$x_1 = A'+B\cos(\omega_2 t+\phi_2)+C\cos(\omega_3 t+\phi_3)+x_{01}$$

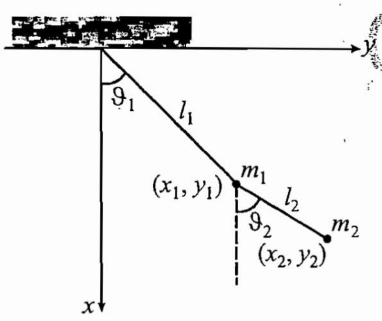
Similarly, $$x_2 = \alpha Q_1 + 0 - \frac{2m}{M}\gamma Q_3 = A'-\frac{2m}{M}C\cos(\omega_3 t+\phi_3)+x_{02} \qquad (\because \gamma f_3 = C)$$

and $$x_3 = \alpha Q_1 - \beta Q_2 + \gamma Q_3 = A'-B\cos(\omega_2 t+\phi_2)+C\cos(\omega_3 t+\phi_3)+x_{03}$$

where A' represents a constant corresponding to rigid translation and as stated in the begining x_{0i} is the equilibrium position of an atom.

Double pendulum

Determine the normal vibrations and frequencies.



Coordinates of the double pendulum

The Lagrangian is

$$L = T - V = \frac{1}{2}m_1 l_1^2\dot{\vartheta}_1^2 + \frac{1}{2}m_2\left[l_1^2\dot{\vartheta}_1^2 + l_2^2\dot{\vartheta}_2^2 + 2l_1 l_2\dot{\vartheta}_1\dot{\vartheta}_2\cos(\vartheta_1-\vartheta_2)\right]$$
$$-m_1 g\left[l_1+l_2-l_1\cos\vartheta_1\right]-m_2 g\left[l_1+l_2-(l_1\cos\vartheta_1+l_2\cos\vartheta_2)\right].$$

The Lagrange equations with ϑ_1 and ϑ_2 read

$$\frac{d}{dt}\left(\frac{\partial L}{\partial\dot{\vartheta}_1}\right)-\frac{\partial L}{\partial\vartheta_1}=0,\quad \frac{d}{dt}\left(\frac{\partial L}{\partial\dot{\vartheta}_2}\right)-\frac{\partial L}{\partial\vartheta_2}=0.$$

One has