Mechanics: Lagrangian Mechanics

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I. 1-D SYMMETRIC MOLECULAR VIBRATION

For a molecule like CO_2, we have a system with three particles aligning a line. The Lagrangian of this system can be written as

$$L = \frac{m_1}{2}\dot{x}_1^2 + \frac{m_2}{2}\dot{x}_2^2 + \frac{m_3}{2}\dot{x}_3^2 - U(|x_1 - x_2|) - U(|x_2 - x_3|).$$

This system owns the translation invariance, so the C.M momentum is conserved. therefore the motion of the centre of mass must be uniform. Hence one should be able to separate the C.M motion from the inner motions of the molecule. We can adopt the new coordinate:

$$\begin{aligned}
x_1 &= R_{CM} + \frac{m_2 + m_3}{m_2 + m_2 + m_3}x_{12} + \frac{m_3}{m_1 + m_2 + m_3}x_{23}, \\
x_2 &= R_{CM} - \frac{m_1}{m_2 + m_2 + m_3}x_{12} + \frac{m_3}{m_1 + m_2 + m_3}x_{23}, \\
x_3 &= R_{CM} - \frac{m_1 + m_2}{m_2 + m_2 + m_3}x_{12} - \frac{m_1}{m_1 + m_2 + m_3}x_{23},
\end{aligned}$$

For many molecule, $m_1{=}m_3$, then it is convenient to set $A{=}\frac{m_1+m_2}{2m_1+m_2}$ and $B{=}\frac{m_1}{2m_1+m_3}$.

$$x_1 = R_{CM} + Ax_{12} + Bx_{23},\ x_2 = R_{CM} - Bx_{12} + Bx_{23},\ x_3 = R_{CM} - Bx_{12} - Ax_{23},$$

Now we can write down the kinetic energy T of each particle as follows,

$$\begin{aligned}
\frac{m_1}{2}\dot{x}_1^2 &= \frac{m_1}{2}(\dot{R}_{CM}^2 + A^2\dot{x}_{12}^2 + B^2\dot{x}_{23}^2 + 2A\dot{R}_{CM}\dot{x}_{12} + 2B\dot{R}_{CM}\dot{x}_{23} + 2AB\dot{x}_{12}\dot{x}_{23}) \\
\frac{m_2}{2}\dot{x}_2^2 &= \frac{m_2}{2}(\dot{R}_{CM}^2 + B^2\dot{x}_{12}^2 + B^2\dot{x}_{23}^2 - 2B\dot{R}_{CM}\dot{x}_{12} + 2B\dot{R}_{CM}\dot{x}_{23} - 2B^2\dot{x}_{12}\dot{x}_{23}) \\
\frac{m_3}{2}\dot{x}_3^2 &= \frac{m_1}{2}(\dot{R}_{CM}^2 + B^2\dot{x}_{12}^2 + A^2\dot{x}_{23}^2 - 2B\dot{R}_{CM}\dot{x}_{12} - 2A\dot{R}_{CM}\dot{x}_{23} + 2AB\dot{x}_{12}\dot{x}_{23})
\end{aligned}$$

Since we have

$$m_1A - m_2B - m_1B = \frac{m_1(m_1 + m_2) - m_2m_1 - m_1^2}{2m_1 + m_2} = 0.$$

Therefore we have

$$L = \frac{m_2 + 2m_1}{2}\dot{R}_{CM}^2 + \left(\frac{m_1A^2 + m_2B^2 + m_1B^2}{2}\right)\dot{x}_{12}^2$$
$$+ \left(\frac{m_1A^2 + m_2B^2 + m_1B^2}{2}\right)\dot{x}_{23}^2 + (4m_1AB - 2m_2B^2)\dot{x}_{12}\dot{x}_{23} - U(x_{12}) - U(x_{23}).$$

Set $\alpha{=}\left(\frac{m_1A^2+m_2B^2+m_1B^2}{2}\right)$ and $\beta{=}(4m_1AB - 2m_2B^2)$ then

$$L = \frac{M}{2}\dot{R}_{CM}^2 + \alpha\dot{x}_{12}^2 + \alpha\dot{x}_{23}^2 + \beta\dot{x}_{12}\dot{x}_{23} - U(x_{12}) - U(x_{23}).$$

The equations of the motions are

$$2\alpha\ddot{x}_{12} + \beta\ddot{x}_{23} = -\frac{dU(x_{12})}{dx_{12}},\ \ 2\alpha\ddot{x}_{23} + \beta\ddot{x}_{12} = -\frac{dU(x_{23})}{dx_{23}}.$$

The positions of the equilibrium are given as

$$\frac{dU(x_{12})}{dx_{12}}|_{x_{12}=\bar{x}} = 0,\ \ \frac{dU(x_{23})}{dx_{23}}|_{x_{23}=\bar{x}} = 0.$$

Making Taylor expansion around the equilibrium point,

$$\frac{dU(x_{12})}{dx_{12}} = \frac{d^2U(x_{12})}{dx_{12}^2}|_{x_{12}=\bar{x}}(x_{12}-\bar{x})+\mathcal{O}((x_{12}-\bar{x})^2),\ \ \frac{dU(x_{23})}{dx_{23}} = \frac{d^2U(x_{23})}{dx_{23}^2}|_{x_{23}=\bar{x}}(x_{23}-\bar{x})+\mathcal{O}((x_{23}-\bar{x})^2),$$

Set $\xi{=}x_{12} - \bar{x}$ and $\eta{=}x_{23} - \bar{x}$ and $\frac{d^2U(x)}{dx^2}|_{x=\bar{x}}{=}\kappa$. Hence we have

$$2\alpha\ddot{\xi} + \beta\ddot{\eta} = -\kappa\xi,\ \ 2\alpha\ddot{\eta} + \beta\ddot{\xi} = -\kappa\eta.$$

By adding and subtracting the two equations we reach the following equations,

$$(2\alpha + \beta)\ddot{\zeta} = -\kappa\zeta,\ \ (2\alpha - \beta)\ddot{\sigma} = -\kappa\sigma.$$

here $\zeta{=}\xi + \eta$ and $\sigma{=}\xi - \eta$. The tqo equations are independent so we reach the answer,

$$\zeta(t) = \zeta(0)\cos\left(\sqrt{\frac{\kappa}{2\alpha+\beta}}\right)t + \frac{\dot{\zeta}(0)}{\sqrt{\frac{\kappa}{2\alpha+\beta}}}\sin\left(\sqrt{\frac{\kappa}{2\alpha+\beta}}\right)t,$$
$$\sigma(t) = \sigma(0)\cos\left(\sqrt{\frac{\kappa}{2\alpha-\beta}}\right)t + \frac{\dot{\sigma}(0)}{\sqrt{\frac{\kappa}{2\alpha-\beta}}}\sin\left(\sqrt{\frac{\kappa}{2\alpha-\beta}}\right)t,$$

The motions of the molecule is completely determined.

II. HOW TO FIND THE NORMAL MODES

The above method is not applicable in general. Here we bring the general method to solve the same question. The basic idea is that we assume there are some particular modes of the motion which owns only one frequency. This kind of mode is called normal mode. In principle if one can find the normal modes then the general solution must be constructed from the linear combinations of those modes. How to find those modes? The first step is to assume that

$$\xi = Ae^{i\omega t},\ \eta = Be^{i\omega t}.$$

Insert these ansatz one obtains

$$-2\alpha\omega^2 A - \beta\omega^2 B = -\kappa A,\ \ -2\alpha\omega^2 B - \beta\omega^2 A = -\kappa B.$$

One can rewrite the equations as the matrix form,

$$\begin{pmatrix} -2\alpha\omega^2+\kappa & -\beta\omega^2 \\ -\beta\omega^2, & -2\alpha\omega^2+\kappa \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Now we expect this 2×2 matrix cannot be inverted, otherwise A and B must be zero. Therefore we have the following equation,

$$\det\begin{pmatrix} -2\alpha\omega^2+\kappa & -\beta\omega^2 \\ -\beta\omega^2, & -2\alpha\omega^2+\kappa \end{pmatrix} = 0.$$

This equation determines the values of the characteristic frequencies.

$$(-2\alpha\omega^2+\kappa)^2 - \beta^2\omega^4 = 0 \longrightarrow \omega^2 = \frac{\kappa}{2\alpha+\beta}, \frac{\kappa}{2\alpha-\beta}.$$

When $\omega^2{=}\frac{\kappa}{2\alpha+\beta}$, one can find the corresponding mode by inserting the value of ω,

$$\begin{pmatrix} \frac{\beta\kappa}{2\alpha+\beta} & \frac{-\beta\kappa}{2\alpha+\beta} \\ \frac{-\beta\kappa}{2\alpha+\beta} & \frac{\beta\kappa}{2\alpha+\beta} \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \Longrightarrow A = B.$$

On the other hand, when $\omega^2{=}\frac{\kappa}{2\alpha-\beta}$,we have

$$\begin{pmatrix} \frac{-\beta\kappa}{2\alpha-\beta} & \frac{-\beta\kappa}{2\alpha-\beta} \\ \frac{-\beta\kappa}{2\alpha-\beta} & \frac{-\beta\kappa}{2\alpha-\beta} \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \Longrightarrow A = -B.$$

Since the equation only determine ω, the frequency can be either ω or $-\omega$. However, the When $\pm\omega_+ {=} \pm\sqrt{\frac{\kappa}{2\alpha+\beta}}$,

$$\begin{aligned}\xi(t) &= q_1^*(t) = \frac{1}{2}\left((A_+^R + iA_+^I)e^{i\omega_+ t} + (A_+^R - iA_+^I)e^{-i\omega_+ t}\right)\\ &= A_+^R \cos\sqrt{\frac{\kappa}{2\alpha+\beta}}t - A_+^I \sin\sqrt{\frac{\kappa}{2\alpha+\beta}}t.\ \ \eta(t) = \xi(t).\end{aligned}$$

When $\pm\omega_- {=} \pm\sqrt{\frac{\kappa}{2\alpha-\beta}}$,

$$\begin{aligned}\xi(t) &= q_1^*(t) = \frac{1}{2}\left((A_-^R + iA_-^I)e^{i\omega_+ t} + (A_-^R - iA_-^I)e^{-i\omega_+ t}\right)\\ &= A_-^R \cos\sqrt{\frac{\kappa}{2\alpha-\beta}}t - A_-^I \sin\sqrt{\frac{\kappa}{2\alpha-\beta}}t.\ \ \eta(t) = -q_1(t).\end{aligned}$$

The general solutions of $q_1(t)$ and $q_2(t)$ are

$$\begin{aligned}\xi(t) &= A_+^R \cos\sqrt{\frac{\kappa}{2\alpha+\beta}}t - A_+^I \sin\sqrt{\frac{\kappa}{2\alpha+\beta}}t\\ &+ A_-^R \cos\sqrt{\frac{\kappa}{2\alpha-\beta}}t - A_-^I \sin\sqrt{\frac{\kappa}{2\alpha-\beta}}t,\\ \eta(t) &= A_+^R \cos\sqrt{\frac{\kappa}{2\alpha+\beta}}t - A_+^I \sin\sqrt{\frac{\kappa}{2\alpha+\beta}}t\\ &- A_-^R \cos\sqrt{\frac{\kappa}{2\alpha-\beta}}t + A_-^I \sin\sqrt{\frac{\kappa}{2\alpha-\beta}}t,\end{aligned}$$

$$\begin{aligned}\xi(0) &= A_+^R + A_-^R,\ \ \eta(0) = A_+^R - A_-^R,\\ \dot{\xi}(0) &= -\sqrt{\frac{\kappa}{2\alpha+\beta}}A_+^I - \sqrt{\frac{\kappa}{2\alpha-\beta}}A_-^I,\\ \dot{\eta}(0) &= -\sqrt{\frac{\kappa}{2\alpha+\beta}}A_+^I + \sqrt{\frac{\kappa}{2\alpha-\beta}}A_-^I,\end{aligned}$$

$$A_+^R = \frac{1}{2}\left(\xi(0) + \eta(0)\right)\ \ A_-^R = \frac{1}{2}\left(\xi(0) - \eta(0)\right)$$
$$A_+^I = -\sqrt{\frac{2\alpha+\beta}{4\kappa}}(\dot{\xi}(0) + \dot{\eta}(0))\ \ A_+^I = \sqrt{\frac{2\alpha-\beta}{4\kappa}}(-\dot{\xi}(0) + \dot{\eta}(0)).$$

The whole otion of this molecule is determined by these four initial conditions.