52nd—24th INTERNATIONAL-RUDOLF ORTVAY PROBLEM SOLVING CONTEST IN PHYSICS
Problem 10

Nguyen Thanh Long

March 20, 2022

The potential that given in this problem doesn't have any explicit dependence on coordinates so the momentum of our triatomic molecule is a constant. Therefore, the center of mass frame is a inertial frame of reference, then we will choose this frame with the center of mass is the origin. We can see that the stable equilibrium is a equilateral triangle with egde L, so that we will choose the coordinate system as shown below (figure 1) .

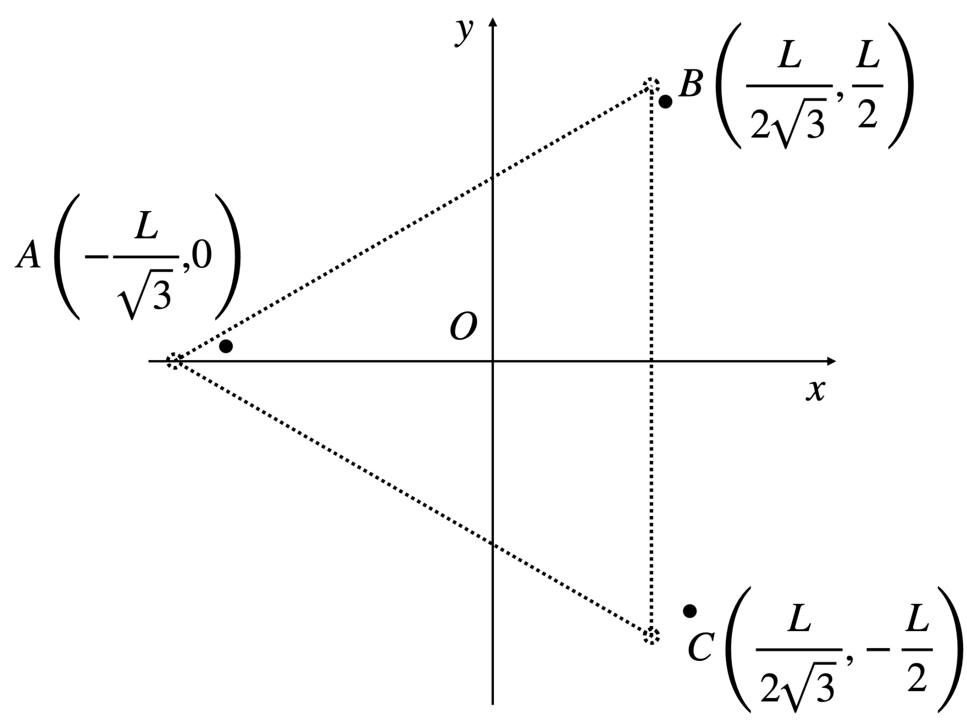

Figure 1: A, B and C are three particle of the molecule and dotted line is the equilibrium.

When three particles are moving, the coordinates of them can be write:

$$x_B = \frac{L}{2\sqrt{3}} + \eta_1. \qquad y_B = \frac{L}{2} + \zeta_1.$$

$$x_C = \frac{L}{2\sqrt{3}} + \eta_2. \qquad y_C = -\frac{L}{2} + \zeta_2.$$

$$x_A = -\frac{L}{\sqrt{3}} - (\eta_1 + \eta_2). \qquad y_A = -(\zeta_1 + \zeta_2).$$

Thus, we note the perimeter and area of :

$$P = \sqrt{(x_B - x_A)^2 + (y_B - y_A)^2} + \sqrt{(x_C - x_A)^2 + (y_C - y_A)^2} + \sqrt{(x_B - x_C)^2 + (y_B - y_C)^2}.$$
$$A = \frac{1}{2}\left[(x_C - x_A)(y_B - y_A) - (x_B - x_A)(y_C - y_A)\right].$$

The Kinetic energy of triatomic molecule:

$$\begin{aligned} T &= \frac{1}{2}m\left(\dot{\eta}_1^2 + \dot{\zeta}_1^2\right) + \frac{1}{2}m\left(\dot{\eta}_2^2 + \dot{\zeta}_2^2\right) + \frac{1}{2}m\left[(\dot{\eta}_1 + \dot{\eta}_2)^2 + \left(\dot{\zeta}_1 + \dot{\zeta}_2\right)^2\right] \\ &= m\left(\dot{\eta}_1^2 + \dot{\eta}_2^2 + \dot{\eta}_1\dot{\eta}_2 + \dot{\zeta}_1^2 + \dot{\zeta}_2^2 + \dot{\zeta}_1\dot{\zeta}_2\right). \end{aligned}$$

Then the Lagrangian of them is:

$$L = m\left(\dot{\eta}_1^2 + \dot{\eta}_2^2 + \dot{\eta}_1\dot{\eta}_2 + \dot{\zeta}_1^2 + \dot{\zeta}_2^2 + \dot{\zeta}_1\dot{\zeta}_2\right) - V_0\left(\frac{P}{L} + \frac{3\sqrt{3}}{8}\frac{L^2}{A}\right).$$

Using the Euler-Lagrange equation $\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) = \frac{\partial L}{\partial x}$, we have 4 differential equation:

$$\begin{aligned} 2\ddot{\eta}_1 + \ddot{\eta}_2 &\approx -\frac{V_0}{mL^2}\left(\frac{45}{4}\eta_1 + 9\eta_2 + \frac{9\sqrt{3}}{4}\zeta_1\right). \\ \ddot{\eta}_1 + 2\ddot{\eta}_2 &\approx -\frac{V_0}{mL^2}\left(9\eta_1 + \frac{45}{4}\eta_2 - \frac{9\sqrt{3}}{4}\zeta_2\right). \\ 2\ddot{\zeta}_1 + \ddot{\zeta}_2 &\approx -\frac{V_0}{mL^2}\left(\frac{9\sqrt{3}}{4}\eta_1 + \frac{27}{4}\zeta_1\right). \\ \ddot{\zeta}_1 + 2\ddot{\zeta}_2 &\approx -\frac{V_0}{mL^2}\left(-\frac{9\sqrt{3}}{4}\eta_2 + \frac{27}{4}\zeta_2\right). \end{aligned}$$

Using matrices, we write them again:

$$\begin{aligned} &\begin{pmatrix} 2 & 1 & 0 & 0 \\ 1 & 2 & 0 & 0 \\ 0 & 0 & 2 & 1 \\ 0 & 0 & 1 & 2 \end{pmatrix}\begin{pmatrix} \ddot{\eta}_1 \\ \ddot{\eta}_2 \\ \ddot{\zeta}_1 \\ \ddot{\zeta}_2 \end{pmatrix} = -\frac{V_0}{mL^2}\begin{pmatrix} \frac{45}{4} & 9 & \frac{9\sqrt{3}}{4} & 0 \\ 9 & \frac{45}{4} & 0 & -\frac{9\sqrt{3}}{4} \\ \frac{9\sqrt{3}}{4} & 0 & \frac{27}{4} & 0 \\ 0 & -\frac{9\sqrt{3}}{4} & 0 & \frac{27}{4} \end{pmatrix}\begin{pmatrix} \eta_1 \\ \eta_2 \\ \zeta_1 \\ \zeta_2 \end{pmatrix} \\ \Rightarrow &\begin{pmatrix} \ddot{\eta}_1 \\ \ddot{\eta}_2 \\ \ddot{\zeta}_1 \\ \ddot{\zeta}_2 \end{pmatrix} = -\frac{V_0}{mL^2}\begin{pmatrix} \frac{9}{2} & \frac{9}{4} & \frac{3\sqrt{3}}{2} & \frac{3\sqrt{3}}{4} \\ \frac{9}{4} & \frac{9}{2} & -\frac{3\sqrt{3}}{4} & -\frac{3\sqrt{3}}{2} \\ \frac{3\sqrt{3}}{2} & \frac{3\sqrt{3}}{4} & \frac{9}{2} & -\frac{9}{4} \\ -\frac{3\sqrt{3}}{4} & -\frac{3\sqrt{3}}{2} & -\frac{9}{4} & \frac{9}{2} \end{pmatrix}\begin{pmatrix} \eta_1 \\ \eta_2 \\ \zeta_1 \\ \zeta_2 \end{pmatrix} \end{aligned}$$

The vibrational frequencies angular of this molecule ω satisfy $\ddot{x} = -\omega^2 x$. Thus, $\frac{m\omega^2 L^2}{V_0}$ is the eigenvalues of the matrice:

$$\begin{pmatrix} \frac{9}{2} & \frac{9}{4} & \frac{3\sqrt{3}}{2} & \frac{3\sqrt{3}}{4} \\ \frac{9}{4} & \frac{9}{2} & -\frac{3\sqrt{3}}{4} & -\frac{3\sqrt{3}}{2} \\ \frac{3\sqrt{3}}{2} & \frac{3\sqrt{3}}{4} & \frac{9}{2} & -\frac{9}{4} \\ -\frac{3\sqrt{3}}{4} & -\frac{3\sqrt{3}}{2} & -\frac{9}{4} & \frac{9}{2} \end{pmatrix}$$

We have found 3 eigenvalues of that matrice: 0 , $\frac{9}{2}$ (twice), 9 so that we have 2 frequencies angular of this molecule: $\omega_1 = 3\sqrt{\frac{V_0}{mL^2}}$, $\omega_2 = \frac{3}{\sqrt{2}}\sqrt{\frac{V_0}{mL^2}}$ ($\omega_3 = 0$ is meaningless so we won't talk about it) Or the vibrational frequencies of this molecule: $f_1 = \frac{3}{2\pi}\sqrt{\frac{V_0}{mL^2}}$ and $f_2 = \frac{3}{2\sqrt{2}\pi}\sqrt{\frac{V_0}{mL^2}}$.