

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

Problem 10

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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) .

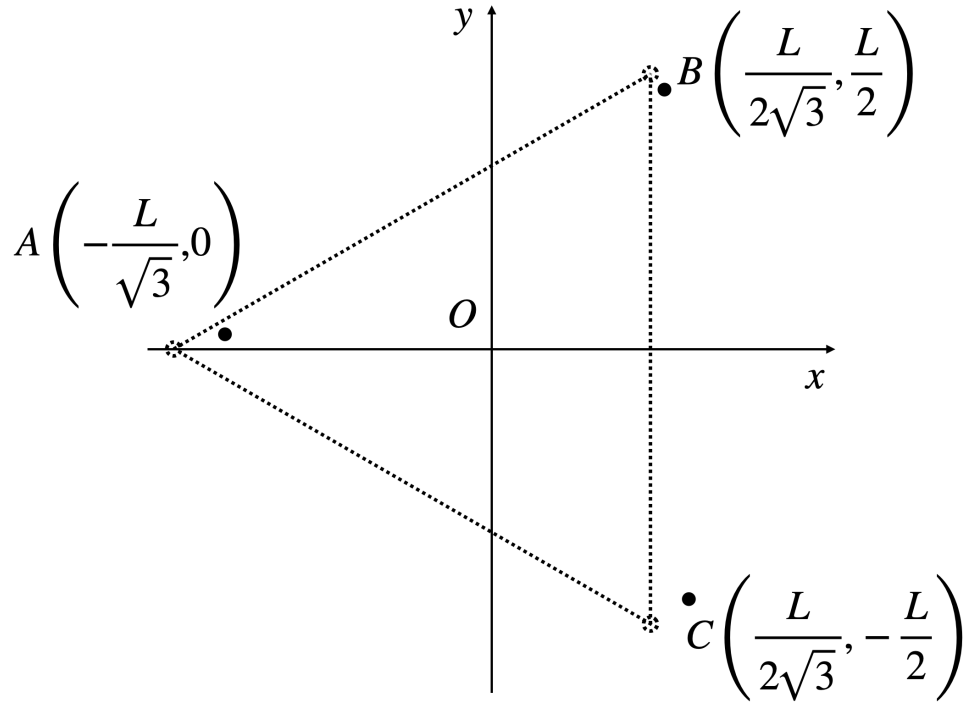


Figure 1: A , B and C are three particle of the molecule and dotted line is the equilibrium.

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

$$\begin{aligned} x_B &= \frac{L}{2\sqrt{3}} + \eta_1. & y_B &= \frac{L}{2} + \zeta_1. \\ x_C &= \frac{L}{2\sqrt{3}} + \eta_2. & y_C &= -\frac{L}{2} + \zeta_2. \\ x_A &= -\frac{L}{\sqrt{3}} - (\eta_1 + \eta_2). & y_A &= -(\zeta_1 + \zeta_2). \end{aligned}$$

Thus, we note the perimeter and area of :

$$P = \sqrt{(x_B - x_A)^2 + (y_B - y_A)^2} + \sqrt{(x_C - x_A)^2 + (y_C - y_A)^2} + \sqrt{(x_B - x_C)^2 + (y_B - y_C)^2}.$$

$$A = \frac{1}{2} [(x_C - x_A)(y_B - y_A) - (x_B - x_A)(y_C - y_A)].$$

The Kinetic energy of triatomic molecule:

$$T = \frac{1}{2}m(\dot{\eta}_1^2 + \dot{\zeta}_1^2) + \frac{1}{2}m(\dot{\eta}_2^2 + \dot{\zeta}_2^2) + \frac{1}{2}m[(\dot{\eta}_1 + \dot{\eta}_2)^2 + (\dot{\zeta}_1 + \dot{\zeta}_2)^2]$$

$$= m(\dot{\eta}_1^2 + \dot{\eta}_2^2 + \dot{\eta}_1\dot{\eta}_2 + \dot{\zeta}_1^2 + \dot{\zeta}_2^2 + \dot{\zeta}_1\dot{\zeta}_2).$$

Then the Lagrangian of them is:

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

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:

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

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

$$2\ddot{\zeta}_1 + \ddot{\zeta}_2 \approx -\frac{V_0}{mL^2} \left(\frac{9\sqrt{3}}{4}\eta_1 + \frac{27}{4}\zeta_1 \right).$$

$$\ddot{\zeta}_1 + 2\ddot{\zeta}_2 \approx -\frac{V_0}{mL^2} \left(-\frac{9\sqrt{3}}{4}\eta_2 + \frac{27}{4}\zeta_2 \right).$$

Using matrices, we write them again:

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

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

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 matrix: 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 $f_2 = \frac{3}{2\sqrt{2}\pi}\sqrt{\frac{V_0}{mL^2}}$.