

## §32 THE INERTIA TENSOR

## PROBLEM 1.

Determine the principal moments of inertia for the following types of molecule, regarded as systems of particles at fixed distances apart:

(a)

A molecule of collinear atoms.

SOLUTION: Choose the  $x_3$ -axis along the line containing all atoms, and place the origin at the centre of mass. Then each particle has coordinates  $(0, 0, x_a)$ , so the inertia tensor is diagonal in the basis  $(x_1, x_2, x_3)$ , with

$$I_3 = 0, \quad I_1 = I_2.$$

Indeed, since the distance to the  $x_1$ -axis (or  $x_2$ -axis) is  $|x_a - x_{CM}|$  for each particle,

$$I_1 = I_2 = \sum_a m_a (x_a - x_{CM})^2, \quad x_{CM} = \frac{1}{\mu} \sum_a m_a x_a, \quad \mu = \sum_a m_a.$$

Expanding and using the definition of  $x_{CM}$  gives

$$\begin{aligned} I_1 = I_2 &= \sum_a m_a x_a^2 - 2x_{CM} \sum_a m_a x_a + \mu x_{CM}^2 \\ &= \sum_a m_a x_a^2 - \frac{1}{\mu} \left( \sum_a m_a x_a \right)^2. \end{aligned}$$

To rewrite this in terms of pairwise separations, expand the square:

$$\left( \sum_a m_a x_a \right)^2 = \sum_a m_a^2 x_a^2 + 2 \sum_{a < b} m_a m_b x_a x_b.$$

Hence

$$\begin{aligned} I_1 = I_2 &= \sum_a m_a x_a^2 - \frac{1}{\mu} \sum_a m_a^2 x_a^2 - \frac{2}{\mu} \sum_{a < b} m_a m_b x_a x_b \\ &= \frac{1}{\mu} \sum_a m_a (\mu - m_a) x_a^2 - \frac{2}{\mu} \sum_{a < b} m_a m_b x_a x_b. \end{aligned}$$

Now note that  $\mu - m_a = \sum_{b \neq a} m_b$ , so

$$\sum_a m_a (\mu - m_a) x_a^2 = \sum_a \sum_{b \neq a} m_a m_b x_a^2 = \sum_{a < b} m_a m_b (x_a^2 + x_b^2).$$

Therefore

$$\begin{aligned} I_1 = I_2 &= \frac{1}{\mu} \sum_{a < b} m_a m_b (x_a^2 + x_b^2) - \frac{2}{\mu} \sum_{a < b} m_a m_b x_a x_b \\ &= \frac{1}{\mu} \sum_{a < b} m_a m_b (x_a - x_b)^2. \end{aligned}$$

Since for collinear atoms the pair distance is  $l_{ab} = |x_a - x_b|$ , we finally obtain

ANSWER TO PROBLEM 1 (A).

$$\begin{aligned} I_1 = I_2 &= \frac{1}{\mu} \sum_{a < b} m_a m_b l_{ab}^2 \\ I_3 &= 0 \end{aligned}$$

(b)

A triatomic molecule which is an isosceles triangle (Fig. 36).

SOLUTION: Let the molecule lie in the  $(x_1, x_2)$ -plane, with  $x_1$  along the base and  $x_2$  along the axis of symmetry. The two base atoms have equal masses  $m_1$  and are separated by a distance  $a$ ; the apex atom has mass  $m_2$  and is at height  $h$  above the base midpoint. Denote the total mass by

$$\mu = 2m_1 + m_2.$$

Choose coordinates (before shifting to the centre of mass):

$$(x_1, x_2)_{(1)} = \left(-\frac{a}{2}, 0\right), \quad (x_1, x_2)_{(3)} = \left(+\frac{a}{2}, 0\right), \quad (x_1, x_2)_{(2)} = (0, h),$$

where atoms (1) and (3) have mass  $m_1$  and atom (2) has mass  $m_2$ . By symmetry  $x_{1,CM} = 0$ , and

$$x_{2,CM} = \frac{m_2 h}{\mu}.$$

The symmetry implies that the axes through the centre of mass parallel to  $x_1$ ,  $x_2$ , and  $x_3$  are principal. Hence,

$$I_1 = \sum_a m_a (x_{2,a} - x_{2,CM})^2, \quad I_2 = \sum_a m_a (x_{1,a} - x_{1,CM})^2, \quad I_3 = I_1 + I_2,$$

since the molecule is planar ( $x_3 \equiv 0$ ). Using the pair-distance identity in one dimension,

$$\sum_a m_a (x_{2,a} - x_{2,CM})^2 = \frac{1}{\mu} \sum_{a < b} m_a m_b (x_{2,a} - x_{2,b})^2,$$

and noting that the only non-zero vertical separations are between the apex and each base atom, equal to  $h$ , we obtain

$$I_1 = \frac{1}{\mu} (m_1 m_2 h^2 + m_1 m_2 h^2) = \frac{2m_1 m_2}{\mu} h^2.$$

Similarly,

$$I_2 = \sum_a m_a (x_{1,a} - x_{1,CM})^2 = \frac{1}{\mu} \sum_{a < b} m_a m_b (x_{1,a} - x_{1,b})^2.$$

The horizontal separations are between the two base atoms, and between the apex and either base atom. Hence

$$I_2 = \frac{1}{\mu} \left( m_1^2 a^2 + 2m_1 m_2 \left(\frac{a}{2}\right)^2 \right) = \frac{1}{\mu} \left( m_1^2 a^2 + \frac{1}{2} m_1 m_2 a^2 \right) = \frac{1}{2} m_1 a^2.$$

Therefore

$$I_3 = I_1 + I_2 = \frac{2m_1 m_2}{\mu} h^2 + \frac{1}{2} m_1 a^2.$$

ANSWER TO PROBLEM 1 (B).

$$I_1 = \frac{2m_1 m_2}{\mu} h^2$$

$$I_2 = \frac{1}{2} m_1 a^2$$

$$I_3 = I_1 + I_2.$$

(c)

A tetratomic molecule which is an equilateral-based tetrahedron (Fig. 37).

SOLUTION: The base is an equilateral triangle of side  $a$  in the plane  $x_3 = 0$ , with three equal masses  $m_1$  at its vertices. A fourth atom of mass  $m_2$  lies on the symmetry axis through the base centroid at height  $h$  above the base. Let

$$\mu = 3m_1 + m_2.$$

Let  $\rho$  be the distance from the base centroid to a base vertex. For an equilateral triangle,

$$\rho = \frac{a}{\sqrt{3}}, \quad \rho^2 = \frac{a^2}{3}.$$

By symmetry the centre of mass lies on the symmetry axis. Measuring  $x_3$  from the base plane,

$$x_{3,CM} = \frac{m_2 h}{\mu}.$$

The symmetry axis is a principal axis; any two orthogonal axes through the centre of mass perpendicular to it are also principal and have equal moments. Thus

$$I_1 = I_2, \quad I_3 \text{ about the symmetry axis } (x_3).$$

The apex mass lies on the axis and contributes nothing. Each base mass is at distance  $\rho$  from the axis, hence

$$I_3 = 3m_1 \rho^2 = 3m_1 \frac{a^2}{3} = m_1 a^2.$$

Let  $x_1$  be any axis through the centre of mass perpendicular to  $x_3$ . Then

$$I_1 = \sum_a m_a (y_a^2 + z_a^2),$$

where  $y$  is a coordinate orthogonal to  $x_1$  in the plane perpendicular to the axis, and  $z$  is measured along  $x_3$  from the centre of mass. The vertical coordinates relative to the centre of mass are

$$z_{\text{base}} = -x_{3,CM} = -\frac{m_2 h}{\mu}, \quad z_{\text{apex}} = h - x_{3,CM} = h \left(1 - \frac{m_2}{\mu}\right) = \frac{3m_1}{\mu} h.$$

For the three vertices of an equilateral triangle, for any in-plane axis through the centroid,

$$\sum_{\text{base}} y^2 = \frac{3}{2} \rho^2 = \frac{3}{2} \cdot \frac{a^2}{3} = \frac{1}{2} a^2.$$

Therefore,

$$\begin{aligned} I_1 &= m_1 \left( \sum_{\text{base}} y^2 \right) + 3m_1 z_{\text{base}}^2 + m_2 z_{\text{apex}}^2 \\ &= \frac{1}{2} m_1 a^2 + 3m_1 \left( \frac{m_2^2 h^2}{\mu^2} \right) + m_2 \left( \frac{9m_1^2 h^2}{\mu^2} \right) \\ &= \frac{1}{2} m_1 a^2 + \frac{3m_1 m_2}{\mu} h^2. \end{aligned}$$

Hence  $I_2 = I_1$ .

ANSWER TO PROBLEM 1 (C).

$$\begin{aligned} I_1 = I_2 &= \frac{3m_1 m_2}{\mu} h^2 + \frac{1}{2} m_1 a^2 \\ I_3 &= m_1 a^2 \end{aligned}$$