☹ me-que-14002

Show that the principal moments of inertia of a linear chain consisting of two kinds of atoms a, b, with origin chosen to coincide with the centre of mass, is given by

$$I_1 = I_2 = \frac{1}{M}\sum_{i\neq j} m_i m_j\, d_{ij}^2, \qquad I_3 = 0.$$

where the summation includes each pair of i, j atoms once and $d_{ij}$is the distance between atoms in the pair and M is the total mass. Verify that this gives correct answer for a triatomic molecule. [6+4]

☺ **Solution:** Let the positions of the masses be x_i measured from some origin on the line joining the atoms. The moment of inertia about the origin, I_0 is given by

$$I_0 = \sum_i m_i x_i^2.$$

Letting $I_{\rm cm}$ denote the moment of inertia about the centre of mass. Using the parallel axes theorem we have

$$I_0 = I_{\rm cm} + MX^2,$$

where

$$X = \frac{1}{M}\sum_i m_i x_i$$

is the position of the centre of mass and M is the total mass. Therefore we get

$$\begin{aligned}
I_{\rm cm} &= I_0 - MX^2 = \frac{1}{M}\Big\{M\sum_i x_i^2 - \Big(\sum_i m_i x_i\Big)^2\Big\} && (1)\\
&= \frac{1}{M}\Big\{\Big(\sum_j m_j\Big)\sum_i (m_i x_i^2) - \Big(\sum_i m_i x_i\Big)\Big(\sum_j m_j x_j\Big)\Big\} && (2)\\
&= \frac{1}{M}\sum_{ij}\Big\{m_j m_i (x_i^2 - x_i x_j)\Big\} && (3)\\
&= \frac{1}{M}\sum_{i\neq j}\Big\{m_j m_i (x_i^2 - x_i x_j)\Big\} && (4)\\
&= \frac{1}{2M}\sum_{i\neq j}\Big\{m_j m_i (x_i^2 - 2x_i x_j + x_j)^2\Big\} && (5)
\end{aligned}$$

In the last step, for S_{ij} symmetric under exchange $i \leftrightarrow j$, we have used

$$\sum_{ij} S_{ij} T_{ij} = \frac{1}{2}\sum_{ij} S_{ij}(T_{ij} + T_{ji})$$

In the sum in (5), each pair ij is counted twice, hence we get

$$I_{\rm cm} = \frac{1}{M}\sum_{\rm pairs}\left\{m_j m_i(x_i^2 - 2x_i x_j + x_j)^2\right\} \tag{6}$$

$$= \frac{1}{M}\sum_{\rm pairs}(x_i - x_j)^2. \tag{7}$$

where now each pair is counted once.