PROBLEM ⌷2⌷ : THE LONGITUDINAL MOTION OF A LINEAR MOLECULE

In this problem you will analyze the longitudinal motion of a linear molecule, i.e., the motion along the molecular axis. The rotational motion and the bending of the molecule are not considered. The molecule is assumed to consist of N atoms of mass m_1, m_2, ..., m_N, respectively. Each atom is assumed to be connected to its neighbors by a chemical bond. Each bond is approximated by a massless spring which obeys Hooke's law with spring constants k_1, k_2, ... k_{N-1}. The molecule is shown in Fig. 1.
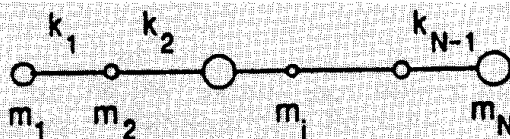

Fig.1. A linear molecule with N atoms.

Use the following facts when solving this problem: The longitudinal vibrational motion of a linear molecule consists of a superposition of separate vibrational motions called normal vibrations, or normal modes. In a normal mode all atoms vibrate in simple harmonic motion with the same frequency and pass through their equilibrium positions simultaneously.

Questions

1) Let x_i be the displacement of atom i from its equilibrium position. Express the force F_i acting on each atom i as a function of the displacements x_1, x_2 ,..., x_N and the spring constants k_1, k_2, ..., k_{N-1}. What relationship is there among the forces F_1, F_2, ..., F_N? Using this relationship, derive a relationship between the displacements x_1, x_2, ..., x_N and give a physical interpretation of this relationship.

2) Analyze the motion of a diatomic molecule AB (Fig. 2). The value of the spring constant is k. Derive an expression for the forces acting on atoms A and B. Determine the possible types of motion of the molecule. Determine the corresponding vibrational frequencies and interpret the result. In particular, how is it possible for the atoms to vibrate with the same frequency even though their masses are not the same?
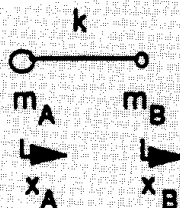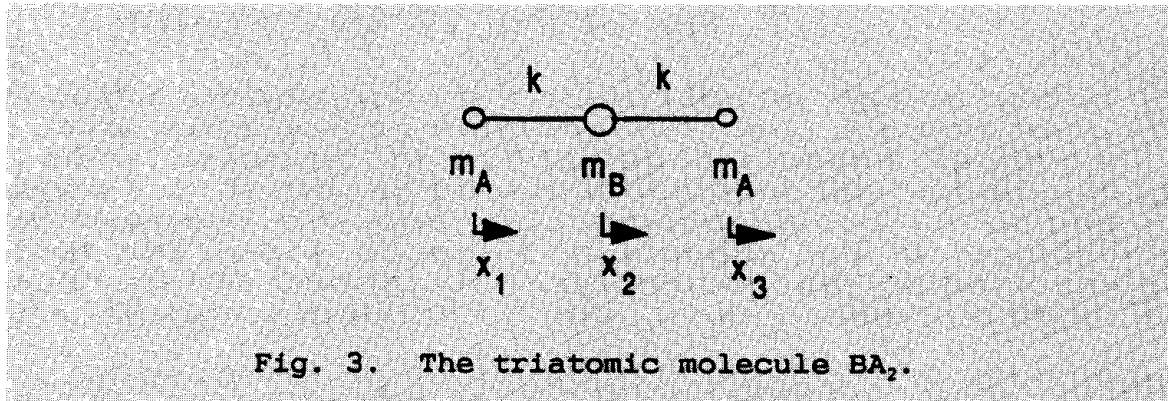

Fig. 2. The diatomic molecule AB

3) Analyze the motion of the triatomic molecule BA_2 (Fig. 3)

Fig. 3. The triatomic molecule BA_2.

Express the net force on each atom as a function of its displacement only. Deduce the possible motions of the molecule and the corresponding vibrational frequencies.

4) The frequencies of the two longitudinal modes of vibration of the CO_2 molecule are 3.998×10^{13} Hz and 7.042×10^{13} Hz, respectively. Determine a numerical value for the spring constant of the CO bond.

How well do you think this approximation for the bond structure of the molecule describes the vibrational motion of the real molecule?

The atomic mass of the carbon atom = 12 amu and that of the oxygen atom = 16 amu. The atomic mass unit = 1.660×10^{-27} kg.