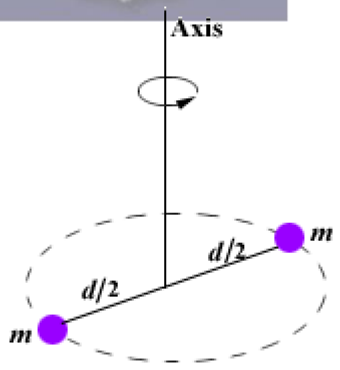
754.

<u>Problem 51.33 (RHK)</u>

We have to show that in a diatomic molecule consisting of two atoms of equal mass m separated by a distance d and rotating about an axis, the energy levels can be written as

$$E_l = \frac{h^2 l(l+1)}{4\pi^2 m d^2},\ l = 1, 2, 3..$$

(b) *We have to calculate the energies of the lowest three levels of the* O_2 *molecule, for which the two atoms are* 121 pm *apart. The mass of the oxygen atom is* 16.0 u.



<u>Solution:</u>

(a)

Classically the energy of this system in terms of its angular momentum L can be expressed as

$$E = 2\times\left(\frac{1}{2}mv^2\right),$$

and

$$L = 2\times mv\times\frac{d}{2} = mvd,$$

or

$$E = \frac{L^2}{md^2}.$$

According to the quantization of angular momentum

$$L^2 = l\left(l+1\right)\mathrm{h}^2,\ l = 0,1,2,3..$$

Therefore, the energy values of the quantum rotator are

$$E = \frac{l\left(l+1\right)h^2}{4\pi^2 md^2},\ l = 1,2,3..$$

(b)

We will calculate next using this model the ground state energy in eV of the O_2 molecule with $d = 121\ \mathrm{pm}$ and $m = 16.0\ \mathrm{u}$.

We will use the following data and values:

$$m = 16.0\ \mathrm{u} = 16.0\times1.66\times10^{-27}\ \mathrm{kg}$$
$$= 26.56\times10^{-27}\ \mathrm{kg}.$$

$d = 121 \times 10^{-12}$ m,

and

$h = 1.054 \times 10^{-34}$ J s

The ground state of the O_2 molecule will correspond to $n = 1$. Substituting the above data, we get

$$\frac{h^2}{md^2} = \frac{\left(1.054 \times 10^{-34}\right)^2}{26.56 \times 10^{-27} \times \left(121 \times 10^{-12}\right)^2} \text{ J}$$

$$= 2.86 \times 10^{-23} \text{ J.}$$

As $1\text{J} = 6.242 \times 10^{18}$ eV,

we get

$$\frac{h^2}{md^2} = 2.86 \times 10^{-23} \times 6.242 \times 10^{18} \text{ eV}$$

$$= 1.78 \times 10^{-4} \text{ eV.}$$

The energies of the lowest three levels of the O_2 molecule will therefore be

$l = 1,\ E_1 = 3.56 \times 10^{-4}$ eV;

$l = 2,\ E_2 = 10.68 \times 10^{-4}$ eV;

$l = 3,\ E_3 = 21.36 \times 10^{-4}$ eV.