Gasiorowicz 3rd edition April 14, 2008

P7-1.

Consider the molecule CN, which may be described by a dumbbell consisting of two masses M_1 and M_2 attached by a rigid rod of length a. The dumbbell rotates in a plane about an axis going through the center of mass and perpendicular to it.

(a) Write down the Hamiltonian that describes the motion.

(b) What is the energy spectrum?

(c) Write down an expression for the difference in energy between the ground state and the first excited state in terms of the masses and a.

Solution:

(a)

If x is the distance of the center of mass from M_1:

$$M_1 x = M_2 (a - x) \Rightarrow x(M_1 + M_2) = M_2 a$$

$$\Rightarrow x = \frac{M_2 a}{M_1 + M_2}$$

$$\therefore \text{Moment of intertia} = I = M_1 x^2 + M_2 (a - x)^2$$

$$= M_1 \left(\frac{M_2 a}{M_1 + M_2} \right)^2 + M_2 \left(a - \frac{M_2 a}{M_1 + M_2} \right)^2$$

$$= M_1 \left(\frac{M_2 a}{M_1 + M_2} \right)^2 + M_2 \left(\frac{M_1 a}{M_1 + M_2} \right)^2$$

$$= \frac{M_1 M_2{}^2 a^2 + M_1{}^2 M_2 a^2}{(M_1 + M_2)^2}$$

$$= \frac{M_1 M_2 (M_1 + M_2) a^2}{(M_1 + M_2)^2}$$

$$= \frac{M_1 M_2 a^2}{(M_1 + M_2)}$$

$$= \mu a^2 \quad \text{where } \mu \text{ is the reduced mass, } \mu = \frac{M_1 M_2}{M_1 + M_2}$$

$$\therefore H = \frac{L^2}{2I} \quad \text{where } I = \frac{M_1 M_2}{M_1 + M_2} a^2 \text{ and L is the angular momentum.}$$

(b)

Since $H = \frac{L^2}{2I}$, so $[H, L^2] = 0$.

$L^2\psi = \ell(\ell+1)\hbar^2$

$$\therefore E = \frac{\ell(\ell+1)\hbar^2}{2I} = \frac{\ell(\ell+1)\hbar^2}{2\left(\frac{M_1 M_2}{M_1 + M_2}\right)a^2} = \frac{(M_1 + M_2)\ell(\ell+1)\hbar^2}{2M_1 M_2 a^2} \qquad \ell = 0,1,2,.....$$

(c)

$$E_0 = \frac{(M_1 + M_2)\cdot 0\cdot(0+1)\hbar^2}{2M_1 M_2 a^2} = 0$$

$$E_1 = \frac{(M_1 + M_2)\cdot 1\cdot(1+1)\hbar^2}{2M_1 M_2 a^2} = \frac{2(M_1 + M_2)\hbar^2}{2M_1 M_2 a^2} = \frac{(M_1 + M_2)\hbar^2}{M_1 M_2 a^2}$$

$$\therefore E_1 - E_0 = \frac{(M_1 + M_2)\hbar^2}{M_1 M_2 a^2}$$