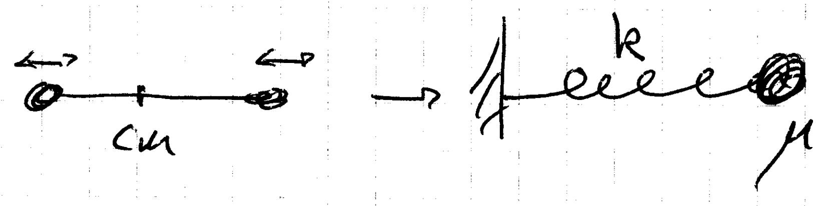
H.O.

CM



$$V(x) = \frac{1}{2} k x^2$$

Q.M

$$\hat{H} = -\frac{\hbar^2}{2\mu}\nabla^2 + \frac{1}{2} k x^2$$

in 1d

$$\hat{H} = -\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2} + \frac{1}{2} k x^2$$

$$\hat{H}\Psi_n = E_n \Psi_n$$

$$E_n = h\nu(n+1/2)$$

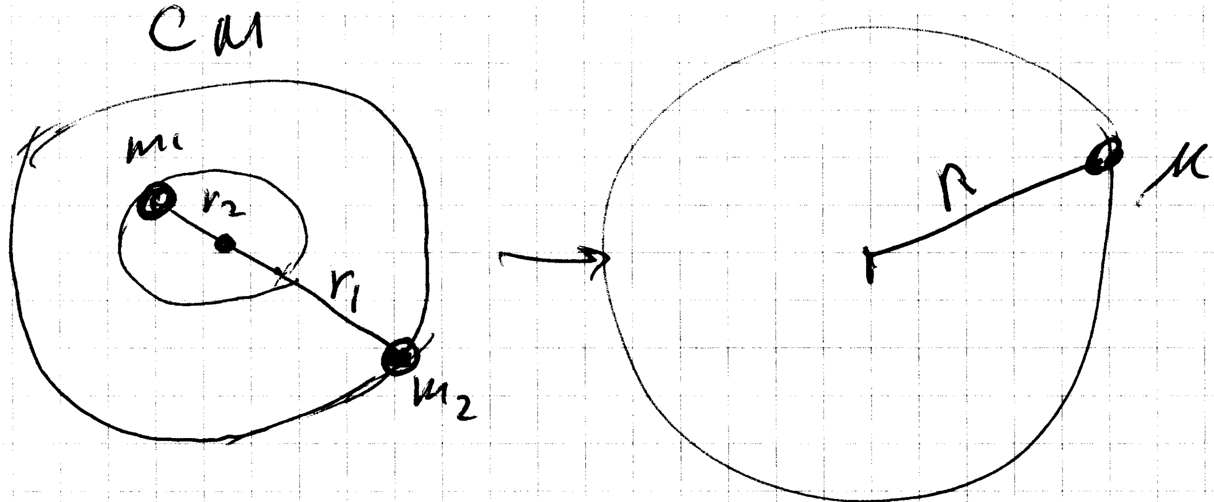
$$\Psi_n(x) \sim H_n(\sqrt{\alpha}x)\, e^{-\frac{1}{2}\alpha x^2}$$

$$\Delta E_{n\to n+1} = h\nu$$

$$\nu = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}}$$

RR

CM



$$K = \frac{1}{2}\frac{L^2}{I} \qquad R = r_1 + r_2$$

$$I = \mu R^2 \qquad \mu = \frac{m_1 m_2}{m_1 + m_2}$$

$$E = \frac{1}{2}\frac{L^2}{I} \qquad V(r) = 0$$

QM

$$\hat{H} = \hat{K} = -\frac{\hbar^2}{2\mu}\nabla^2$$

$$(x, y, z) \longrightarrow (r, \theta, \varphi)$$

$$\hat{H} = + \frac{1}{2I} \hat{L}^2$$

$$\hat{L}^2 = -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \sin\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\varphi^2} \right]$$

SPECTROSCOPY

IN THE CASE OF THE QM HO THE ONLY TRANSITIONS ALLOWED ARE BETWEEN ADJACENT LEVELS (CHE401)

$$\Delta n = \pm 1$$

IN THE CASE OF RIGID ROTATOR

$$\Delta J = \pm 1$$

FOR Q.M. H.O.

$$\Delta E_{viB} = \pm h\nu$$

RIGID ROTATOR

$J \rightarrow J+1$ $\quad \Delta E_{Rot} = \frac{\hbar^2}{I}(J+1)$ $\quad$ R- BRANCH $\Delta J = +1$

$J \rightarrow J-1$ $\quad \Delta E_{Rot} = -\frac{\hbar^2}{I} J$ $\quad$ P-BRANCH $\Delta J = -1$

FOR THE Q.M. H.O.

$$\nu = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}} = \frac{1}{2\pi}\sqrt{\frac{500\ N\,m^{-1}}{8.5\times10^{-27}\,kg}}\ \frac{100}{(10^{-26})}$$

$$\sim 4\times10^{13}\ s^{-1} \quad - \quad 5\times10^{12}\ s^{-1}$$

$$h\nu \sim 3\times10^{-20}\ J \quad - \quad 3\times10^{-21}\ J$$

$$\sim 5\times10^{-3}\ eV \quad - \quad 5\times10^{-4}\ eV$$

$$\frac{1}{\lambda} \sim 4\times10^{3}\ cm^{-1} \qquad 5\times10^{2}\ cm^{-1}$$

$$4000\ cm^{-1} \qquad 500\ cm^{-1}$$

$$t_{vib} \sim 25\ fs \qquad 200\ fs$$

RR

$$\nu_{OBS} = \frac{h}{4\pi^2 I}(J+1) \equiv 2B(J+1)$$

$$B \equiv \frac{h}{8\pi^2 I} = \frac{1}{2}\frac{\hbar}{I}$$

FOR A DIATOMIC MOLECULE

$\mu \sim 10^{-25} - 10^{-26}$ Kg

$r \sim 100$ pm

$I \sim 10^{-45} - 10^{-46}$ Kg m^2

$\nu \sim 2\times10^{10}$ Hz — 10^{11} Hz

$\sim 2B$ MICROWAVE REGION

$h\nu \sim 10^{-6}$ eV

$\frac{1}{\lambda} \sim 2\ cm^{-1}$ — $10\ cm^{-1}$

$t_{ROT} \sim 50\,000$ fs — $50{,}00$ fs