Note Title 04-02-2011

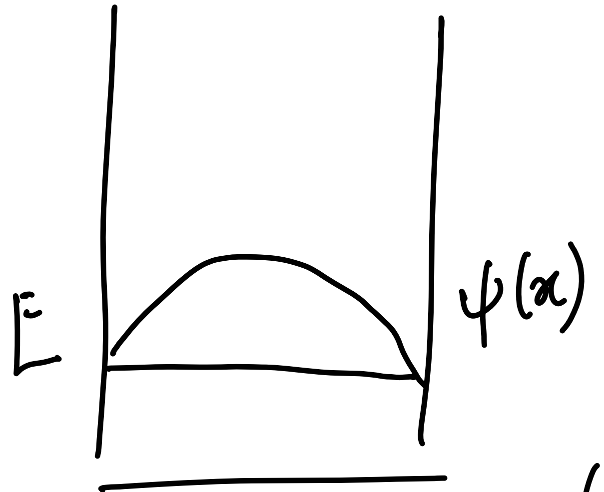
Correction in the Hermite polynomial recursion relation

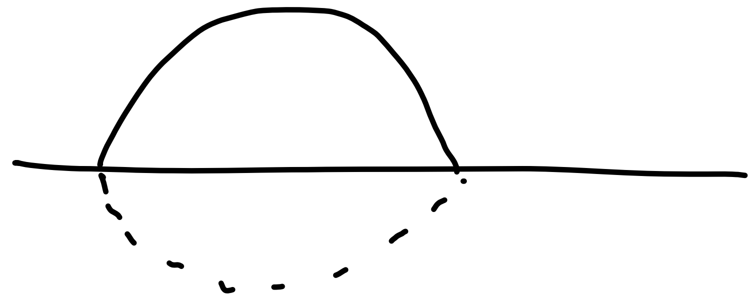
$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$$

$$H_0(x) = 1$$

$$H_1(x) = 2x$$

$$\vdots$$

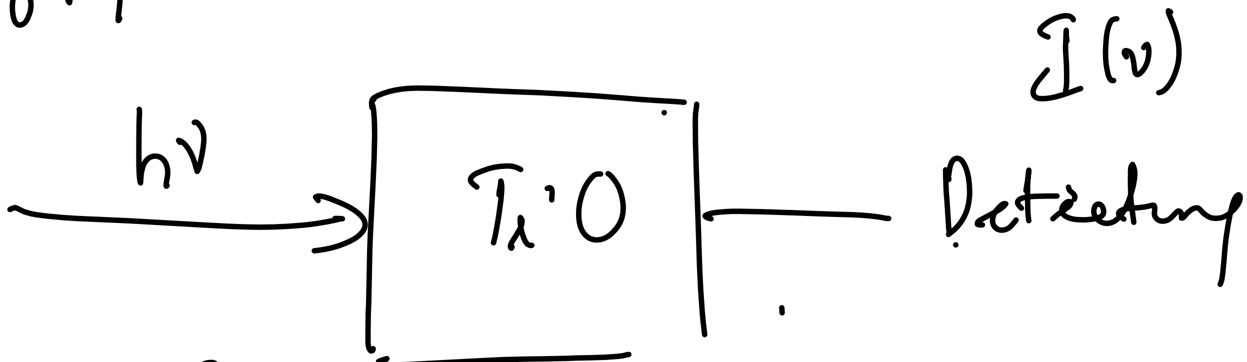




$$(4x^2 - 2)\, e^{-\alpha x^2/2}$$

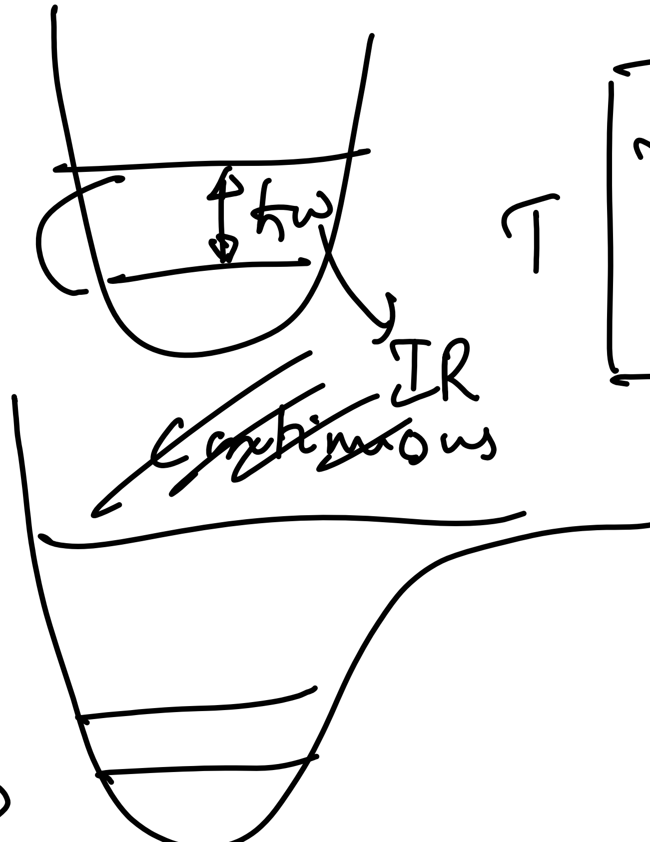
$k \sim 1000\ \mathrm{N/m}$

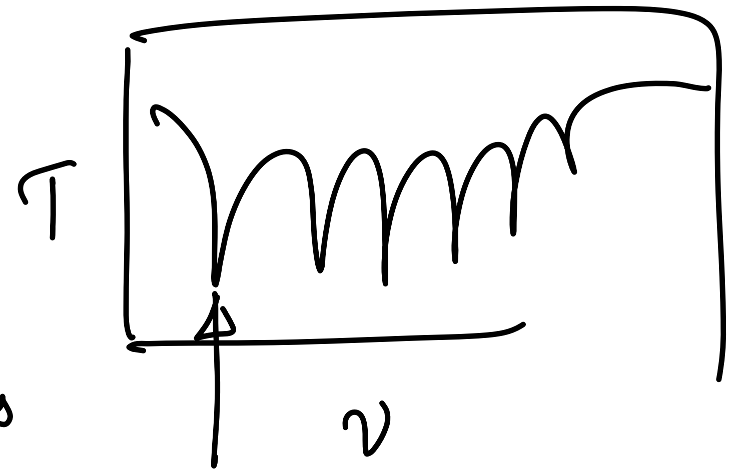
$$\omega = \sqrt{\frac{k}{\mu}}$$



$\sim 10^{13}/\mathrm{s} \rightarrow$ Infrared of the EM spectrum

$\Delta v = \pm 1$ → selection rule





$\omega = 2\pi\nu \rightarrow 1/s$

$\Delta E = \hbar\omega$
$= h\nu$
$= hc\tilde{\nu}$

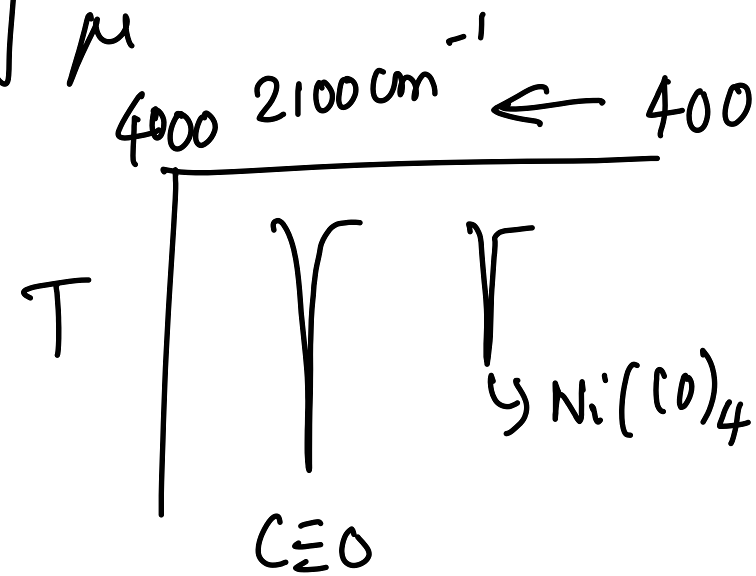
$cm^{-1} \rightarrow 400 - 4000\ cm^{-1}$

$$\boxed{C \equiv O}$$

$$\omega = \sqrt{\frac{k}{\mu}}$$

$Ni(CO)_4$

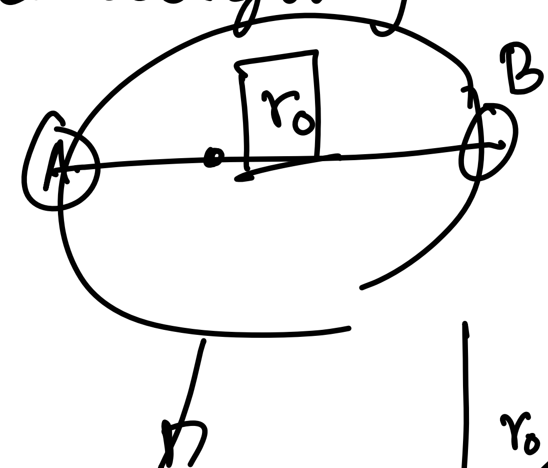
Σ

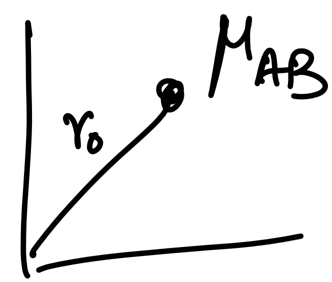


Note Title 04-02-2011

Rotational motion

Reduced mass at a fixed distance (equilibrium bond length) undergoing rotational motion





Note Title 04-02-2011

$$\mathcal{H} = \hat{T} \qquad V = 0 \qquad M$$

$$\hat{T} = \frac{\hat{p}^2}{2m} = \frac{\hat{L}^2}{2I} \qquad I = \mu r_0^2$$

$$L^2 = \vec{\hat{L}} \cdot \vec{\hat{L}} \qquad \vec{L} = \begin{vmatrix} i & j & k \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix}$$

$$\hat{L}_x , \hat{L}_y , \hat{L}_z$$

Note Title 04-02-2011

Verify at home!

$$\hat{L}_x = (y p_z - z p_y) -$$

$$\hat{L}_y = (z p_x - x p_z) - \left[i\hbar \frac{\partial}{\partial x}, x \right]$$

$$[p_x, x] = ? \quad -i\hbar$$

$$[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$$

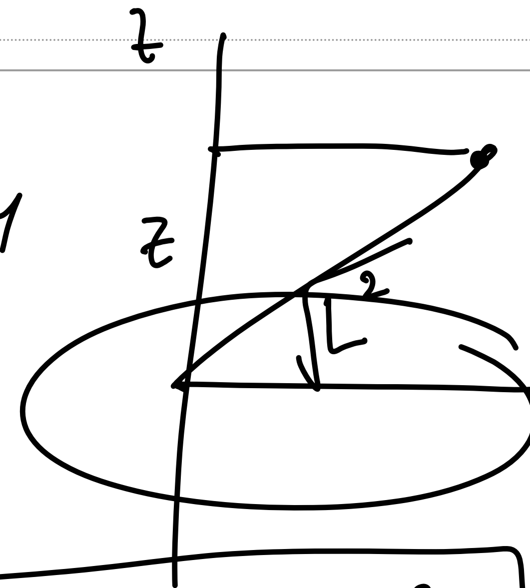
cyclic permutations

$$[L_y, L_z] = i\hbar \hat{L}_x$$

$$[L^2, L_x] = 0 = [L^2, L_y] = [L^2, L_z]$$

Note Title 04-02-2011

L^2 & L_z → completely arbitrary



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

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

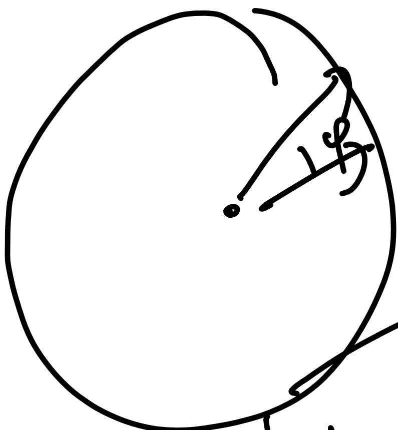
Motion confined to the xy-plane $\sin\theta = 1$

$$\hat{L}^2 = L_z^2 = -\hbar^2 \frac{\partial^2}{\partial\varphi^2}$$

Note Title 04-02-2011

Rotor confined to a plane

$$\boxed{\hat{\mathcal{H}} = \frac{-\hbar^2}{2\mu r^2}\frac{\partial^2}{\partial \varphi^2}}$$



$$\mathcal{H}\psi = E\psi$$

$$\Delta L_z \, \Delta\varphi \geq \hbar/2$$