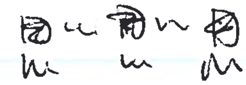
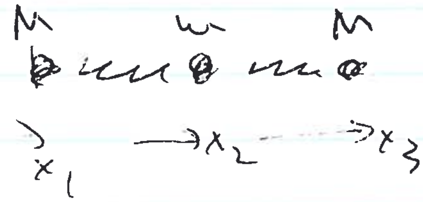
10/30/2017

Modes of molecule : CO_2





$$\begin{cases} F_1 = M\ddot{x}_1 = -k(x_1 - x_2) = +k(x_2 - x_1) \\ F_2 = m\ddot{x}_2 = -k(x_2 - x_3) - k(x_2 - x_1) \\ F_3 = M\ddot{x}_3 = -k(x_3 - x_2) \end{cases}$$

$$\ddot{x}_1 = -\frac{k}{M} x_1 + \frac{k}{M} x_2$$

$$\ddot{x}_2 = +\frac{k}{m} x_1 - \frac{2k}{m} x_2 + \frac{k}{m} x_3$$

$$\ddot{x}_3 = +\frac{k}{M} x_2 - \frac{k}{m} x_3$$

$$\begin{pmatrix} \ddot{x}_1 \\ \ddot{x}_2 \\ \ddot{x}_3 \end{pmatrix} = \begin{pmatrix} -k/m & k/m & 0 \\ +\frac{k}{m} & -2k/m & +\frac{k}{m} \\ 0 & +\frac{k}{M} & -\frac{k}{M} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

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oscillatory solutions : $x_i = A_i e^{-i\omega t}$

$(A_i \cos\omega t)$

$$\boxed{\overleftrightarrow{M}\cdot\vec{A} = -\omega^2\vec{A}}$$

$$(\overleftrightarrow{M} + \omega^2 \mathbb{1})\cdot\vec{A} = 0$$

$$\det(\overleftrightarrow{M} + \omega^2 \mathbb{1}) = 0.$$

$$\det\begin{pmatrix} \omega^2 - \frac{k}{M} & \frac{k}{M} & 0 \\ k/m & \omega^2 - \frac{2k}{m} & \frac{k}{m} \\ 0 & \frac{k}{M} & \omega^2 - \frac{k}{M} \end{pmatrix}$$

$$= \left(\omega^2 - \frac{k}{M}\right)^2\left(\omega^2 - \frac{2k}{m}\right) - 2\left(\frac{k}{M}\right)^2\left(\omega^2 - \frac{k}{M}\right)$$

$$= \left(\omega^2 - \frac{k}{M}\right)\left[\left(\omega^2 - \frac{k}{M}\right)\left(\omega^2 - \frac{2k}{m}\right) - 2\left(\frac{k}{M}\right)^2\right] = 0$$

$$\left(\omega^2 - \frac{k}{M}\right)\cdot\omega^2\left(\omega^2 - \left(\frac{2k}{m} + \frac{k}{M}\right)\right) = 0$$

displacement (vectors).

$\omega^2=0$ $\qquad -\frac{k}{M}x_1+\frac{k}{M}x_2=0 \qquad x_1=x_2$

$$\frac{k}{M}x_2-\frac{k}{m}x_3=0 \qquad x_2=x_3$$

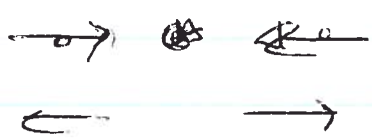
$$-\frac{k}{m}x_1+\frac{2k}{m}x_2-\frac{k}{m}x_3=0$$

springs unstretched | c.m. motion

$\omega^2=\frac{k}{M}$ $\qquad \cancel{-\frac{k}{m}x_1} = \cancel{-\frac{k}{m}x_1}+\frac{k}{m}x_2 \qquad x_2=0$

$$-\frac{k}{m}x_3 = \frac{k}{m}x_2 - \cancel{\frac{k}{m}x_3}$$

$$\cancel{-\frac{k}{M}x_2}=\frac{k}{M}x_1-\frac{2k}{m}x_2+\frac{k}{m}x_3 \qquad x_1+x_3=0$$



molecule at rest,

stretches, squeezes

$$\omega^2 = \frac{2k}{m} + \frac{k}{M}$$

$$\left(-\frac{2k}{m} - \cancel{\frac{k}{M}}\right)x_1 = -\cancel{\frac{k}{M}}x_1 + \frac{k}{M}x_2$$

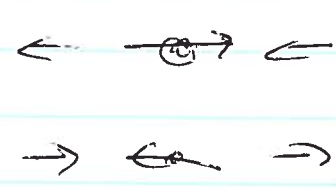
$$-\frac{2k}{m}x_1 = \frac{k}{M}x_2 \qquad \cancel{m x_1 = -\frac{1}{2}M}$$

$$\boxed{M x_1 = -\frac{1}{2} m x_2}$$

$$\left(-\frac{2k}{m} - \cancel{\frac{k}{M}}\right)x_3 = \frac{k}{M}x_2 - \cancel{\frac{k}{M}x_3}$$

$$M x_3 = -\frac{1}{2} m x_2$$

$$\left(\cancel{-\frac{2k}{m}} - \frac{k}{M}\right)x_2 = \frac{k}{M}x_1 \cancel{-\frac{2k}{m}x_2} + \frac{k}{m}x_3$$



c.m. fixed

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vectors $\begin{pmatrix}1\\1\\1\end{pmatrix}$ $\begin{pmatrix}-1\\0\\1\end{pmatrix}$ $\begin{pmatrix}+1\\-c\\+1\end{pmatrix}$

orthogonal (almost) (mass weighted).

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complex

$\boxed{Mv = \lambda v}$ $\quad M_{ij} v_j = \lambda v_i$

$(u, Mv) = (u_i)^* (M_{ij} v_j) = u^\dagger M v$

$(u, v) = u^\dagger v = (u^T)^* v$ $\quad (u, u) = u_i^* u_i \geq 0$

QM: $v \to |\psi\rangle$

$\langle\phi|\psi\rangle$ inner product. "Dirac Bracket"

$\langle\phi|M|\psi\rangle$ matrix element

$= \langle\psi|M|\phi\rangle^*$

$Mv_1 = \lambda_1 v_1$

$Mv_2 = \lambda_2 v_2$

$(v_2, Mv_1) = v_2^\dagger M v_1 = v_2^\dagger \lambda_1 v_1 = \lambda_1 (v_2^\dagger v_1)$

$v_1^\dagger M v_2 = v_1^\dagger \lambda_2 v_2 = \lambda_2 (v_1^\dagger v_2)$

Adjoint: $v_2^\dagger M^\dagger v_1 = \lambda_2^* v_2^\dagger v_1$

"Self-adjoint" $M^\dagger = M$ $\quad M_{ij}^* = M_{ji}$

$(M^T)^* = M$

$$v_2^\dagger M v_1 = \lambda_1 v_2^\dagger v_1 = \lambda_2^* v_2^\dagger v_1$$

$$\boxed{(\lambda_1 - \lambda_2^*)(v_2^\dagger v_1) = 0}$$

Two results: $v_1 = v_2$ $\quad v^\dagger v = \sum_i |v_i|^2 > 0.$

$\rightarrow \lambda = \lambda^*$ real eigenvalues

$\lambda_1 \neq \lambda_2$ $\quad v_2^\dagger v_1 = 0$

Eigenvectors orthogonal

$$Kx = \lambda Mx$$

$$x_2^\dagger K x_1 = \lambda_1 x_2^\dagger M x_1 \qquad x_1^\dagger K x_2 = \lambda_2 x_1^\dagger M x_2$$

$$x_2^\dagger K x_1 = \lambda_2^* x_2^\dagger M x_1$$

$K^\dagger = K$ $\qquad (\lambda_1 - \lambda_2^*)\, x_2^\dagger$

$M^\dagger = M$

weighted inner product.

$$\underline{\langle v_1, v_2\rangle} = v_1^{+} M \underline{v_2}$$

$$\left(\underline{Kx = \lambda \cancel{M} x} \right)$$

$Kx_1 = \lambda_1 \cancel{M} x_1$

$Kx_2 = \lambda_2 \cancel{M} x_2$

$$x_2^{+} M K x_1 = \lambda_1$$

$$x_2^{+} M K x_1 = \lambda_1 \, x_2^{+} M x_1$$

$$x_1^{+} M K x_2 = \lambda_2 \, x_1^{+} M x_2$$

$$x_2^{+} K^{+} M^{+} x_1 = \lambda_2^{+} \, x_2^{+} M^{+} x_1$$

diagonal, real positive

$M^{+} = M$.

$MK = K^{+} M^{+}$

$$(\lambda_1 - \lambda_2^{+}) \, x_2^{+} M x_1$$