RECAP V EQUILIBRIUM AT $\{(q_{i_0})\}$

$$q_i = q_{i_0} + \eta_i \quad \text{new coords}$$

$$T = \sum_{ij} \tfrac{1}{2} T_{ij} \dot{\eta}_i \dot{\eta}_j \qquad V_{ij} = \left.\frac{\partial^2 V}{\partial q_i \partial q_j}\right|_0$$

$$V = \tfrac{1}{2} V_{ij} \eta_i \eta_j \qquad \mathcal{L} = T - V$$

EOM: $T_{ij} \ddot{\eta}_j + V_{ij} \eta_j = 0$

$$\overleftrightarrow{T} \ddot{\vec{\eta}} + \overleftrightarrow{V} \vec{\eta} = 0$$

OSCILLATORY ANSATZ $\begin{cases} \eta_i = C a_i e^{-i\omega t} \\ \vec{\eta} = C \vec{a} e^{-i\omega t} \end{cases}$

EOM $-\omega^2 \overleftrightarrow{T} \vec{a} + \overleftrightarrow{V} \vec{a} = 0$

$$\lambda_k = \omega_k^2 \qquad (\overleftrightarrow{V} - \lambda_k \overleftrightarrow{T}) \vec{a}_k = 0$$

$$(\lambda_k - \lambda_l) \vec{a}_l^T \overleftrightarrow{T} \vec{a}_k = 0$$

if $k \neq l$, $\lambda_k \neq \lambda_l$ (NON DEGENERATE)

$$\vec{a}_l^T \overleftrightarrow{T} \vec{a}_k = 0 \quad l \neq k$$

NORMALIZATION $\vec{a}_k^T \overleftrightarrow{T} \vec{a}_k = 1$

$$(a_1 \cdots a_n)_k \begin{pmatrix} & & \\ & T & \\ & & \end{pmatrix} \begin{pmatrix} a_1 \\ \vdots \\ a_n \end{pmatrix}_k = 1 \qquad \overleftrightarrow{A}$$

$\overleftrightarrow{A}^T$

$$\begin{pmatrix} (a_1 \cdots a_n)_1 \\ (a_1 \cdots a_n)_2 \\ \vdots \\ (a_1 \cdots a_n)_n \end{pmatrix} \begin{pmatrix} & & \\ & T & \\ & & \end{pmatrix} \left(\begin{pmatrix} a_1 \\ \vdots \\ a_n \end{pmatrix}_1 \begin{pmatrix} a_1 \\ \vdots \\ a_n \end{pmatrix}_2 \cdots \begin{pmatrix} a_1 \\ \vdots \\ a_n \end{pmatrix}_n \right) = \overleftrightarrow{\mathbb{1}}$$

$$\overleftrightarrow{A}^T \overleftrightarrow{T} \overleftrightarrow{A} = \begin{pmatrix} \vec{a}_1^T \overleftrightarrow{T} \vec{a}_1 & \vec{a}_1^T \overleftrightarrow{T} \vec{a}_2 & \\ \vec{a}_2^T \overleftrightarrow{T} \vec{a}_1 & \vec{a}_2^T \overleftrightarrow{T} \vec{a}_2 & \\ \vdots & \vdots & \ddots \\ \vec{a}_n^T \overleftrightarrow{T} a_1 & & \vec{a}_n^T \overleftrightarrow{T} \vec{a}_n \end{pmatrix} = \underline{\overleftrightarrow{1}}$$

$$= \begin{pmatrix} 1 & & & O \\ & 1 & & \\ & & 1 & \\ O & & & \ddots \\ & & & & 1 \end{pmatrix}$$

$a_{jk} = j^{th}$ value of the k^{th} eigenvector

$$\overleftrightarrow{C}' = \overleftrightarrow{A}^T \overleftrightarrow{C} \overleftrightarrow{A}$$

IF $\overleftrightarrow{A}$ ORTHOGONAL $\overleftrightarrow{A}^T = \overleftrightarrow{A}^{-1}$

$$\overleftrightarrow{A}^T \overleftrightarrow{T} \overleftrightarrow{A} = \overleftrightarrow{1}$$

$\overleftrightarrow{A}$ TRANSFORMS $\overleftrightarrow{T}$ TO $\underline{\overleftrightarrow{1}}$

$$\lambda_{ik} \equiv \lambda_k \delta_{ij} \quad \text{(no sum)} \qquad \overleftrightarrow{\lambda} = \begin{pmatrix} \lambda_1 & & O \\ & \lambda_2 & \\ O & & \ddots \\ & & & \lambda_n \end{pmatrix}$$

$$\overleftrightarrow{V} \vec{a}_k = \lambda_k \overleftrightarrow{T} \vec{a}_k \quad \text{(no sum)}$$

$$\sum_j V_{ij} \underbrace{(a_j)_k}_{a_{jk}} = \sum_l T_{ij} a_{jl} \lambda_{lk}$$

$$\overleftrightarrow{V} \overleftrightarrow{A} = \overleftrightarrow{T} \overleftrightarrow{A} \overleftrightarrow{\lambda}$$

$$\overleftrightarrow{\mathbb{V}}\,\overleftrightarrow{A} = \overleftrightarrow{\mathbb{T}}\,\overleftrightarrow{A}\,\overleftrightarrow{\lambda}$$

MULTIPLY BY $\overleftrightarrow{A}^T$

$$\overleftrightarrow{A}^T\,\overleftrightarrow{\mathbb{V}}\,\overleftrightarrow{A} = \underbrace{\overleftrightarrow{A}^T\,\overleftrightarrow{\mathbb{T}}\,\overleftrightarrow{A}}_{\mathbb{1}}\,\overleftrightarrow{\lambda} = \overleftrightarrow{\lambda}$$

$$\overleftrightarrow{\mathbb{V}}_{diag} = \overleftrightarrow{\lambda}$$

EITHER USE

NORMALIZED CARTESIAN COORDS

$$T_{ij} = \delta_{ij} \quad \left(\overleftrightarrow{\mathbb{T}} = \overleftrightarrow{\mathbb{1}}\right)$$

SOLVE $\overleftrightarrow{A}^T\,\overleftrightarrow{A} = \overleftrightarrow{\mathbb{1}}$ $\quad \overleftrightarrow{A}^T\,\overleftrightarrow{\mathbb{V}}\,\overleftrightarrow{A} = \overleftrightarrow{\mathbb{V}}_{diag}$

OR GENERAL COORDS $\overleftrightarrow{\mathbb{T}} \neq \overleftrightarrow{\mathbb{1}}$

SOLVE $\overleftrightarrow{A}^T\,\overleftrightarrow{\mathbb{T}}\,\overleftrightarrow{A} = \overleftrightarrow{\mathbb{1}}$ $\quad \overleftrightarrow{A}^T\,\overleftrightarrow{\mathbb{V}}\,\overleftrightarrow{A} = \overleftrightarrow{\mathbb{V}}_{DIAG}$

GENERAL SOLUTION $\quad \eta_i = \sum_k C_k a_{ik} e^{-i\omega_k t}$

$\omega = \pm\sqrt{\lambda}$ IRRELEVANT SINCE WE TAKE THE REAL PART AND C_k IS COMPLEX

$$\eta_i(0) = \sum_k \mathrm{Re}\left(C_k a_{ik}\right) \Rightarrow \underline{\vec{\eta}(0) = \overleftrightarrow{A}\, \mathrm{Re}\, \vec{C}}$$

$$\dot{\eta}_i(0) = \sum_k \mathrm{Im}\left(C_k a_{ik} \omega_k\right) \qquad \vec{C} = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix}$$

MULTIPLY BY $\overleftrightarrow{A}^T \overleftrightarrow{T}$

$$\underbrace{\overleftrightarrow{A}^T \overleftrightarrow{T} \overleftrightarrow{A}}_{\mathbb{1}} \mathrm{Re}\, \vec{C} = \overleftrightarrow{A}^T \overleftrightarrow{T} \vec{\eta}(0)$$

$$\mathrm{Re}\, C_\ell = \sum_{jk} a_{j\ell} T_{jk} \eta_k(0)$$

$$\mathrm{Im}\, C_\ell = \frac{1}{\omega_\ell} \sum_{jk} a_{j\ell} T_{jk} \dot{\eta}_k(0)$$

$C \Rightarrow$ amplitude and phase of the different resonant modes

NOW TRANSFORM TO "NORMAL" COORDS

$$\eta_i = a_{ij} \xi_j \Leftrightarrow \vec{\eta} = \overleftrightarrow{A} \vec{\xi} \qquad \vec{\eta}^T = \vec{\xi}^T \overleftrightarrow{A}^T$$

$$V = \frac{1}{2} \vec{\eta}^T \overleftrightarrow{V} \vec{\eta} = \frac{1}{2} \vec{\xi}^T \underbrace{\overleftrightarrow{A}^T \overleftrightarrow{V} \overleftrightarrow{A}}_{\overleftrightarrow{\lambda}} \vec{\xi}$$

$$= \frac{1}{2} \vec{\xi}^T \overleftrightarrow{\lambda} \vec{\xi} = \frac{1}{2} \sum_k \omega_k^2 \xi_k^2$$

$$T = \frac{1}{2} \dot{\vec{\xi}}^T \underbrace{\overleftrightarrow{A}^T \overleftrightarrow{T} \overleftrightarrow{A}}_{\mathbb{1}} \dot{\vec{\xi}} = \frac{1}{2} \dot{\vec{\xi}}^T \dot{\vec{\xi}} = \frac{1}{2} \sum_i \dot{\xi}_i^2$$

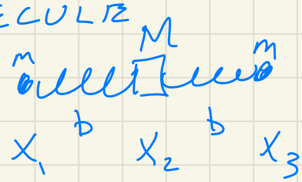
$$\mathcal{L} = T - V = \frac{1}{2}\sum_k \left(\dot{\xi}_k^2 - \omega_k^2 \xi_k^2\right)$$

EOM $\quad \ddot{\xi}_k + \omega_k^2 \xi_k = 0$

$$\Rightarrow \quad \xi_k = C_k e^{-i\omega_k t}$$

$$q_i = q_{i_0} + \eta_i \quad \Rightarrow \quad \eta_i \to \xi_i$$

LINEAR TRIATOMIC MOLECULE



$$V = \frac{k}{2}\left(x_2 - x_1 - b\right)^2 + \frac{k}{2}\left(x_3 - x_2 - b\right)^2$$

$$\eta_i = x_i - x_{0_i} \qquad x_{0_2} - x_{0_1} = b = x_{0_3} - x_{0_2}$$

$$V = \frac{k}{2}\left(\eta_2 - \eta_1\right)^2 + \frac{k}{2}\left(\eta_3 - \eta_2\right)^2$$

$$= \frac{k}{2}\left(\eta_1^2 + 2\eta_2^2 + \eta_3^2 - 2\eta_1\eta_2 - 2\eta_2\eta_3\right)$$

$$V_{ij} = \frac{\partial^2 V}{\partial\eta_i \partial\eta_j} \qquad \overleftrightarrow{V} = \begin{pmatrix} k & -k & 0 \\ -k & 2k & -k \\ 0 & -k & k \end{pmatrix}$$

$$T = \frac{1}{2} m\left(\dot{\eta}_1^2 + \dot{\eta}_3^2\right) + \frac{1}{2} M \dot{\eta}_2^2$$

$$\overleftrightarrow{T} = \begin{pmatrix} m & & 0 \\ & M & \\ 0 & & m \end{pmatrix} \qquad \overleftrightarrow{V} - \omega^2 \overleftrightarrow{T} \; ?$$

$$\left| \overleftrightarrow{\mathbb{V}} - w^2 \overleftrightarrow{\mathbb{T}} \right| = \begin{vmatrix} k-w^2 m & -k & 0 \\ -k & 2k-w^2 M & -k \\ 0 & -k & k-w^2 m \end{vmatrix} = 0$$

skipping algebra

$$\Rightarrow w^2 (k - w^2 m)\left(k(M+2m) - w^2 M m\right) = 0$$

$$w_1 = 0 \qquad w_2 = \sqrt{\frac{k}{m}} \qquad w_3 = \left[\frac{k}{m}\left(1 + \frac{2m}{M}\right)\right]^{1/2}$$

$$\Rightarrow \ddot{\xi}_1 = 0$$ MOTION OF CM

WE ASSUMED 3 FREQ. OF OSCILLATION
BUT THERE ARE ONLY ~~E~~ 2

CAN TRANSFORM TO FRAME WHERE

$$\dot{\vec{R}} = 0 \qquad \left(\sum m_i\right) \vec{R} = m(\vec{r}_1 + \vec{r}_3) + M \vec{r}_2 = 0$$

$$\left(\overleftrightarrow{\mathbb{V}} - w_i^2 \overleftrightarrow{\mathbb{T}}\right) \vec{a}_i = 0$$

$$\begin{pmatrix} k - w_i^2 m & -k & 0 \\ -k & 2k - w_i^2 M & -k \\ 0 & -k & k - w_i^2 m \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}_i = 0$$

$$(k - w_j^2 m) a_{1_j} - k a_{2_j} = 0$$

$$-k a_{1_j} + (2k - w_j^2 M) a_{2_j} - k a_{3_j} = 0$$

$$-k a_{2_j} + (k - w_j^2 m) a_{3_j} = 0$$

$$\overleftrightarrow{A}^{T} \overleftrightarrow{\mathbb{T}} \overleftrightarrow{A} = \overleftrightarrow{\mathbb{1}} \qquad \vec{a}^{T} \overleftrightarrow{\mathbb{T}} \vec{a} = 1$$

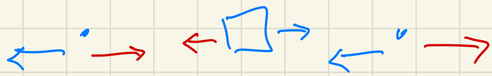
NORMALIZATION $\quad m(a_{1_j}^2 + a_{3_j}^2) + M a_{2_j}^2 = 1$

$$w_1 = 0 \Rightarrow a_{11} = a_{21} = a_{31} = \frac{1}{\sqrt{2m+M}}$$

$$\omega_2 = k/m \qquad k - \omega_2^2 m = 0 \Rightarrow a_{22} = 0$$

$$a_{12} = -a_{32} = \frac{1}{\sqrt{2m}}$$

$$\omega_3 = \left[\frac{k}{m}\left(1 + \frac{2m}{M}\right)\right]^{1/2} \Rightarrow a_{13} = a_{33} = \frac{-k}{k - \omega_3^2 m} a_{23}$$



$$\begin{cases} \xi_1 = \dfrac{1}{\sqrt{2m+M}}\left(m\eta_1 + M\eta_2 + m\eta_3\right) & \text{CM MOTION} \\ \xi_2 = \sqrt{\dfrac{m}{2}}\left(\eta_1 - \eta_3\right) \\ \xi_3 = \sqrt{\dfrac{\mu}{2}}\left(\eta_1 + \eta_3 - 2\eta_2\right) \end{cases}$$

NORMAL MODES

3D 9 DEGREES OF FREEDOM

3 TRANSLATIONAL MODE

3 ROTATIONAL MODES

$\Rightarrow$ 3 VIBRATIONAL MODES

LINEAR MOLECULE

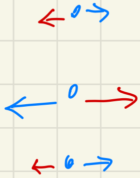
3 TRANS

2 ROTATIONAL

$\Rightarrow$ 4 VIBRATIONAL

WE KNOW 2 OF THEM

TWO TRANSVERSE ~~MO~~ VIBRATIONAL MODES MUST BE DEGENERATE



COMBINE TWO LINEAR MOTIONS

TO GET

a) LINEAR MOTION

OR

b) ELLIPTICAL MOTION

DEPENDING ON RELATIVE PHASE