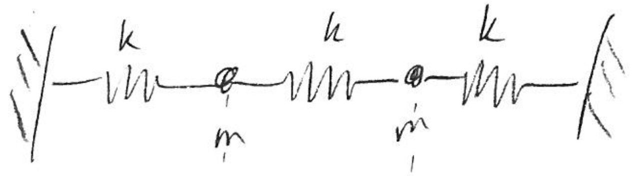
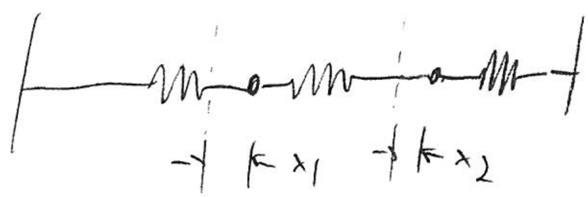
Oscillations   example first, then general case



: equilibrium



: stretched (1-d motion only)

$$L = \frac{m}{2}\left(\dot{x}_1^2 + \dot{x}_2^2\right) - \frac{1}{2} k \left[\underbrace{(x_1 - x_2)^2 + x_1^2 + x_2^2}_{2\left(x_1^2 + x_2^2 - x_1 x_2\right)} \right]$$

$$\left.\begin{aligned} m\ddot{x}_1 &= -2k x_1 + k x_2 \\ m\ddot{x}_2 &= -2k x_2 + k x_1 \end{aligned}\right\} + \text{initial conditions for } x_i \;\&\; \dot{x}_i \quad i=1,2$$

As in the single SHO, look for $x_i = a_i e^{-i\omega t}$

$$-m\omega^2 a_1 = -2k a_1 + k a_2$$
$$-m\omega^2 a_2 = -2k a_2 + k a_1$$

: homogeneous eq for $a_{1,2}$; soln iff

$$\det \begin{pmatrix} m\omega^2 - 2k & k \\ k & m\omega^2 - 2k \end{pmatrix} = (m\omega^2 - 2k)^2 - k^2 = 0$$

or $\omega^2 - 2\omega_0^2 = \pm \omega_0^2$, $\omega_0^2 \equiv \frac{k}{m}$

$\rightarrow \omega^2 = \omega_0^2$ or $3\omega_0^2$

$\omega^2 = \omega_0^2$. $\quad -m\cdot\frac{k}{m} a_1 = -2k_1 a_1 + k a_2 \to a_1 = a_2$

$\omega^2 = 3\omega_0^2 \quad -m\cdot\frac{3k}{m} a_1 = -2k_1 a_1 + k a_2 \to a_1 = -a_2$.

un compressed
usual stiffness

all compressed/expanded
- stiffer

In the space $\underline{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$, $\omega = \omega_0 \to \hat{a}_1(t) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} e^{-i\omega_0 t}$

$\omega = \sqrt{3}\omega_0 \to \hat{a}_2(t) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} e^{-\sqrt{3} i\omega_0 t}$

general solution $\underline{x}(t) = c_1 \hat{a}_1(t) + c_2 \hat{a}_2(t)$.

$$= \begin{pmatrix} \frac{1}{\sqrt{2}}\left(c_1 e^{-i\omega_0 t} + c_2 e^{-i\sqrt{3}\omega_0 t}\right) \\ \frac{1}{\sqrt{2}}\left(\quad '' \quad - \quad '' \quad \right) \end{pmatrix}$$

for IC write $\underline{x}(0) = \frac{1}{\sqrt{2}}\begin{pmatrix} c_1 + c_2 \\ c_1 - c_2 \end{pmatrix}$

$$\dot{\underline{x}}(0) = \frac{-i\omega_0}{\sqrt{2}}\begin{pmatrix} c_1 + \sqrt{3}c_2 \\ c_1 - \sqrt{3}c_2 \end{pmatrix}$$

This is complex notation: really $\underline{x}(t) = \mathrm{Re}\,\frac{1}{\sqrt{2}}(\cdots)$

$\dot{x} = \mathrm{Im}\,\frac{-\omega_0}{\sqrt{2}}(\cdots)$

The $\hat{a}_i(t)$ are "normal modes" of frequency ω_i

→ purely harmonic motion of entire system

General motion = superposition of normal modes.

Advantage:

Let $x_i = \sum_j a_{ij} y_j \qquad \underline{y} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$ = new coord. vector

$$(a_{ij}) = \underline{\underline{A}} = \begin{pmatrix} \hat{a}_1 & \hat{a}_2 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$L = \frac{1}{2} \underline{\dot{x}}^T \begin{pmatrix} m & 0 \\ 0 & m \end{pmatrix} \underline{\dot{x}} - \frac{1}{2} \underline{x}^T \begin{pmatrix} 2k & -k \\ -k & 2k \end{pmatrix} \underline{x}$$

$$= \frac{1}{2} \underline{\dot{x}}^T \underline{\underline{T}}\, \underline{\dot{x}} - \frac{1}{2} \underline{x}^T \cdot \underline{\underline{U}} \cdot \underline{x}$$

$$= \frac{1}{2} \underline{\dot{y}}^T \cdot \underbrace{\left(\underline{\underline{A}}^T \underline{\underline{T}}\, \underline{\underline{A}} \right)}_{= \begin{pmatrix} m & 0 \\ 0 & m \end{pmatrix}} \cdot \underline{\dot{y}} - \frac{1}{2} \underline{y}^T \cdot \underbrace{\left(\underline{\underline{A}}^T \underline{\underline{U}}\, \underline{\underline{A}} \right)}_{= \begin{pmatrix} k & 0 \\ 0 & 3k \end{pmatrix}} \cdot \underline{y}$$

$$= \left(\frac{1}{2} m_1 \dot{y}_1^2 - \frac{1}{2} k y_1^2 \right) + \left(\frac{1}{2} m \dot{y}_2^2 - \frac{3}{2} k y_2^2 \right)$$

→ the problem is diagonalized in terms of the normal modes.

Small oscillations in general:

$$T = \sum_\alpha \tfrac{1}{2} m_\alpha \dot{\underline{r}}_\alpha^2 \xrightarrow[\underline{r}_\alpha = \underline{r}_\alpha(q_1 \cdots q_n)]{} \sum_{ij} \tfrac{1}{2} m_{ij}\, \dot q_i \dot q_j$$

where $m_{ij}(q) = \sum_\alpha m_\alpha \frac{\partial \underline{r}_\alpha}{\partial q_i} \cdot \frac{\partial \underline{r}_\alpha}{\partial q_j}$

by having $\underline{r}_\alpha = \underline{r}_\alpha(q, \cancel{t})$, assume no time-dependent constraints

If $U = U(\{\underline{r}_\alpha\}) \to U(q)$ only then

Lagrange eq are

$$\frac{d}{dt} \sum_j m_{ij}(q)\, \dot q_j = -\frac{\partial U}{\partial q_i}$$

Assume $\exists$ unstretched equilibrium state where

and $q_i = q_i^0 =$ constant, $\left.\frac{\partial U}{\partial q_i}\right|_{q^0} = 0$

Expand about equil $\quad q_i = q_i^0 + x_i$

$$U(q) = U(q^0) + \sum_i x_i \underbrace{\left.\frac{\partial U}{\partial q_i}\right|_0}_{0} + \frac{1}{2}\sum_{ij} x_i x_j \left(\left.\frac{\partial^2 U}{\partial q_i \partial q_j}\right|_0\right) + \cdots$$

with $|x_i|$ small enough to drop $\partial^3 U$ etc terms

$$T(\underline{q}, \dot{\underline{q}}) = \frac{1}{2} \sum_{ij} m_{ij} (\underline{q}^0 + \underline{x})(\dot{x}_i \dot{x}_j + \cdots)$$

$$\simeq \frac{1}{2} \sum_{ij} T_{ij} \dot{x}_i \dot{x}_j \quad ; \quad T_{ij} = m_{ij}(\underline{q}^0)$$

$$L = \sum_{ij} \frac{1}{2} \left(T_{ij} \dot{x}_i \dot{x}_j - U_{ij} x_i x_j \right)$$

$$\rightarrow \quad \sum_j T_{ij} \ddot{x}_j + U_{ij} x_j = 0$$

For normal modes look for $x_j(t) = a_j e^{-i\omega t}$

$$\rightarrow \quad \sum_j \left(U_{ij} - \omega^2 T_{ij} \right) a_j = 0 \quad \forall i.$$

or $\left(\underline{\underline{U}} - \omega^2 \underline{\underline{T}} \right) \cdot \underline{a} = 0$

More complicated eigenvalue problem because $\underline{\underline{T}} \neq \underline{\underline{1}}$ in general, but will show $\exists$ a complete set of real eigenvectors with non-negative real eigenvalues (for ω^2).

Notice T + U are real + symmetric → hermitian

so if $\underline{\underline{U}} \cdot \underline{a} = \lambda \underline{\underline{T}} \cdot \underline{a}$ $\quad \lambda = \omega^2$

then $\underline{a}^\dagger \cdot \underline{\underline{U}} \cdot \underline{a} = \lambda \underline{a}^\dagger \cdot \underline{\underline{T}} \cdot \underline{a}$

$$= (\underline{\underline{U}} \cdot \underline{a})^\dagger \cdot \underline{a} = (\lambda \underline{\underline{T}} \cdot \underline{a})^\dagger \underline{a} = \lambda^* \underline{a}^\dagger \underline{\underline{T}} \underline{a}$$

so $\lambda = \lambda^*$ + then $\underline{\underline{U}} \cdot \underline{a}^* = \lambda \underline{\underline{T}} \cdot \underline{a}^*$

→ $\frac{1}{2}(\underline{a} + \underline{a}^*) = \mathrm{Re}\, \underline{a}$ is an eigenvector

Also $\lambda = \dfrac{\underline{a}^T \cdot \underline{\underline{U}} \cdot \underline{a}}{\underline{a}^T \cdot \underline{\underline{T}} \cdot \underline{a}}$ = pos. or zero

because denom = KE > 0

numerator = energy cost for an osc = pos or zero

(if negative, system would be unstable)

If λ + λ' are distinct eigenvalues then

$\underline{a}'^T \underline{\underline{U}} \cdot \underline{a} = \underline{a}'^T (\lambda \underline{\underline{T}}) \underline{a} = \lambda \underline{a}'^T \cdot \underline{\underline{T}} \cdot \underline{a}$

↳ $(\underline{\underline{U}} \underline{a}')^T \cdot \underline{a} = (\lambda' \underline{\underline{T}} \underline{a}')^T \cdot \underline{a} = \lambda' \underline{a}'^T \underline{\underline{T}} \underline{a}$

→ $\underline{a}' \underline{\underline{T}} \cdot \underline{a} = 0$ ~ orthogonality w weight fn

So if the char eq. $\det(\underline{\underline{U}} - \lambda \underline{\underline{T}}) = 0$ has

n distinct roots, there are n "orthogonal" eigenvectors,

If λ = double root, $\exists$ 2 corresp. eigenvectors $\underline{a}_1, \underline{a}_2$,

& can use Gram-Schmidt to make them "orthogonal"

$$\rightarrow \quad \hat{a}_1 = \frac{1}{N_1} \underline{a}_1 \qquad \text{where } N_1^2 = \underline{a}_1^T \underline{\underline{T}} \cdot \underline{a}$$

$$\hat{a}_2 = \frac{1}{N_2} \left[\underline{a}_2 - \hat{\underline{a}}_1 \left(\hat{\underline{a}}_1^T \circ \underline{\underline{T}} \cdot \underline{a}_2 \right) \right] \rightarrow \hat{\underline{a}}_1 \underline{\underline{T}} \underline{a}_2 = 0$$

So, cleaning up the notation, have n "unit" eigenvectors

$$\hat{a}_1 \cdots \hat{a}_n \quad \text{with e-v } \lambda_1 \cdots \lambda_n \ni \hat{a}_i^T \underline{\underline{T}} \hat{a}_j = \delta_{ij}$$

$$\text{which also} \Rightarrow \quad \hat{\underline{a}}_i^T \cdot \underline{\underline{U}} \cdot \hat{a}_j = \lambda_i \delta_{ij}$$

Let $\underline{A} = \left(\hat{a}_1 \cdots \hat{a}_n \right)$ — or $A_{ij} = (\hat{a}_j)_i$

$$\text{so} \quad \underline{\underline{A}}^T \cdot \underline{\underline{T}} \cdot \underline{\underline{A}} = \begin{pmatrix} \hat{a}_1^T \\ \vdots \\ \hat{a}_n^T \end{pmatrix} \cdot \underline{\underline{T}} \cdot \left(\hat{a}_1 \cdots \hat{a}_n \right) = \underline{\underline{1}}$$

$$\underline{\underline{A}}^T \cdot \underline{\underline{U}} \cdot \underline{\underline{A}} = \begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{pmatrix} \equiv \underline{\underline{\Lambda}}.$$

ie, $\underline{\underline{A}}$ simultaneously diagonalizes $\underline{\underline{T}}$ & $\underline{\underline{U}}$.

General solution is then

$$\underline{x}(t) = \mathrm{Re} \sum_k c_k \hat{a}_k e^{-i\omega_k t}$$

$$\Leftrightarrow \quad x_i(t) = \mathrm{Re} \sum_k c_k \underbrace{(\hat{a}_k)_i}_{= A_{ik}} e^{-i\omega_k t}$$

$$= \mathrm{Re}\, \underline{\underline{A}} \cdot \underline{c}(t), \qquad \underline{c}(t) \equiv \begin{pmatrix} c_1 e^{-i\omega_1 t} \\ \vdots \\ c_n e^{-i\omega_n t} \end{pmatrix}$$

$$\rightarrow \underline{x}(0) = \mathrm{Re} \left(\underline{\underline{A}} \cdot \underline{c}(0) \right)$$

$$\dot{\underline{x}}(0) = -\mathrm{Im} \left(\underline{\underline{A}} \cdot \underline{\underline{\Lambda}}^{1/2} \cdot \underline{c}(0) \right)$$

but $\underline{\underline{A}}$ real so $\rightarrow$ $\mathrm{Re}\, \underline{c}(0) = \underline{\underline{A}}^{-1} \cdot \underline{x}(0)$

$$\mathrm{Im}\, \underline{c}(0) = -\underline{\underline{\Lambda}}^{-1/2} \underline{\underline{A}}^{-1} \dot{\underline{x}}(0)$$

Normal modes: let $\underline{x} = \underline{\underline{A}} \cdot \underline{y}$

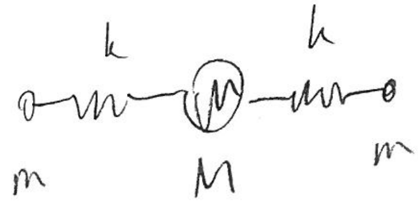
$$L = \frac{1}{2} \dot{\underline{x}}^T \cdot \underline{\underline{T}} \cdot \dot{\underline{x}} - \frac{1}{2} \underline{x}^T \cdot \underline{\underline{U}} \cdot \underline{x}$$

$$= \frac{1}{2} \dot{\underline{y}}^T \underbrace{(A^T T A)}_{\underline{\underline{1}}} \dot{\underline{y}} - \frac{1}{2} \underline{y}^T \underbrace{(A^T U A)}_{\underline{\underline{\Lambda}}} \cdot \underline{y}$$

$$= \frac{1}{2} \sum_i \dot{y}_i^2 - \omega_i^2 y_i^2$$

$$\rightarrow \ddot{y}_i = -\omega_i^2 y_i \quad \ldots$$

Example - molecular vibrations



$l \equiv$ unstretched length

x_i = separations

$$L = \frac{m}{2}\left(\dot{x}_1^2 + \dot{x}_3^2\right) + \frac{M}{2}\dot{x}_2^2$$
$$- \frac{k}{2}\left(x_2 - x_1\right)^2 - \frac{k}{2}\left(x_3 - x_2\right)^2$$

so $$\underline{\underline{T}} = \begin{pmatrix} m & & 0 \\ & M & \\ 0 & & m \end{pmatrix} \qquad \underline{\underline{U}} = \begin{pmatrix} k & -k & 0 \\ -k & 2k & -k \\ 0 & -k & k \end{pmatrix}$$

$$\det\left|\underline{\underline{U}} - \omega^2 \underline{\underline{T}}\right| = \det\begin{pmatrix} k-\omega^2 m & -k & 0 \\ -k & 2k-\omega^2 M & -k \\ 0 & -k & k-\omega^2 m \end{pmatrix}$$

$$= \left(k-\omega^2 m\right)\left[\left(2k-\omega^2 M\right)\left(k-\omega^2 m\right) - k^2\right]$$
$$+ k\left[-k\left(k-\omega^2 m\right)\right]$$
$$= \omega^2\left(k-\omega^2 m\right)\left(\omega^2 M m - k\left(M+2m\right)\right)$$
$$= 0 \rightarrow \omega_1^2 = 0, \quad \omega_2^2 = \frac{k}{m}, \quad \omega_3^2 = k\,\frac{M+2m}{Mm}$$

Mode 1 $\omega_1^2 = 0$ eigenvectors satisfy

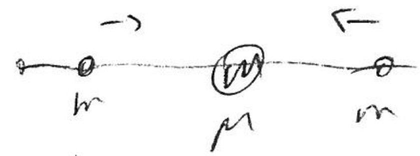
$$k\begin{pmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = 0$$

$$\left.\begin{aligned} \to\ x_1 &= x_2 \\ x_2 &= x_3 \\ -x_1 + 2x_2 - x_3 &= 0 \end{aligned}\right\}\quad x_1 = x_2 = x_3$$

This is just uniform translation of whole molecule,
obviously costs no energy
always an eigenmode ($x_i \to x_i + v_0 t$ a symmetry)
avoid by working with relative coordinates alone.

Mode 2: Simple harmonic osc. mode

$$\to\ \pm\alpha\,(1, 0, -1)$$



Mode 3: Interesting case:

$$\to\ \pm\alpha\left(\sqrt{\frac{M}{m}},\ -2\sqrt{\frac{m}{M}},\ \sqrt{\frac{M}{m}}\right)$$

Details of normalization - exercise/book