Normal Modes

1) What is a normal mode: periodic vs. quasiperiodic motion
2) Small oscillation limit: oscill. near <u>stable</u> equilibrium.
3) Construct Lagrangian $\mathcal{L}(\vec{q},\dot{\vec{q}}) = T - V$

$\uparrow$ generalized coordinates (position, angle, ...)

Pick $\vec{q}=0$ at equilibrium ($\dot{\vec{q}}$ has to be 0)

Kinetic Energy:

$$T = \sum_{i,j} \frac{1}{2} M_{ij}\dot{q}_i\dot{q}_j + \text{h.o.t} = \frac{1}{2}\dot{\vec{q}}^{\,t} M \dot{\vec{q}} + \text{h.o.t.}$$

Potential Energy:

$$V = V(\vec{q}) = V_0 + \sum_i \underbrace{\frac{\partial V}{\partial q_i}}_{=0 \text{ (equilibrium)}} q_i + \frac{1}{2}\sum_{i,j}\frac{\partial^2 V}{\partial q_i \partial q_j} q_i q_j + \text{h.o.t}$$

$$= V_0 + \sum_{i,j}\frac{1}{2}U_{ij}q_iq_j + \text{h.o.t.} = V_0 + \frac{1}{2}\vec{q}^{\,t} U \vec{q} + \text{h.o.t.}$$

Note: We are free to split cross-terms, so that both M and U are symmetric

Lagrange's equations:

$$0 = \frac{\delta \mathcal{L}}{\delta q} = -\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}_i} + \frac{\partial \mathcal{L}}{\partial q_i} = -\frac{d}{dt}\sum_j\left(\frac{1}{2}M_{ij}\dot{q}_j + \frac{1}{2}\dot{q}_j M_{ji}\right) - \sum_j\left(\frac{1}{2}U_{ij}q_j + \frac{1}{2}q_j U_{ji}\right) =$$

$$= -\sum_j\left(M_{ij}\ddot{q}_j + U_{ij}q_j\right)$$

$$\Rightarrow \boxed{M\ddot{\vec{q}} + U\vec{q} = 0}$$

Seek special solutions: $q_j = \mathrm{Re}\{a_j e^{i\omega t}\} \rightarrow \ddot{q}_j = -\omega^2 q_j$

$$\Rightarrow -\omega^2 M\vec{q} + U\vec{q} = \boxed{(U - \omega^2 M)\vec{q} = 0}$$

almost eigenvalue problem!

Can convert into actual EV problem:

$$M\vec{q} \equiv \vec{Q} \quad \Rightarrow \quad \left(MUM^{-1} - \omega^2 \mathbb{1}\right) M\vec{q} = \left(U' - \omega^2 \mathbb{1}\right)\vec{Q} = 0$$

$(U - \omega^2 M)\vec{q} = 0$ ← system (homogeneous) of algebraic eq's.

has nontrivial solutions when $\boxed{\det(U - \omega^2 M) = 0}$

equation for normal frequencies

For each ω_i find normal mode $\vec{q}_i$: $\vec{q} = \sum_i \alpha_i \vec{q}_i$

Example (CO_2 – molecule)

Coordinates: $\vec{q} = (x_1, x_2, x_3, y_1, y_2, y_3, z_1, z_2, z_3)$

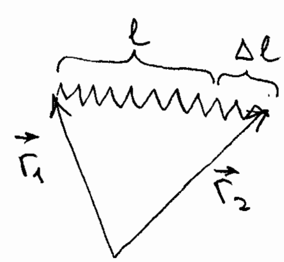
K.E.:

$$T = \frac{m}{2}\dot{\vec{r}}_1^{\,2} + \frac{M}{2}\dot{\vec{r}}_2^{\,2} + \frac{m}{2}\dot{\vec{r}}_3^{\,2}$$

$$= \frac{m}{2}(\dot{x}_1^2 + \dot{y}_1^2 + \dot{z}_1^2) + \frac{M}{2}(\dot{x}_2^2 + \dot{y}_2^2 + \dot{z}_2^2) + \frac{m}{2}(\dot{x}_3^2 + \dot{y}_3^2 + \dot{z}_3^2)$$

P.E.:

$$V = \frac{k}{2}(\Delta l_{12})^2 + \frac{k}{2}(\Delta l_{23})^2$$



$$\Delta l_{12} = |\vec{r}_1 - \vec{r}_2| - l$$

$$\vec{r}_1 = \begin{pmatrix} -l + x_1 \\ y_1 \\ z_1 \end{pmatrix}, \quad \vec{r}_2 = \begin{pmatrix} x_2 \\ y_2 \\ z_2 \end{pmatrix}$$

$$|\vec{r}_1 - \vec{r}_2| = \sqrt{(-l + x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2} =$$

$$= \sqrt{l^2 - 2l(x_1 - x_2) + (x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2} =$$

$$= l\left(1 - 2\frac{x_1 - x_2}{l} + O(l^{-2})\right)^{\frac{1}{2}} = l - (x_1 - x_2) + O(l^{-1})$$

$$\Rightarrow \Delta l_{12} = -(x_1 - x_2) + O(l^{-1})$$

$$V = \frac{k}{2}(x_1 - x_2)^2 + \frac{k}{2}(x_2 - x_3)^2 =$$
$$= \frac{1}{2}\left(kx_1^2 - 2kx_1x_2 + kx_2^2 + kx_2^2 - 2kx_2x_3 + kx_3^2\right)$$

$$M = \left(\begin{array}{ccc|ccc|ccc} m & & 0 & & & & & & \\ & M & & & 0 & & & 0 & \\ 0 & & m & & & & & & \\ \hline & & & m & & & & & \\ & 0 & & & M & & & 0 & \\ & & & & & m & & & \\ \hline & & & & & & m & & 0 \\ & 0 & & & 0 & & & M & \\ & & & & & & 0 & & m \end{array}\right) \qquad \mathcal{V} = \left(\begin{array}{ccc|ccc|ccc} k & -k & 0 & & & & & & \\ -k & 2k & -k & & 0 & & & 0 & \\ 0 & -k & k & & & & & & \\ \hline & & & & & & & & \\ & 0 & & & 0 & & & 0 & \\ & & & & & & & & \\ \hline & & & & & & & & \\ & 0 & & & 0 & & & 0 & \\ & & & & & & & & \end{array}\right)$$

Normal frequencies:

$$\det(\mathcal{V} - \omega^2 M) = \left[\left((k-\omega^2 m)(2k - \omega^2 M) - k^2\right)(k - \omega^2 m) + (k - \omega^2 m)(-k^2)\right] \times$$
$$\times \underbrace{(0 - \omega^2 m)^4 (0 - \omega^2 M)^2}_{\omega^2 = 0,\ 6\text{ times}} = 0.$$

$\leftarrow$ y, z - directions

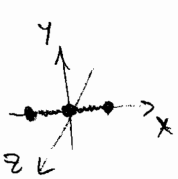
$$\left((k-\omega^2 m)(2k - \omega^2 M) - k^2 - k^2\right)(k - \omega^2 m) =$$
$$= \left(2k^2 - k^2 - k^2 - k(2m+M)\omega^2 + mM\omega^4\right)(k - \omega^2 m) =$$
$$= \omega^2\left(\omega^2 mM - k(2m+M)\right)(k - \omega^2 m) = 0$$
$$\Downarrow$$
$$\omega^2 = 0, \quad \omega^2 = \frac{k}{m}, \quad \omega^2 = k\frac{2m+M}{mM} \quad \leftarrow \text{x-direction}$$

Normal modes:

"0"s: $\vec{e}_y^{\,(1,2,3)}$, $\vec{e}_z^{\,(1,2,3)}$, $\vec{e}_x^{\,1} + \vec{e}_x^{\,2} + \vec{e}_x^{\,3}$ ← check! (total of 7)

$\vec{q} = \vec{e}_y^{\,1} + \vec{e}_y^{\,2} + \vec{e}_y^{\,3}$: $y_1 = y_2 = y_3$ — uniform translation along y-axis

same for x, z-axis



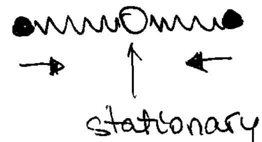
$\vec{q} = \vec{e}_y^{\,1} - \vec{e}_y^{\,3}$: $y_1 = -y_3,\ y_2 = 0$ — rigid body rotation about z-axis

same for y-axis

that's 3+2 = 5. What are the other 2 "0" modes?

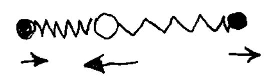
$$\omega^2 = \frac{k}{m}: \quad \begin{pmatrix} k & -k & 0 \\ -k & 2k & -k \\ 0 & -k & k \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = k \begin{pmatrix} x_1 - x_2 \\ -x_1 + 2x_2 - x_3 \\ x_3 - x_2 \end{pmatrix} = \frac{k}{m} \begin{pmatrix} m x_1 \\ M x_2 \\ m x_3 \end{pmatrix}$$

$$\Rightarrow x_2 = 0, \; x_1 = -x_3$$



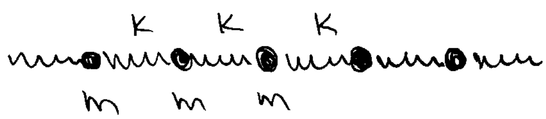
$$\omega^2 = k \frac{2m+M}{mM}: \quad k \begin{pmatrix} x_1 - x_2 \\ -x_1 + 2x_2 - x_3 \\ x_3 - x_2 \end{pmatrix} = k \frac{2m+M}{mM} \begin{pmatrix} m x_1 \\ M x_2 \\ m x_3 \end{pmatrix}$$

$$\Rightarrow x_1 = +x_3, \; x_2 = -2\frac{m}{M} x_1$$



Center of mass stationary in both cases!

Example: (Elastic medium – another comps. exercise)



K.E.: $T = \sum_i \frac{1}{2} m \dot{x}_i^2$

P.E.: $V = \sum_i \frac{1}{2} k (x_i - x_{i-1})^2$

$$M = \begin{pmatrix} \ddots & & & \\ & m & & 0 \\ & & m & \\ 0 & & & m \; \ddots \end{pmatrix}, \qquad U = \underbrace{\begin{pmatrix} \ddots & \ddots & & & 0 \\ \ddots & 2k & -k & & \\ & -k & 2k & -k & \\ & & -k & 2k & \ddots \\ 0 & & & \ddots & \ddots \end{pmatrix}}_{N=\infty} \Big\} N = \infty$$

Can diagonalize by choosing:

$$x_j = \mathrm{Re}\left\{ a e^{iqj + i\omega t} \right\}$$

translational symmetry in space (discrete)

translational symmetry in time (continuous)

$$-\pi < q < \pi$$

Lagrange's eq's:

$$\frac{\delta \mathcal{L}}{\delta q_\ell} = -\sum_j \left(M_{\ell j} \ddot{x}_j + U_{\ell j} x_j \right) =$$

$$= -\sum_j m \delta_{\ell j} a\, e^{iqj + i\omega t} (-\omega^2)$$

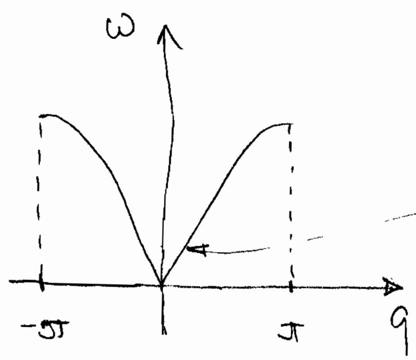
$$- \sum_j k \delta_{\ell j} a \left(-e^{iq(j-1)+i\omega t} + 2 e^{iqj + i\omega t} - e^{iq(j+1)+i\omega t} \right)$$

$$= - ma(-\omega^2) e^{iq\ell + i\omega t} - ka \underbrace{\left(-e^{-iq} + 2 - e^{iq}\right)}_{2(1-\cos q) = 4\sin^2(q/2)} e^{iq\ell + i\omega t}$$

$$\Rightarrow \quad m\omega^2(q) = k \cdot 4 \sin^2(q/2)$$

$$\Rightarrow \quad \omega^2(q) = 4 \sin^2(q/2) \cdot \frac{k}{m}$$

Dispersion relation: normal frequency vs. wavenumber of normal mode

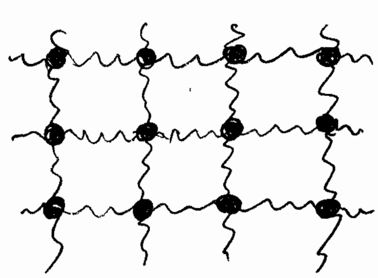


linear for small q: $\omega \approx \sqrt{\frac{k}{m}}\, q$

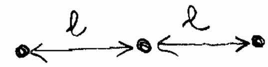
Solution:

$$x_j = \mathrm{Re} \left\{ \int_{-\pi}^{\pi} a(q) \exp\left[iqj + i\, 2\sqrt{k/m}\, \left|\sin(q/2)\right| t \right] dq \right\}$$

Can easily generalize for 2-d, 3-d



Continuum limit



$j \to y/\ell$

$q \to \ell q'$

$\frac{m}{\ell} = \rho$ - density , $\kappa\ell = T$ - elastic modulus

$$X(y) = \lim_{\ell \to 0} \mathrm{Re}\left\{ \int_{-\pi/\ell}^{\pi/\ell} a(q'\ell) \exp\left[iq'y + 2i \frac{\sqrt{T/\rho}}{\ell} \left|\sin(q'\ell/2)\right| t \right] dq' \cdot \ell \right\}$$

$$= \mathrm{Re}\left\{ \int_{-\infty}^{\infty} A(q') \exp\left[iq'y + i\sqrt{T/\rho}\,|q'|\,t \right] dq' \right\}$$

Dispersion relation: