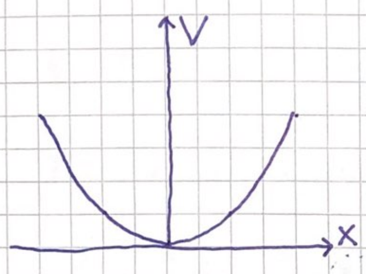
6. Oscillations

Applications:
Vibrations in molecules, solids and mechanical systems
Oscillations in coupled electrical circuits
Acoustics

Brief review of 1D harmonic oscillator:



$V(x) = \frac{1}{2} k x^2$

Curvature $k = \partial^2 V / \partial x^2$

N2: $F = m\ddot{x}$ with $F = -\partial V/\partial x = -kx$

$\Rightarrow m\ddot{x} + kx = 0 \quad \Rightarrow x(t) = \mathrm{Re}\{A e^{-i\omega_0 t}\}$; $\omega_0 = \sqrt{k/m}$

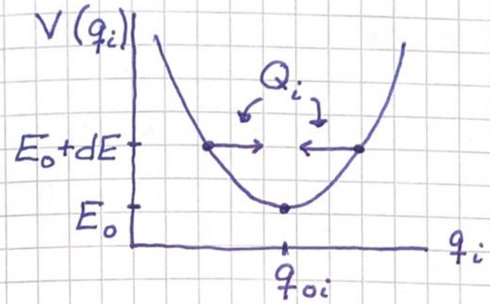
We will generalize the simple harm. osc. to a system of coupled harm. osc. Assume a conservative system with $n = 3N - k$ degrees of freedom (i.e. N particles and k holonomic constraints), where we have transformed from $\vec{r}_j$ ($j = 1,..,N$) to generalized independent coords. q_i ($i = 1,..,n$).

Equilibrium when all generalized forces are zero,

$$Q_i = -(\partial V/\partial q_i)_0 = 0$$

Equilibrium configuration: q_{0i} ($i = 1,..,n$)

Stable equilibrium :



Small disturbance from equilibrium $\Rightarrow$ Small oscillation around equilibrium

$$q_i(t) = q_{0i} + \eta_i(t)$$

η_i = deviation from eq. = new generalized coords.

Taylor expansion of V around eq. : [Sum conv.!]

$$V(\{q_i\}) = V(\{q_{0i}\}) + \left(\frac{\partial V}{\partial q_i}\right)_0 \eta_i + \frac{1}{2}\left(\frac{\partial^2 V}{\partial q_i \partial q_j}\right)_0 \eta_i \eta_j + \dots$$

Eq. condition: $(\partial V/\partial q_i)_0 = 0$

Free choice of $V=0$, e.g., $V(\{q_{0i}\}) = 0$

$$\Rightarrow V = \frac{1}{2}\left(\frac{\partial^2 V}{\partial q_i \partial q_j}\right)_0 \eta_i \eta_j \equiv \frac{1}{2} V_{ij}\, \eta_i \eta_j$$

with symmetric matrix $\mathbb{V}$, i.e., $V_{ij} = V_{ji}$

Kinetic energy T is quadratic in velocities,

$$T = \frac{1}{2} m_{ij}\, \dot{q}_i \dot{q}_j = \frac{1}{2} m_{ij}\, \dot{\eta}_i \dot{\eta}_j$$

$$\text{with } m_{ij}(\{q_i\}) = m_{ij}(\{q_{0i}\}) + (\partial m_{ij}/\partial q_k)_0\, \eta_k + \dots$$
$$\approx m_{ij}(\{q_{0i}\})$$

since T is already quadratic in (the small) $\dot{\eta}_i$

$$\Rightarrow T = \frac{1}{2} T_{ij}\, \dot{\eta}_i \dot{\eta}_j \quad ; \quad T_{ij} \equiv m_{ij}(\{q_{0i}\})$$

with symmetric $\mathbb{T}$, i.e., $T_{ij} = T_{ji}$ [Usually $T_{ij} = T_i\, \delta_{ij}$]

Lagrangian : $L = T - V = \frac{1}{2}(T_{ij}\dot{\eta}_i\dot{\eta}_j - V_{ij}\eta_i\eta_j)$

Eqns. of motion : $\frac{d}{dt}\frac{\partial L}{\partial \dot{\eta}_i} - \frac{\partial L}{\partial \eta_i} = 0$; $i = 1,..,n$

Consider particular i, with sum indices l and j :

$$\frac{\partial L}{\partial \dot{\eta}_i} = \frac{1}{2}T_{lj}\frac{\partial}{\partial \dot{\eta}_i}(\dot{\eta}_l\dot{\eta}_j) = \frac{1}{2}T_{lj}(\delta_{il}\dot{\eta}_j + \delta_{ij}\dot{\eta}_l)$$

$$= \frac{1}{2}T_{ij}\dot{\eta}_j + \frac{1}{2}T_{li}\dot{\eta}_l = T_{ij}\dot{\eta}_j$$

(using $T_{li} = T_{il}$ and renaming sum index $l \to j$)

$$\Rightarrow \frac{d}{dt}\frac{\partial L}{\partial \dot{\eta}_i} = T_{ij}\frac{d}{dt}\dot{\eta}_j = T_{ij}\ddot{\eta}_j$$

Similarly :

$$\frac{\partial L}{\partial \eta_i} = -\frac{\partial V}{\partial \eta_i} = \ldots = -V_{ij}\eta_j$$

$$\Rightarrow \quad T_{ij}\ddot{\eta}_j + V_{ij}\eta_j = 0 \quad ; \quad i = 1,\ldots,n$$

A set of n coupled linear 2. order diff. eqns.
Same <u>form</u> as 1D harm. osc.

$\Rightarrow$ Reasonable ansatz is : $\eta_i(t) = A_i e^{-i\omega t}$
with complex amplitudes A_i, and $\mathrm{Re}\,\eta_i$ = actual movement

$$\Rightarrow V_{ij}A_j - \omega^2 T_{ij}A_j = 0$$

Non-trivial solution when $\det(\mathbb{V} - \omega^2\mathbb{T}) = 0$,
an n^{th} order eqn. for ω^2, with solutions (roots)
ω_α^2 ; $\alpha = 1,..,n$, the <u>eigenfrequencies</u> of the system.

Eigenmodes α :

$A_{i\alpha}$ = amplitude along gen. coord. q_i in mode α

Determined by the set of eqns.

$$(V_{ij} - \omega_\alpha^2 T_{ij}) A_{j\alpha} = 0$$

For a given ω_α, these n eqns. determine $n-1$ components of

$$\vec{A}_\alpha = \begin{pmatrix} A_{1\alpha} \\ A_{2\alpha} \\ \vdots \\ A_{n\alpha} \end{pmatrix}$$

[Cf. Assignment 2, Question 2, double pendulum ; $n=2$]

$\Rightarrow$ <u>One</u> undetermined <u>complex</u> component for each mode α, e.g. $A_{1\alpha}$, with undetermined abs. value and phase

$\Rightarrow$ $2n$ undetermined factors, as expected for n second order diff. eqns.

Gen. coords. for oscillation in eigenmode α :

$$\eta_{j\alpha} = A_{j\alpha} \, e^{-i\omega_\alpha t}$$

General solution is a linear combination of eigenmodes :

$$\eta_j(t) = \sum_{\alpha=1}^{n} \eta_{j\alpha}(t) = \sum_{\alpha=1}^{n} A_{j\alpha} \, e^{-i\omega_\alpha t}$$

Actual movement :

$$\mathrm{Re}\, \eta_j(t) = \sum_{\alpha=1}^{n} \mathrm{Re}\left\{ A_{j\alpha} \, e^{-i\omega_\alpha t} \right\}$$

Normal modes :

$A_{j\alpha}$ is prop. with the cofactor $\Delta_{j\alpha} = (-1)^{j+\alpha} \cdot M_{j\alpha}$ of the determinant $|\mathbb{V} - \omega_\alpha^2 \mathbb{T}|$. The minor (subdeterminant) $M_{j\alpha}$ is evaluated by removing row j and column α in $|\mathbb{V} - \omega_\alpha^2 \mathbb{T}|$.

$$\Rightarrow \mathrm{Re}\,\eta_j(t) = \sum_\alpha \Delta_{j\alpha} \mathrm{Re}\{c_\alpha e^{-i\omega_\alpha t}\} \equiv \sum_\alpha \Delta_{j\alpha} \Theta_\alpha(t)$$

In these normal coordinates Θ_α (and with a suitable scaling of $\Delta_{j\alpha}$) we have

$$T = \frac{1}{2} \sum_\alpha \dot{\Theta}_\alpha^2 \quad ; \quad V = \frac{1}{2} \sum_\alpha \omega_\alpha^2 \Theta_\alpha^2$$

$$\Rightarrow L = \frac{1}{2} \sum_\alpha \left(\dot{\Theta}_\alpha^2 - \omega_\alpha^2 \Theta_\alpha^2 \right)$$

Finally, with $\frac{d}{dt} \frac{\partial L}{\partial \dot{\Theta}_\alpha} - \frac{\partial L}{\partial \Theta_\alpha} = 0$:

$$\ddot{\Theta}_\alpha + \omega_\alpha^2 \Theta_\alpha = 0 \quad ; \quad \alpha = 1, .., n$$

Comments :

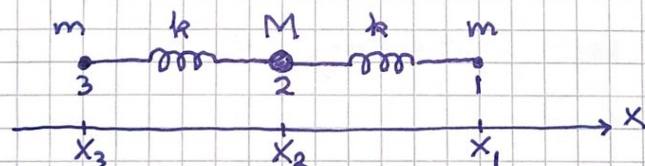
- Decoupled equations, i.e., in some sense orthogonal, hence the name normal modes
- n 2^{nd} order eqns. require $2n$ initial conditions for a complete solution, i.e., to determine abs. value and phase of the complex constants $c_\alpha = |c_\alpha| \exp(i\varphi_\alpha)$
- See compendium for more details (proof)

Ex.1: Particle in 3D harmonic potential

$$V = \frac{1}{2}\left(k_1 x^2 + k_2 y^2 + k_3 z^2\right)$$
$$T = \frac{1}{2} m \left(\dot{x}^2 + \dot{y}^2 + \dot{z}^2\right)$$
$$L = T - V = \frac{1}{2}\sum_{i=1}^{3}\left(m\dot{x}_i^2 - k_i x_i^2\right)$$
$$\Rightarrow \quad m\ddot{x}_i + k_i x_i = 0 \quad ; \quad i = 1, 2, 3 \qquad \text{(No sum here)}$$
$$\Rightarrow \quad x_i = A_i\, e^{-i\omega_i t} \quad \text{with} \quad \omega_i = \sqrt{k_i/m} \quad ; \quad i = 1, 2, 3$$

Here, $\mathbb{V}$ and $\mathbb{T}$ are diagonal from the start, so the cartesian coords. x_i are the normal coords.
<u>Degeneracy</u> if the force field is central, $V = V(r)$, i.e., $k_1 = k_2 = k_3 = k$ and $V(r) = \frac{1}{2}kr^2$. Then $\omega_1 = \omega_2 = \omega_3 = \sqrt{k/m}$

Ex. 2: Linear symmetric 3-atomic molecule



(Ex: CO_2)

Equilibrium bond lengths: $x_{01} - x_{02} = x_{02} - x_{03} = b$
Deviations from equilibrium: $\eta_i = x_i - x_{0i} \quad (i = 1, 2, 3)$
Assume nearest neighbour interaction and harmonic potential:

$$V = \frac{1}{2}k\left[(x_1 - x_2) - b\right]^2 + \frac{1}{2}k\left[(x_2 - x_3) - b\right]^2$$
$$= \frac{1}{2}k\left(\eta_1 - \eta_2\right)^2 + \frac{1}{2}k\left(\eta_2 - \eta_3\right)^2 = \frac{1}{2}V_{ij}\eta_i\eta_j$$
$$T = \frac{1}{2}m_i\dot{x}_i^2 = \frac{1}{2}m\left(\dot{\eta}_1^2 + \dot{\eta}_3^2\right) + \frac{1}{2}M\dot{\eta}_2^2 = \frac{1}{2}T_{ij}\dot{\eta}_i\dot{\eta}_j$$
$$\mathbb{V} = \begin{pmatrix} k & -k & 0 \\ -k & 2k & -k \\ 0 & -k & k \end{pmatrix} \quad ; \quad \mathbb{T} = \begin{pmatrix} m & 0 & 0 \\ 0 & M & 0 \\ 0 & 0 & m \end{pmatrix}$$

Eigenfreqs. given by $\left|\mathbb{V} - \omega^2\mathbb{T}\right| = 0$

$$\Rightarrow \begin{vmatrix} k-\omega^2 m & -k & 0 \\ -k & 2k-\omega^2 M & -k \\ 0 & -k & k-\omega^2 m \end{vmatrix} = 0$$

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

$$\Rightarrow \omega_1 = 0 , \quad \omega_2 = \sqrt{\frac{k}{m}} , \quad \omega_3 = \sqrt{\frac{(2m+M)k}{mM}}$$

The analysis of the atomic movements in the various normal modes $\alpha = 1, 2, 3$ is left as an exercise.

- $\omega_1 = 0$ corresponds to translation of the molecule along the x axis, with

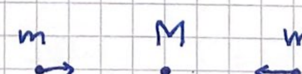
$$\vec{A}_1 \sim \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

- ω_3 is the antisymmetric mode with

$$\vec{A}_3 \sim \begin{pmatrix} 1 \\ -2m/M \\ 1 \end{pmatrix}$$

- ω_2 is the symmetric mode with

$$\vec{A}_2 \sim \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}$$



The "recipe" on p. 77 works for ω_1 and ω_3. For ω_2, $M_{12} = M_{22} = M_{32} = 0$. Then, one must simply solve the set of eqns.

$$\left(V_{ij} - \omega_\alpha^2 T_{ij}\right) A_{j\alpha} = 0$$

Here, 3 eqns. for A_{12}, A_{22} and A_{32}.