Small Oscillations - Introduction

Applications - normal vibration modes in molecules (spectroscopy), solids (phonons, elasticity), optical properties (generalized oscillators)

\[ \text{DF} = 2 \quad \text{DF} = 1 \]

What are small oscillations? Where do inhar conditio enter? Description of general motion -

Since small 2nd Law 2nd order DE
\[ \Rightarrow 2 \times \text{DF inhar condition} \]

Terminology

Normal mode all generalized co-ordinates oscillate with same frequency

Normal mode frequency - frequency of normal mode. There should be N normal frequencies for N DFs.

Normal co-ordinates?
Simple example for ndahon.

\[ k_1 \quad m \quad k_2 \quad m \quad k_1 \]

\[ \cdots \]

\[ k_1 \rightarrow q_1 \]

\[ \cdots \]

\[ k_2 \rightarrow q_2 \]

Select \( q_i \) devahan from equilibrium or generalized co-ordinates.

\[ T = \frac{1}{2} m \left( \ddot{q}_1^2 + \ddot{q}_2^2 \right) \]

\[ U = \frac{1}{2} k_1 (q_1^2 + q_2^2) + \frac{1}{2} k_2 (q_1 - q_2)^2 \]

\[ L = L (q_1, q_2, \dot{q}_1, \dot{q}_2) \]

E-L equations

\[ m \ddot{q}_1 + k_1 q_1 + k_2 (q_2 - q_1) = 0 \]

\[ m \ddot{q}_2 + k_1 q_2 + k_2 (q_1 - q_2) = 0 \]

Solve coupled equations.

Add to eliminate coupling term

\[ m (\ddot{q}_1 + \ddot{q}_2) + k (q_1 + q_2) = 0 \]

Suggests new variable \( \xi_1 = q_1 + q_2 \)

Since still 2 DPs also \( \xi_2 = q_1 - q_2 \)
\[ \ddot{z}_1 + \frac{k_1}{m} z_1 = 0 \Rightarrow \ddot{z}_1(t) = A_1 \cos(\omega_1 t + \phi_1) - q_1(t) + q_2(t) \]

\[ \omega_1 = \sqrt{\frac{k_1}{m}} \]

Notice \( \ddot{z}_1(t) \) doesn't describe either case - more like EM motion.

Subtract 2 equations:

\[ m \left( \ddot{z}_1 - \ddot{z}_2 \right) + (k_1 + 2k_2)(\dot{z}_1 - \dot{z}_2) = 0 \]

\[ \ddot{z}_2(t) = A_2 \cos(\omega_2 t + \phi_2) - \frac{k_2}{m} \ddot{z}_1(t) \]

\[ \omega_2 = \sqrt{\frac{k_2 + 2k_2}{m}} \]

hence \( \ddot{z}_2(t) \) describes relative motion.

4 constants from initial conditions.

Example. \( q_1(0) = x_0 \) everything else zero.

\[ q_1(t) = \frac{1}{2} (\ddot{z}_1(t) + \ddot{z}_2(t)) = \frac{1}{2} (A_1 \cos \phi_1 S_1 + A_2 \cos \phi_2 S_2) \]

\[ \ddot{q}_1(t) = \frac{1}{2} (\ddot{z}_1(t) + \ddot{z}_2(t)) = \frac{1}{2} (\omega_1 \cos \phi_1 S_1 + \omega_2 \cos \phi_2 S_2) \]

... etc.

Solve set at 4:

\[ S_1 = S_2 = 0, A_1 = A_2 = x_0 \]

\[ z_1(t) = x_0 \cos \omega_1 t \quad z_2(t) = x_0 \cos \omega_2 t \]
\[ q_1(t) = \frac{x_0}{2} (\cos \omega_1 t + \cos \omega_2 t) \]
\[ q_2(t) = \frac{x_0}{2} (\cos \omega_1 t - \cos \omega_2 t) \]

See solution in "natural" co-ordinates has 2 parts of different frequencies.

Using \( \cos A \pm \cos B = 2 \left[ \cos \frac{A+B}{2} \cos \frac{A-B}{2} \right] \)

\[ q_1 = x_0 \cos \left( \frac{\omega_1 - \omega_2}{2} t \right) \cos \left( \frac{\omega_1 + \omega_2}{2} t \right) \]
\[ q_2 = x_0 \sin \left( \frac{\omega_1 - \omega_2}{2} t \right) \sin \left( \frac{\omega_1 + \omega_2}{2} t \right) \]

**General observation - N DEs**

\( E-L \rightarrow N \) linear coupled ODEs
- decoupling \( \rightarrow \) new generalized co-ordinates
- 2N initial conditions provide unique solutions
- N independent solutions

**Normal co-ordinates - generalized co-ordinates that describe a normal mode**

Will develop this as eigenvector problem.
In this problem
\[ Q_1 = \sqrt{\frac{m}{2}} Z_1 \quad Q_2 = \sqrt{\frac{m}{2}} Z_2 \]

\[ q_1 = \frac{Q_1 + Q_2}{\sqrt{2m}} \quad q_2 = \frac{Q_1 - Q_2}{\sqrt{2m}} \]

The transformation changes Lagrangian
\[ L = \left( \frac{1}{2} \dot{q}_1^2 - \frac{1}{2} \omega_1^2 q_1^2 \right) + \left( \frac{1}{2} \dot{q}_2^2 - \frac{1}{2} \omega_2^2 q_2^2 \right) \]

separable
- will later describe reason for normalization
  (not that significant)

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General Approach from Lagrangian

N DEs  N generalized co-ordinate
\[ L = T(q_1, q_2, ..., q_n; \dot{q}_1, ..., \dot{q}_n) - V(q_1, ..., q_n) \]

Initially restrict to conservative forces

at equilibrium \( \frac{\partial V}{\partial q_i} \bigg|_{q_i=0} = 0 \)
Now assume:
- small displacement only
- Taylor series expansion.
- 2nd derivative not zero
- higher orders (non-linear terms) small.
- generalized co-ordinates and constraints time independent.

\[ q_i = q_{i0} + \eta_i \quad \eta_i \text{ small} \]

**Kinetic energy**

\[ T = \frac{1}{2} \sum \sum m_i \left( \ddot{x}_i + \dot{\eta}_i \dot{\eta}_i + \ddot{\eta}_i \right) \quad N_0 = \text{# particles} \]

\[ \dot{x}_i = \sum \frac{\partial x_i}{\partial q_j} \dot{q}_j \quad (\text{let } x_i \text{ include } \eta_i \text{ and } \dot{\eta}_i) \quad q_i, \dot{q}_i \in \mathbb{R} \]

\[ T = \frac{1}{2} \sum_{i} N_0 \sum_{j} m_i \left( \sum_{j} \frac{\partial x_j}{\partial q_{i0}} \dot{q}_{i0} \right)^2 \]

\[ = \frac{1}{2} \sum_{i} N_0 \sum_{j} \sum_{k} \left( \frac{\partial x_j}{\partial q_{i0}} \right) \left( \frac{\partial x_k}{\partial q_{i0}} \right) \dot{q}_{i0} \dot{q}_{i0} \]

\[ = \frac{1}{2} \sum_{j,k} \sum_{i} m_i \left[ \sum_{i} \frac{\partial x_j}{\partial q_{i0}} \frac{\partial x_k}{\partial q_{i0}} \right] \dot{q}_{i0} \dot{q}_{i0} \]

\[ = m_{jk} \left( q_1, \ldots, q_n \right) \]
mass matrix \( M_{jk} \) has "position" dependence but since only looking at small oscillation treat constant

\[
M_{jk} (q_1, \ldots, q_N) = M_{jk,0} + \sum_{i=1}^{N} \frac{\Theta m_{jk,i} n_i}{\epsilon q_i} \quad \text{Small,}
\]

\[
\Rightarrow T = \frac{1}{2} \sum_{j<k}^{N} M_{jk,0} \tilde{n}_j \tilde{n}_k
\]

\text{Symmetric, constant}

Similar for potential but since at \( q_0 \):

\[
V = V_0 + \sum_{i}^{N} \frac{\Theta V_0}{\epsilon q_{i,0}} n_i + \frac{1}{2} \sum_{i}^{N} \frac{\Theta V}{\epsilon q_{i,0}^2} n_i n_i
\]

\[
= V_0 + \sum_{i}^{N} V_{j0} n_i n_j
\]

\text{Symmetric, real, shop}

\[
L = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} (m_{ij,0} \tilde{n}_i \tilde{n}_j - V_{ij} n_i n_j) - V_0
\]

\[
E-L \sum_{i}^{N} (m_{ii} n_i^2 + V_{ii} n_i) = 0 \quad j = 1 \ldots N
\]

\text{All coupled}