Physics 106a — Classical Mechanics

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Lecture 18: Normal Modes

Outline

- General setup
- Linear algebra theory of normal modes
- Examples
  - Two coupled pendulums
  - Linear triatomic molecule CO_2
  - Triangular molecule O_3

Equations of motion and eigenvalue problem

- Lagrangian

$$L = \frac{1}{2}\tilde{\dot{\boldsymbol{q}}} \cdot \boldsymbol{T} \cdot \dot{\boldsymbol{q}} - \frac{1}{2}\tilde{\boldsymbol{q}} \cdot \boldsymbol{V} \cdot \boldsymbol{q}$$

- Euler-Lagrange equations

$$\boldsymbol{T} \cdot \ddot{\boldsymbol{q}} + \boldsymbol{V} \cdot \boldsymbol{q} = 0$$

- Look for sinusoidal solution

$$\boldsymbol{q}(t) = \boldsymbol{\Phi} e^{i\omega t}$$

- Generalized eigenvalue problem ⇒ characteristic equation

$$\boldsymbol{V} \cdot \boldsymbol{\Phi} - \omega^2 \boldsymbol{T} \cdot \boldsymbol{\Phi} = 0 \quad \Rightarrow \quad \det(\boldsymbol{V} - \omega^2 \boldsymbol{T}) = 0$$

- Solution
  - N solutions for ω_α^2 (the eigenvalues): ω_α are the *normal mode frequencies.*
  - Corresponding eigenvectors $\boldsymbol{\Phi}^{(\alpha)}$ are the *normal modes*
  - Components $\Phi_i^{(\alpha)}$ give the relative sizes of q_i if the αth mode is excited

Theorems

The following results can be proved (e.g. Hand and Finch §9.6):

- the eigenvalues ω_α^2 are real
- the eigenvectors $\mathbf{\Phi}^{(\alpha)}$ may be chosen real
- assuming $\boldsymbol{T}$ is positive definite, then if $\boldsymbol{V}$ is positive definite, corresponding to a stable equilibrium, $\omega_\alpha^2 > 0$ and the mode frequencies ω_α are real
- a symmetry may lead to no change in potential energy for some displacement: this will give a zero eigenvalue and a *zero frequency mode*
- different eigenvectors can be chosen orthonormal (orthogonal and normalized to 1) in the sense

$$\tilde{\mathbf{\Phi}}^{(\alpha)} \cdot \boldsymbol{T} \cdot \mathbf{\Phi}^{(\beta)} = \delta_{\alpha\beta}$$

- the eigenvectors form a basis (complete orthonormal set)

General solution

Equations of motion $\boldsymbol{T} \cdot \ddot{\boldsymbol{q}} + \boldsymbol{V} \cdot \boldsymbol{q} = 0$

A general set of displacements can be expanded in the normal mode basis

$$\boldsymbol{q}(t) = \sum_{\alpha} \rho_\alpha(t) \boldsymbol{\Phi}^{(\alpha)} \quad \Rightarrow \quad q_i(t) = \sum_{\alpha} \rho_\alpha(t) \Phi_i^{(\alpha)}$$

The $\rho_\alpha(t)$ are called *normal mode coordinates.* Substituting into the EOM

$$0 = \sum_{\alpha} (\ddot{\rho}_\alpha \boldsymbol{T} \cdot \boldsymbol{\Phi}^{(\alpha)} + \rho_\alpha \boldsymbol{V} \cdot \boldsymbol{\Phi}^{(\alpha)}) = \sum_{\alpha} (\ddot{\rho}_\alpha + \omega_\alpha^2 \rho_\alpha) \boldsymbol{T} \cdot \boldsymbol{\Phi}^{(\alpha)}$$

so that they satisfy *independent* SHO equations

$$\ddot{\rho}_\beta + \omega_\beta^2 \rho_\beta = 0$$

Using the orthogonality of the $\boldsymbol{\Phi}^{(\alpha)}$ we can calculate the inverse relation

$$\rho_\beta(t) = \tilde{\boldsymbol{\Phi}}^{(\beta)} \cdot \boldsymbol{T} \cdot \boldsymbol{q}(t)$$

Driven motion

Equations of motion: $\boldsymbol{T} \cdot \ddot{\boldsymbol{q}} + \boldsymbol{V} \cdot \boldsymbol{q} = \boldsymbol{F}(t)$

Expand the solution in the normal modes

$$\boldsymbol{q}(t) = \sum_{\alpha} \rho_{\alpha}(t) \boldsymbol{\Phi}^{(\alpha)}$$

Substituting into the EOM

$$\sum_{\alpha} (\ddot{\rho}_{\alpha} + \omega_{\alpha}^{2} \rho_{\alpha}) \boldsymbol{T} \cdot \boldsymbol{\Phi}^{(\alpha)} = \boldsymbol{F}$$

so that the normal mode coordinates satisfy the equations

$$\ddot{\rho}_{\beta} + \omega_{\beta}^{2} \rho_{\beta} = \mathcal{F}_{\beta} \quad \text{with} \quad \mathcal{F}_{\beta} = \tilde{\boldsymbol{\Phi}}^{(\beta)} \cdot \boldsymbol{F}$$

Initial conditions

Often convenient to use complex notation for the normal mode oscillations

$$\rho_\alpha(t) = \mathrm{Re}[A_\alpha e^{i\omega_\alpha t}]$$

The general solution can now be written

$$\boldsymbol{q}(t) = \sum_\alpha \mathrm{Re}[A_\alpha e^{i\omega_\alpha t}]\boldsymbol{\Phi}^{(\alpha)}$$

and then

$$\dot{\boldsymbol{q}}(t) = \sum_\alpha \mathrm{Re}[i\omega_\alpha A_\alpha e^{i\omega_\alpha t}]\boldsymbol{\Phi}^{(\alpha)}$$

Suppose initial conditions for $\boldsymbol{q}(0)$ and velocities $\dot{\boldsymbol{q}}(0)$. Use the orthogonality relation to give

$$\mathrm{Re}\, A_\beta = \tilde{\boldsymbol{\Phi}}^{(\beta)} \cdot \boldsymbol{T} \cdot \boldsymbol{q}(0)$$

$$\omega_\beta \,\mathrm{Im}\, A_\beta = -\tilde{\boldsymbol{\Phi}}^{(\beta)} \cdot \boldsymbol{T} \cdot \dot{\boldsymbol{q}}(0)$$

Transformation matrix

Define the matrix $\boldsymbol{R}$ as the matrix with *columns* given by the normal mode vectors

$$R_{i\alpha} = \Phi_i^{(\alpha)}$$

Then

$$\boldsymbol{q}(t) = \boldsymbol{R} \cdot \boldsymbol{\rho}\,(t)$$

The orthogonality of the normal mode vectors can be expressed as

$$\tilde{\boldsymbol{R}} \cdot \boldsymbol{T} \cdot \boldsymbol{R} = \boldsymbol{I}$$

with $\boldsymbol{I}$ the unit $N \times N$ matrix.

The inverse relation is

$$\boldsymbol{\rho}(t) = \tilde{\boldsymbol{R}} \cdot \boldsymbol{T} \cdot \boldsymbol{q}(t)$$

Diagonalization

The orthogonality of the normal mode vectors gave

$$\tilde{\boldsymbol{R}} \cdot \boldsymbol{T} \cdot \boldsymbol{R} = \boldsymbol{I}$$

Also

$$(\tilde{\boldsymbol{R}} \cdot \boldsymbol{V} \cdot \boldsymbol{R})_{\alpha\beta} = \tilde{\boldsymbol{\Phi}}^{(\alpha)} \cdot \boldsymbol{V} \cdot \boldsymbol{\Phi}^{(\beta)} = \omega_\beta^2 \tilde{\boldsymbol{\Phi}}^{(\alpha)} \cdot \boldsymbol{T} \cdot \boldsymbol{\Phi}^{(\beta)} = \omega_\beta^2 \delta_{\alpha\beta}$$

so that $\boldsymbol{R}$ also diagonalizes $\boldsymbol{V}$

$$\tilde{\boldsymbol{R}} \cdot \boldsymbol{V} \cdot \boldsymbol{R} = \boldsymbol{\Omega}$$

where $\boldsymbol{\Omega}$ is the diagonal matrix with entries ω_α^2.

The *congruence transformation* $\tilde{\boldsymbol{R}} \cdot \boldsymbol{?} \cdot \boldsymbol{R}$ diagonalizes both $\boldsymbol{T}$ and $\boldsymbol{V}$.

Lagrangian and Hamiltonian

It is straightforward to show using $\boldsymbol{q} = \boldsymbol{R} \cdot \boldsymbol{\rho}$

$$T = \tfrac{1}{2}\tilde{\dot{\boldsymbol{q}}} \cdot \boldsymbol{T} \cdot \dot{\boldsymbol{q}} = \tfrac{1}{2}\tilde{\dot{\boldsymbol{\rho}}} \cdot \dot{\boldsymbol{\rho}}$$
$$V = \tfrac{1}{2}\tilde{\boldsymbol{q}} \cdot \boldsymbol{V} \cdot \boldsymbol{q} = \tfrac{1}{2}\tilde{\boldsymbol{\rho}} \cdot \boldsymbol{\Omega} \cdot \boldsymbol{\rho}$$

so that the Lagrangian is

$$L = \tfrac{1}{2}\sum_{\alpha}(\dot{\rho}_{\alpha}^{2} - \omega_{\alpha}^{2}\rho_{\alpha}^{2})$$

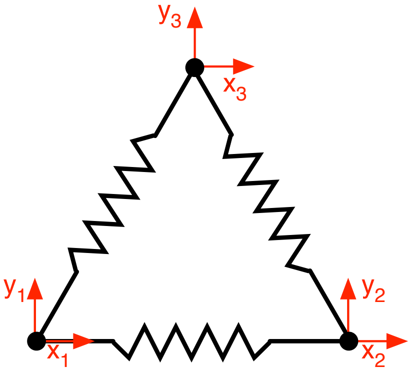
Defining the momentum conjugate to the normal mode coordinate

$$p_{\rho,\alpha} = \frac{\partial L}{\partial \dot{\rho}_{\alpha}} = \dot{\rho}_{\alpha}$$

gives the Hamiltonian

$$H = \tfrac{1}{2}\sum_{\alpha}(p_{\rho,\alpha}^{2} + \omega_{\alpha}^{2}\rho_{\alpha}^{2})$$

Vibrations of Ozone



$$V = \frac{1}{2}k\left\{\left[\frac{1}{2}(x_2 - x_3) + \frac{\sqrt{3}}{2}(y_3 - y_2)\right]^2 + \left[\frac{1}{2}(x_3 - x_1) + \frac{\sqrt{3}}{2}(y_3 - y_1)\right]^2 + (x_2 - x_1)^2\right\}$$

(Only need projection of displacements *along* spring)

Vibrations of Ozone

$$V = \tfrac{1}{2}k\left\{\left[\tfrac{1}{2}(x_2 - x_3) + \tfrac{\sqrt{3}}{2}(y_3 - y_2)\right]^2 + \left[\tfrac{1}{2}(x_3 - x_1) + \tfrac{\sqrt{3}}{2}(y_3 - y_1)\right]^2 + (x_2 - x_1)^2\right\}$$

$$\mathbf{q} = (x_1, y_1, x_2, y_2, x_3, y_3), \qquad V_{14} = \frac{\partial^2 V}{\partial x_1 \partial y_2} \quad \text{etc.}$$

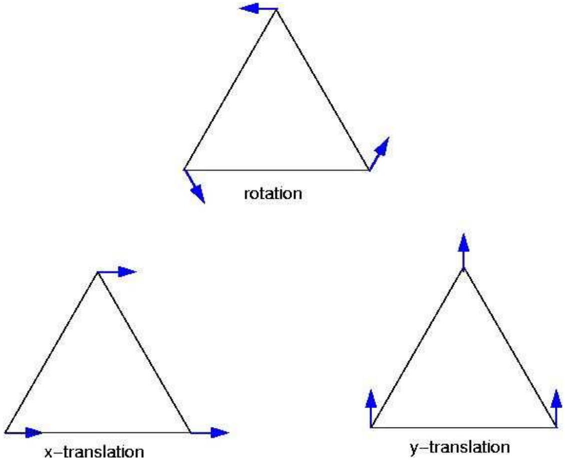
$$\mathbf{V} = k\begin{pmatrix} 5/4 & \sqrt{3}/4 & -1 & 0 & -1/4 & -\sqrt{3}/4 \\ \sqrt{3}/4 & 3/4 & 0 & 0 & -\sqrt{3}/4 & -3/4 \\ -1 & 0 & 5/4 & -\sqrt{3}/4 & -1/4 & \sqrt{3}/4 \\ 0 & 0 & -\sqrt{3}/4 & 3/4 & \sqrt{3}/4 & -3/4 \\ -1/4 & -\sqrt{3}/4 & -1/4 & \sqrt{3}/4 & 1/2 & 0 \\ -\sqrt{3}/4 & -3/4 & \sqrt{3}/4 & -3/4 & 0 & 3/2 \end{pmatrix}$$

$$\mathbf{T} = m\mathbf{I}$$

$$\text{Eigenvalues}[\mathbf{V}/m] : \quad \left\{0, 0, 0, \frac{3k}{2m}, \frac{3k}{2m}, \frac{3k}{m}\right\}$$

Vibrations of Ozone

Zero modes



Vibrations of Ozone

Other modes

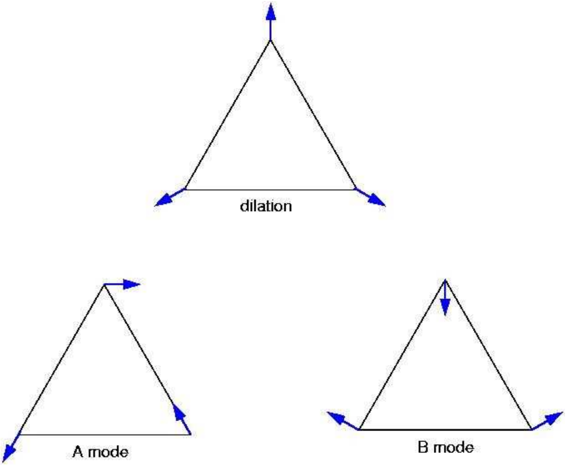
$$\text{Eigenvectors[V][[6]]:} \quad \left\{-\frac{\sqrt{3}}{2}, -\frac{1}{2}, \frac{\sqrt{3}}{2}, -\frac{1}{2}, 0, 1\right\}$$

$$\text{Eigenvectors[V][[5]]:} \quad \left\{-\frac{1}{2}, -\frac{\sqrt{3}}{2}, -\frac{1}{2}, \frac{\sqrt{3}}{2}, 1, 0\right\}$$

$$\text{Eigenvectors[V][[4]]:} \quad \left\{\frac{-\sqrt{3}}{2}, \frac{1}{2}, \frac{\sqrt{3}}{2}, \frac{1}{2}, 0, -1\right\}$$

Vibrations of Ozone

Other modes



A and B modes are *degenerate* — group theory for $\bar{6}m2$ point group