PHY 711 Classical Mechanics and Mathematical Methods
10-10:50 AM MWF in Olin 103

Discussion for Lecture 16 – Chap. 4 (F & W)

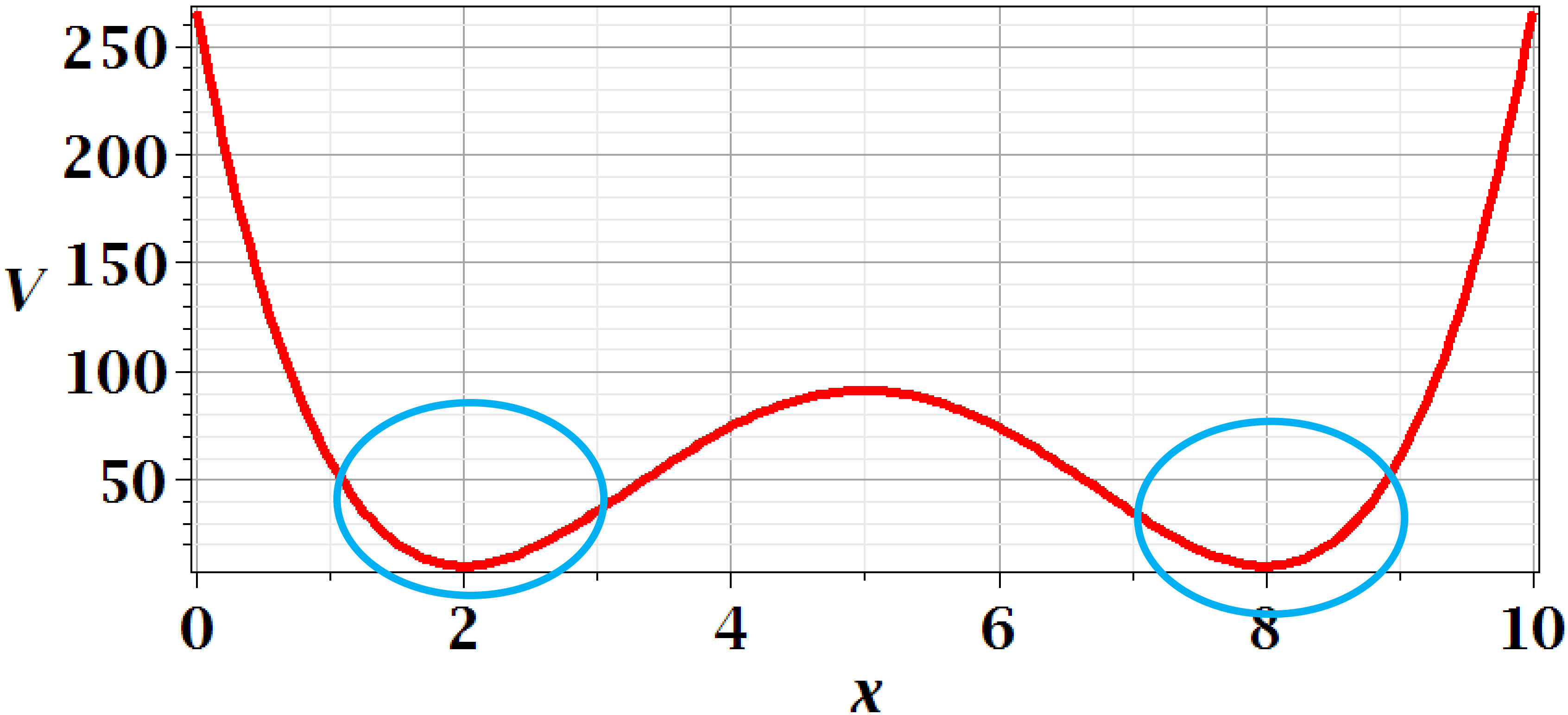
Analysis of motion near equilibrium

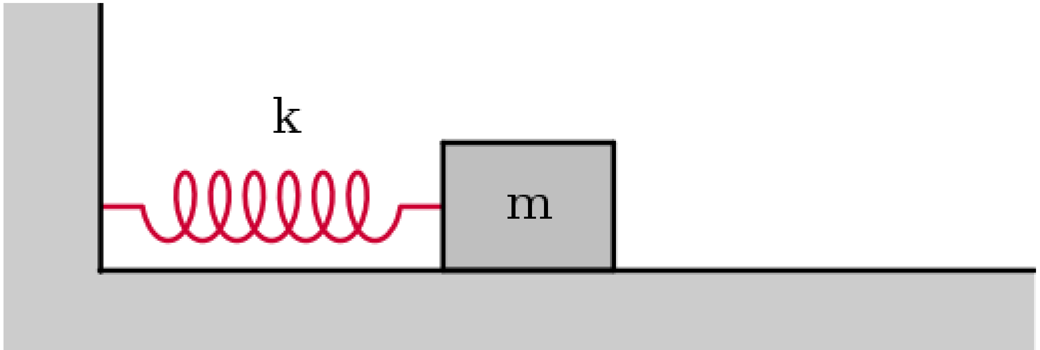
1. Small oscillations about equilibrium
2. Normal modes of vibration

	Date	F&W	Topic	HW
1	Mon, 8/26/2024		Introduction and overview	#1
2	Wed, 8/28/2024	Chap. 3(17)	Calculus of variation	#2
3	Fri, 8/30/2024	Chap. 3(17)	Calculus of variation	#3
4	Mon, 9/02/2024	Chap. 3	Lagrangian equations of motion	#4
5	Wed, 9/04/2024	Chap. 3 & 6	Lagrangian equations of motion	#5
6	Fri, 9/06/2024	Chap. 3 & 6	Lagrangian equations of motion	#6
7	Mon, 9/09/2024	Chap. 3 & 6	Lagrangian to Hamiltonian formalism	#7
8	Wed, 9/11/2024	Chap. 3 & 6	Phase space	#8
9	Fri, 9/13/2024	Chap. 3 & 6	Canonical Transformations	
10	Mon, 9/16/2024	Chap. 5	Dynamics of rigid bodies	#9
11	Wed, 9/18/2024	Chap. 5	Dynamics of rigid bodies	#10
12	Fri, 9/20/2024	Chap. 5	Dynamics of rigid bodies	#11
13	Mon, 9/23/2024	Chap. 1	Scattering analysis	#12
14	Wed, 9/25/2024	Chap. 1	Scattering analysis	#13
15	Fri, 9/27/2024	Chap. 1	Scattering analysis	#14
16	Mon, 9/30/2024	Chap. 4	Small oscillations near equilibrium	
17	Wed, 10/2/2024	Chap. 1-6	Review	THE-10/3-10/24
18	Fri, 10/4/2024	Chap. 4	Normal mode analysis	THE-10/3-10/24

Motivation for studying small oscillations – many interacting systems have stable and meta-stable configurations which are well approximated by:

$$V(x) \approx V(x_{eq}) + \tfrac{1}{2}\left(x - x_{eq}\right)^2 \left.\frac{d^2V}{dx^2}\right|_{x_{eq}} = V(x_{eq}) + \tfrac{1}{2}k\left(x - x_{eq}\right)^2$$





Equations of motion for a single oscillator:

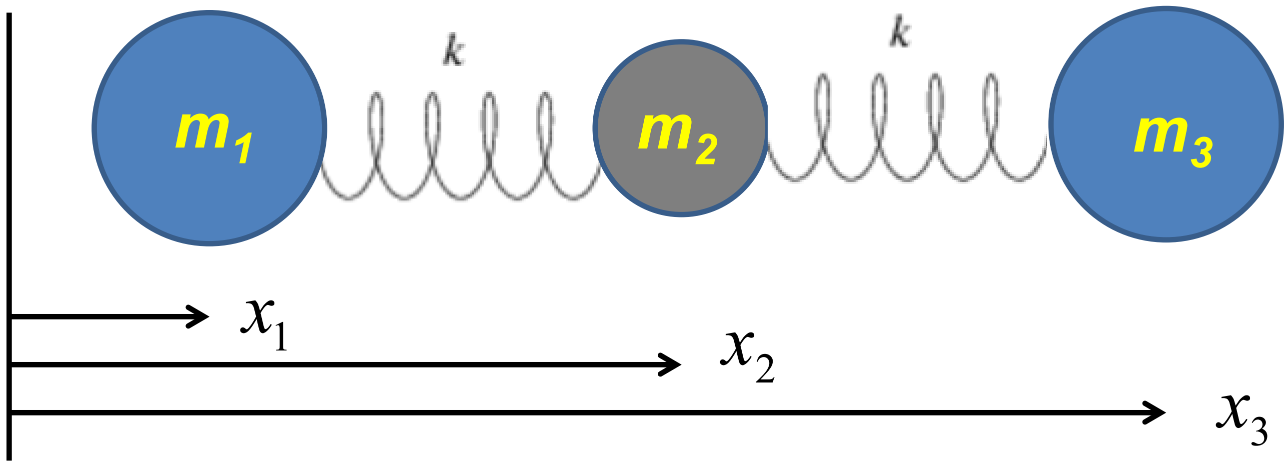
Let $k \equiv m\omega^2$

$$L(x,\dot{x},t) = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2 x^2$$

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} = \frac{\partial L}{\partial x} \qquad \Rightarrow m\ddot{x} = -m\omega^2 x$$

$$x(t) = A\sin(\omega t + \varphi)$$

Coupled oscillators --
Example – linear molecule



$$L = \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2\dot{x}_2^2 + \frac{1}{2}m_3\dot{x}_3^2 - \frac{1}{2}k\left(x_2 - x_1 - \ell_{12}\right)^2 - \frac{1}{2}k\left(x_3 - x_2 - \ell_{23}\right)^2$$

Equilibrium lengths

$$L = \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2\dot{x}_2^2 + \frac{1}{2}m_3\dot{x}_3^2$$
$$-\frac{1}{2}k\left(x_2 - x_1 - \ell_{12}\right)^2 - \frac{1}{2}k\left(x_3 - x_2 - \ell_{23}\right)^2$$

Let: $x_1 \rightarrow x_1 - x_1^0 \quad x_2 \rightarrow x_2 - x_1^0 - \ell_{12} \quad x_3 \rightarrow x_3 - x_1^0 - \ell_{12} - \ell_{23}$

$$L = \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2\dot{x}_2^2 + \frac{1}{2}m_3\dot{x}_3^2 - \frac{1}{2}k\left(x_2 - x_1\right)^2 - \frac{1}{2}k\left(x_3 - x_2\right)^2$$

Coupled equations of motion:

$$m_1\ddot{x}_1 = k\left(x_2 - x_1\right)$$
$$m_2\ddot{x}_2 = -k\left(x_2 - x_1\right) + k\left(x_3 - x_2\right) = k\left(x_1 - 2x_2 + x_3\right)$$
$$m_3\ddot{x}_3 = -k\left(x_3 - x_2\right)$$

Coupled equations of motion :

$$m_1\ddot{x}_1 = k(x_2 - x_1)$$

$$m_2\ddot{x}_2 = -k(x_2 - x_1) + k(x_3 - x_2) = k(x_1 - 2x_2 + x_3)$$

$$m_3\ddot{x}_3 = -k(x_3 - x_2)$$

Let $x_i(t) = X_i^\alpha e^{-i\omega_\alpha t}$ where X_i^α and ω_α are to be determined

$$-\omega_\alpha^2 m_1 X_1^\alpha = k\left(X_2^\alpha - X_1^\alpha\right)$$

$$-\omega_\alpha^2 m_2 X_2^\alpha = k\left(X_1^\alpha - 2X_2^\alpha + X_3^\alpha\right)$$

$$-\omega_\alpha^2 m_3 X_3^\alpha = -k\left(X_3^\alpha - X_2^\alpha\right)$$

Coupled linear equations:

$$-\omega_\alpha^2 m_1 X_1^\alpha = k\left(X_2^\alpha - X_1^\alpha\right)$$

$$-\omega_\alpha^2 m_2 X_2^\alpha = k\left(X_1^\alpha - 2X_2^\alpha + X_3^\alpha\right)$$

$$-\omega_\alpha^2 m_3 X_3^\alpha = -k\left(X_3^\alpha - X_2^\alpha\right)$$

Matrix form:

$$\begin{pmatrix} k-\omega_\alpha^2 m_1 & -k & 0 \\ -k & 2k-\omega_\alpha^2 m_2 & -k \\ 0 & -k & k-\omega_\alpha^2 m_3 \end{pmatrix}\begin{pmatrix} X_1^\alpha \\ X_2^\alpha \\ X_3^\alpha \end{pmatrix} = 0$$

Matrix form:

$$\begin{pmatrix} k-\omega_\alpha^2 m_1 & -k & 0 \\ -k & 2k-\omega_\alpha^2 m_2 & -k \\ 0 & -k & k-\omega_\alpha^2 m_3 \end{pmatrix} \begin{pmatrix} X_1^\alpha \\ X_2^\alpha \\ X_3^\alpha \end{pmatrix} = 0$$

More convenient form:

Let $Y_i \equiv \sqrt{m_i}X_i$ Equations for Y_i take the form:

$$\begin{pmatrix} \kappa_{11}-\omega_\alpha^2 & -\kappa_{12} & 0 \\ -\kappa_{12} & 2\kappa_{22}-\omega_\alpha^2 & -\kappa_{23} \\ 0 & -\kappa_{23} & \kappa_{33}-\omega_\alpha^2 \end{pmatrix} \begin{pmatrix} Y_1^\alpha \\ Y_2^\alpha \\ Y_3^\alpha \end{pmatrix} = 0$$

where $\kappa_{ij} = \kappa_{ji} \equiv \dfrac{k}{\sqrt{m_i m_j}}$

Digression:

Eigenvalue properties of matrices $\mathbf{M}\mathbf{y}_\alpha = \lambda_\alpha \mathbf{y}_\alpha$

Hermitian matrix : $H_{ij} = H^*{}_{ji}$

Theorem for Hermitian matrices :

λ_α have real values and $\mathbf{y}_\alpha^H \cdot \mathbf{y}_\beta = \delta_{\alpha\beta}$

Unitary matrix : $\mathbf{U}\mathbf{U}^H = \mathbf{I}$

$|\lambda_\alpha| = 1$ and $\mathbf{y}_\alpha^H \cdot \mathbf{y}_\beta = \delta_{\alpha\beta}$

Digression on matrices -- continued

Eigenvalues of a matrix are "invariant" under a similarity transformation

Eigenvalue properties of matrix: $\mathbf{M}\mathbf{y}_\alpha = \lambda_\alpha \mathbf{y}_\alpha$

Transformed matrix: $\mathbf{M}'\mathbf{y}'_\alpha = \lambda'_\alpha \mathbf{y}'_\alpha$

If $\mathbf{M}' = \mathbf{S}\mathbf{M}\mathbf{S}^{-1}$ then $\lambda'_\alpha = \lambda_\alpha$ and $\mathbf{S}^{-1}\mathbf{y}'_\alpha = \mathbf{y}_\alpha$

Proof $\mathbf{S}\mathbf{M}\mathbf{S}^{-1}\mathbf{y}'_\alpha = \lambda'_\alpha \mathbf{y}'_\alpha$

$$\mathbf{M}\left(\mathbf{S}^{-1}\mathbf{y}'_\alpha\right) = \lambda'_\alpha \left(\mathbf{S}^{-1}\mathbf{y}'_\alpha\right)$$

Example of transformation:

Original problem written in eigenvalue form:

$$\begin{pmatrix} k/m_1 & -k/m_1 & 0 \\ -k/m_2 & 2k/m_2 & -k/m_2 \\ 0 & -k/m_3 & k/m_3 \end{pmatrix} \begin{pmatrix} X_1^\alpha \\ X_2^\alpha \\ X_3^\alpha \end{pmatrix} = \omega_\alpha^2 \begin{pmatrix} X_1^\alpha \\ X_2^\alpha \\ X_3^\alpha \end{pmatrix}$$

Let $\mathbf{S} = \begin{pmatrix} \sqrt{m_1} & 0 & 0 \\ 0 & \sqrt{m_2} & 0 \\ 0 & 0 & \sqrt{m_3} \end{pmatrix}$; $\quad \mathbf{SMS}^{-1} = \begin{pmatrix} \kappa_{11} & -\kappa_{12} & 0 \\ -\kappa_{12} & 2\kappa_{22} & -\kappa_{23} \\ 0 & -\kappa_{23} & \kappa_{33} \end{pmatrix}$

Let $\mathbf{Y} \equiv \mathbf{SX}$

$$\begin{pmatrix} \kappa_{11} & -\kappa_{12} & 0 \\ -\kappa_{12} & 2\kappa_{22} & -\kappa_{23} \\ 0 & -\kappa_{23} & \kappa_{33} \end{pmatrix} \begin{pmatrix} Y_1^\alpha \\ Y_2^\alpha \\ Y_3^\alpha \end{pmatrix} = \omega_\alpha^2 \begin{pmatrix} Y_1^\alpha \\ Y_2^\alpha \\ Y_3^\alpha \end{pmatrix}$$

where $\quad \kappa_{ij} = \kappa_{ji} \equiv \dfrac{k}{\sqrt{m_i m_j}}$

In our case :

$$\begin{pmatrix} \kappa_{11} & -\kappa_{12} & 0 \\ -\kappa_{12} & 2\kappa_{22} & -\kappa_{23} \\ 0 & -\kappa_{23} & \kappa_{33} \end{pmatrix} \begin{pmatrix} Y_1^\alpha \\ Y_2^\alpha \\ Y_3^\alpha \end{pmatrix} = \omega_\alpha^2 \begin{pmatrix} Y_1^\alpha \\ Y_2^\alpha \\ Y_3^\alpha \end{pmatrix}$$

for $m_1 = m_3 \equiv m_O$ and $m_2 \equiv m_C$ $\quad (CO_2)$

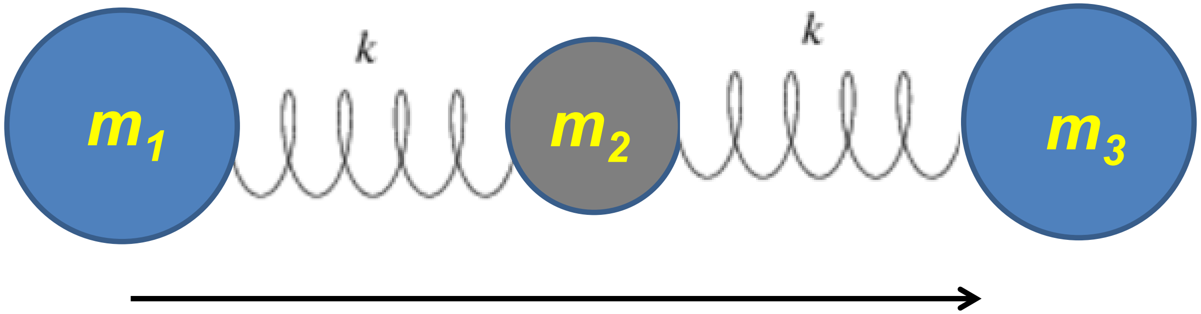
$$\begin{pmatrix} \kappa_{OO} & -\kappa_{OC} & 0 \\ -\kappa_{OC} & 2\kappa_{CC} & -\kappa_{OC} \\ 0 & -\kappa_{OC} & \kappa_{OO} \end{pmatrix} \begin{pmatrix} Y_1^\alpha \\ Y_2^\alpha \\ Y_3^\alpha \end{pmatrix} = \omega_\alpha^2 \begin{pmatrix} Y_1^\alpha \\ Y_2^\alpha \\ Y_3^\alpha \end{pmatrix}$$

Eigenvalues and eigenvectors :

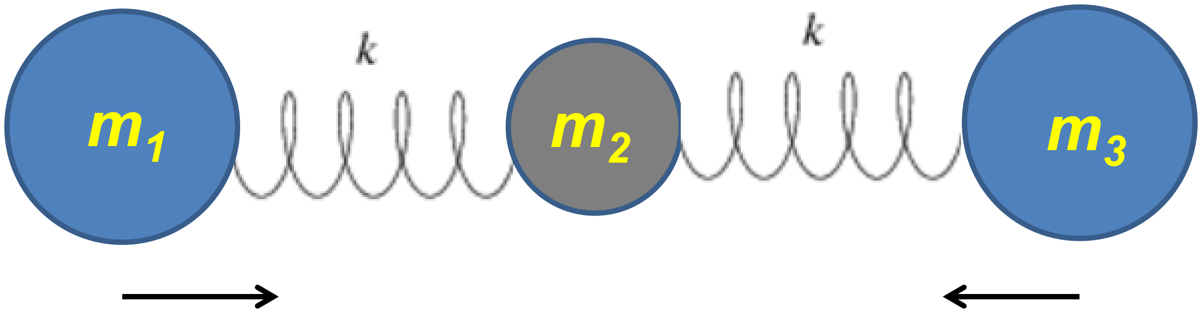
$$\omega_1^2 = 0 \qquad \begin{pmatrix} Y_1^1 \\ Y_2^1 \\ Y_3^1 \end{pmatrix} = N_1 \begin{pmatrix} \sqrt{\frac{m_O}{m_C}} \\ 1 \\ \sqrt{\frac{m_O}{m_C}} \end{pmatrix}, \quad \begin{pmatrix} X_1^1 \\ X_2^1 \\ X_3^1 \end{pmatrix} = N'_1 \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

$$\omega_2^2 = \frac{k}{m_O} \qquad \begin{pmatrix} Y_1^2 \\ Y_2^2 \\ Y_3^2 \end{pmatrix} = N_2 \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}, \quad \begin{pmatrix} X_1^2 \\ X_2^2 \\ X_3^2 \end{pmatrix} = N'_2 \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

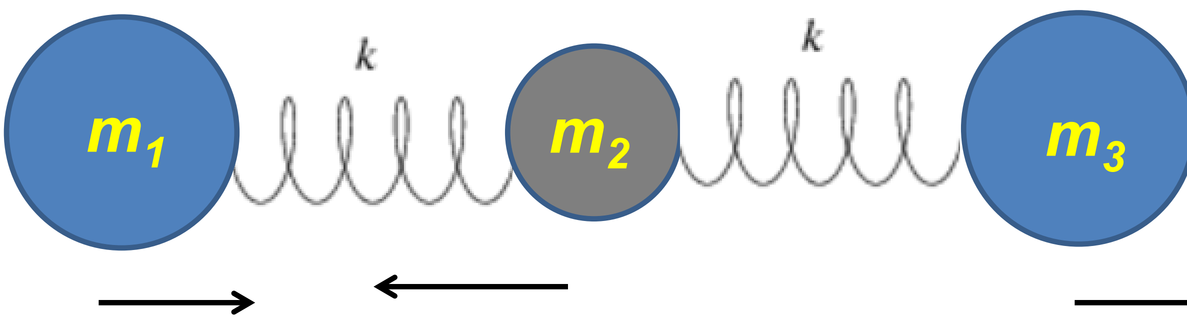
$$\omega_3^2 = \frac{k}{m_O} + \frac{2k}{m_C} \qquad \begin{pmatrix} Y_1^3 \\ Y_2^3 \\ Y_3^3 \end{pmatrix} = N_3 \begin{pmatrix} 1 \\ -2\sqrt{\frac{m_O}{m_C}} \\ 1 \end{pmatrix}, \quad \begin{pmatrix} X_1^3 \\ X_2^3 \\ X_3^3 \end{pmatrix} = N'_3 \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix}$$



$$\omega_1 = 0$$



$$\omega_2 = \sqrt{\frac{k}{m_O}}$$



$$\omega_3 = \sqrt{\frac{k}{m_O} + \frac{2k}{m_C}}$$

General solution :

$$x_i(t) = \Re\left(\sum_\alpha C^\alpha X_i^\alpha e^{-i\omega_\alpha t} \right)$$

For example, normal mode amplitudes

C^α can be determined from initial conditions

Comment on solving for eigenvalues and eigenvectors – while it is reasonable to find these analytically for 2x2 or 3x3 matrices, it is prudent to use Maple or Mathematica for larger systems.

Maple example

Mathematica example

Additional digression on matrix properties

Singular value decomposition

It is possible to factor any real matrix $\mathbf{A}$ into unitary matrices $\mathbf{V}$ and $\mathbf{U}$ together with positive diagonal matrix $\mathbf{\Sigma}$:

$$\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^{\mathbf{H}}$$

$$\mathbf{\Sigma} = \begin{pmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \sigma_N \end{pmatrix}$$

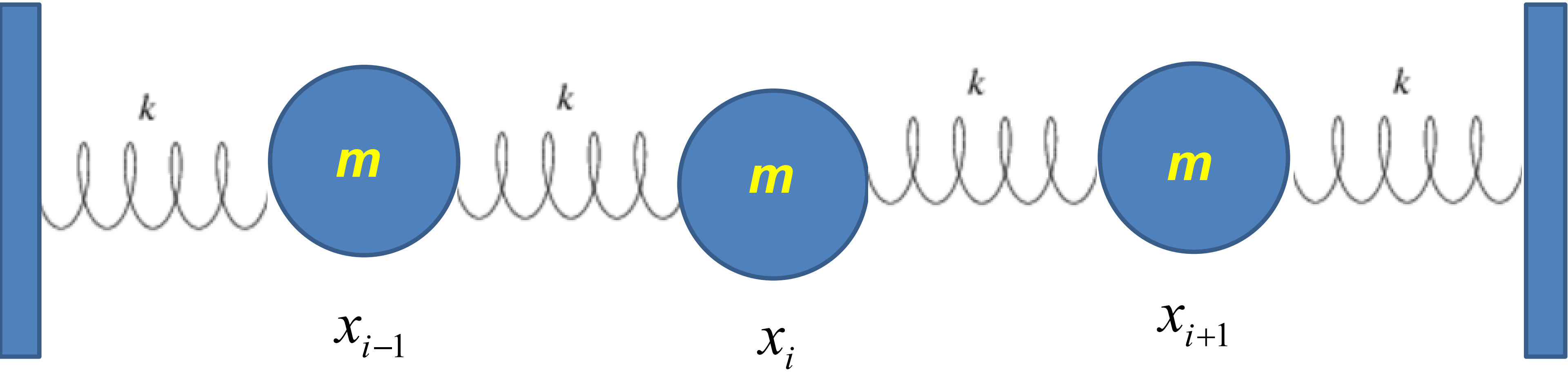
Singular value decomposition -- continued

Consider using SVD to solve a singular linear algebra problem $\qquad \mathbf{A}\mathbf{X} = \mathbf{B}$

$$\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^H$$

$$\mathbf{X} = \sum_{i \text{ for } \sigma_i > \varepsilon} \mathbf{v}_i \frac{\left\langle \mathbf{u}_i^H \mid \mathbf{B} \right\rangle}{\sigma_i}$$

Consider an extended system of masses and springs:



Note: each mass coordinate is measured relative to its equilibrium position x_i^0

$$L = T - V = \frac{1}{2} m \sum_{i=1}^{N} \dot{x}_i^2 - \frac{1}{2} k \sum_{i=0}^{N} \left(x_{i+1} - x_i \right)^2$$

Note: In fact, we have N masses; x_0 and x_{N+1} will be treated using boundary conditions.

$$L = T - V = \frac{1}{2} m \sum_{i=1}^{N} \dot{x}_i^2 - \frac{1}{2} k \sum_{i=0}^{N} \left(x_{i+1} - x_i \right)^2$$

$$x_0 \equiv 0 \text{ and } x_{N+1} \equiv 0$$

From Euler - Lagrange equations :

$$m\ddot{x}_1 = k\left(x_2 - 2x_1\right)$$

$$m\ddot{x}_2 = k\left(x_3 - 2x_2 + x_1\right)$$

....

$$m\ddot{x}_i = k\left(x_{i+1} - 2x_i + x_{i-1}\right)$$

....

$$m\ddot{x}_N = k\left(x_{N-1} - 2x_N\right)$$

Matrix formulation --

Assume $x_i(t) = X_i e^{-i\omega t}$

$$\frac{m}{k}\omega^2 \begin{pmatrix} X_1 \\ X_2 \\ \vdots \\ X_{N-1} \\ X_N \end{pmatrix} = \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ \cdots & \cdots & -1 & 2 & -1 \\ \cdots & \cdots & 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \\ \vdots \\ X_{N-1} \\ X_N \end{pmatrix}$$

Can solve as an eigenvalue problem --

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> with(LinearAlgebra);
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$$> A := \begin{bmatrix} 5 & -1 & 0 & 0 & 0 \\ -1 & 5 & -1 & 0 & 0 \\ 0 & -1 & 5 & -1 & 0 \\ 0 & 0 & -1 & 5 & -1 \\ 0 & 0 & 0 & -1 & 5 \end{bmatrix};$$

$$> Eigenvalues(A); \qquad \begin{bmatrix} 5 \\ 6 \\ 4 \\ 5-\sqrt{3} \\ 5+\sqrt{3} \end{bmatrix}$$

This example also has an algebraic solution --

From Euler-Lagrange equations:

$$m\ddot{x}_j = k\left(x_{j+1} - 2x_j + x_{j-1}\right) \qquad \text{with } x_0 = 0 = x_{N+1}$$

Try: $\quad x_j(t) = Ae^{-i\omega t + iqaj}$

$$-\omega^2 Ae^{-i\omega t + iqaj} = \frac{k}{m}\left(e^{iqa} - 2 + e^{-iqa}\right)Ae^{-i\omega t + iqaj}$$

$$-\omega^2 = \frac{k}{m}\left(2\cos(qa) - 2\right)$$

$$\Rightarrow \omega^2 = \frac{4k}{m}\sin^2\left(\frac{qa}{2}\right)$$

From Euler-Lagrange equations -- continued:

$$m\ddot{x}_j = k\left(x_{j+1} - 2x_j + x_{j-1}\right) \qquad \text{with } x_0 = 0 = x_{N+1}$$

Try: $x_j(t) = Ae^{-i\omega t + iqaj}$ $\qquad \Rightarrow \omega^2 = \frac{4k}{m}\sin^2\left(\frac{qa}{2}\right)$

Note that: $x_j(t) = Be^{-i\omega t - iqaj}$ $\qquad \Rightarrow \omega^2 = \frac{4k}{m}\sin^2\left(\frac{qa}{2}\right)$

General solution:

$$x_j(t) = \Re\left(Ae^{-i\omega t + iqaj} + Be^{-i\omega t - iqaj}\right)$$

Impose boundary conditions:

$$x_0(t) = \Re\left(Ae^{-i\omega t} + Be^{-i\omega t}\right) = 0$$

$$x_{N+1}(t) = \Re\left(Ae^{-i\omega t + iqa(N+1)} + Be^{-i\omega t - iqa(N+1)}\right) = 0$$

Impose boundary conditions -- continued:

$$x_0(t) = \Re\left(Ae^{-i\omega t} + Be^{-i\omega t} \right) = 0$$

$$x_{N+1}(t) = \Re\left(Ae^{-i\omega t + iqa(N+1)} + Be^{-i\omega t - iqa(N+1)} \right) = 0$$

$$\Rightarrow B = -A$$

$$x_{N+1}(t) = \Re\left(Ae^{-i\omega t}\left(e^{iqa(N+1)} - e^{-iqa(N+1)} \right)\right) = 0$$

$$\Rightarrow \sin\left(qa\left(N+1\right)\right) = 0$$

$$\Rightarrow \; qa\left(N+1\right) = \nu\pi \quad \text{where } \nu = 0,1,2\cdots$$

$$qa = \frac{\nu\pi}{N+1}$$

Summary of results:

$$\Rightarrow \omega_\nu^2 = \frac{4k}{m}\sin^2\left(\frac{\nu\pi}{2(N+1)}\right) \qquad x_n = \Re\left(2iA\sin\left(\frac{\nu\pi n}{N+1}\right)\right)$$

$$\nu = 0,1,\ldots N \qquad n = 1,2,\ldots\ldots N$$