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

Plan for Lecture 14:

Start reading Chapter 4

1. **Small oscillations about equilibrium**
2. **Normal modes**

Course schedule

(Preliminary schedule -- subject to frequent adjustment.)

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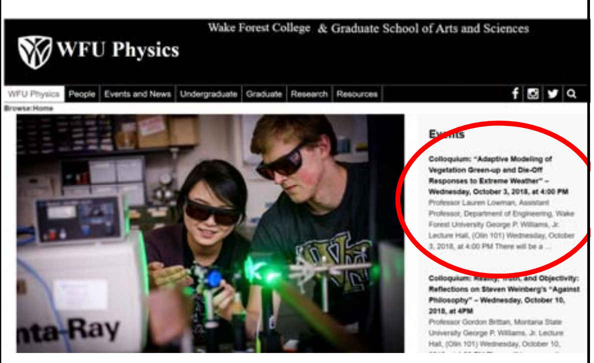
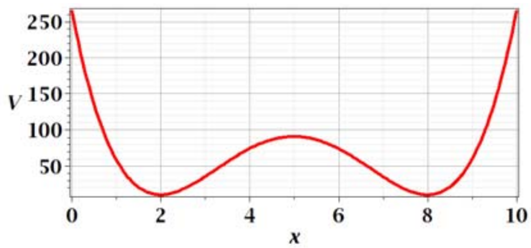
	Date	F&W Reading	Topic	Assignment	Due
1	Mon, 8/27/2018	Chap. 1	Introduction	#1	9/7/2018
	Wed, 8/29/2018	No class			
2	Fri, 8/31/2018	Chap. 1	Scattering theory	#2	9/7/2018
3	Mon, 9/03/2018	Chap. 1	Scattering theory		
4	Wed, 9/05/2018	Chap. 1	Scattering theory	#3	9/10/2018
5	Fri, 9/07/2018	Chap. 2	Non-inertial coordinate systems	#4	9/12/2018
6	Mon, 9/10/2018	Chap. 3	Calculus of Variation	#5	9/12/2018
7	Wed, 9/12/2018	Chap. 3	Calculus of Variation	#6	9/17/2018
	Fri, 9/14/2018	No class	University closed due to weather.		
8	Mon, 9/17/2018	Chap. 3	Lagrangian Mechanics	#7	9/19/2018
9	Wed, 9/19/2018	Chap. 3 and 6	Lagrangian Mechanics and constraints	#8	9/24/2018
10	Fri, 9/21/2018	Chap. 3 and 6	Constants of the motion		
11	Mon, 9/24/2018	Chap. 3 and 6	Hamiltonian formalism	#9	9/28/2018
12	Wed, 9/26/2018	Chap. 3 and 6	Liouville theorem	#10	10/3/2018
13	Fri, 9/28/2018	Chap. 3 and 6	Canonical transformations		
14	Mon, 10/1/2018	Chap. 4	Small oscillations about equilibrium	#11	10/5/2018
15	Wed, 10/3/28/2018	Chap. 4	Normal modes of vibration		
16	Fri, 10/5/2018	Chap. 1-4, 6	Review		



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:

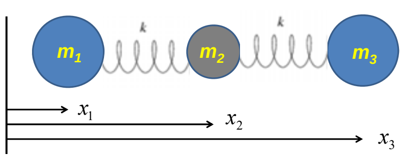
Let $k \equiv m\omega^2$

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

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

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

Example – linear molecule



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

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

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

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

Coupled equations of motion:

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

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Coupled equations of motion:

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

Let $x_i(t)=X_i^\alpha e^{-i\omega_\alpha t}$

$$-\omega_\alpha^2 m_1 X_1^\alpha=k\left(X_2^\alpha-X_1^\alpha\right)$$
$$-\omega_\alpha^2 m_2 X_2^\alpha=k\left(X_1^\alpha-2X_2^\alpha+X_3^\alpha\right)$$
$$-\omega_\alpha^2 m_3 X_3^\alpha=-k\left(X_3^\alpha-X_2^\alpha\right)$$

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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:

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

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

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

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 $m_2 \equiv m_C$ $\quad (CO_2)$

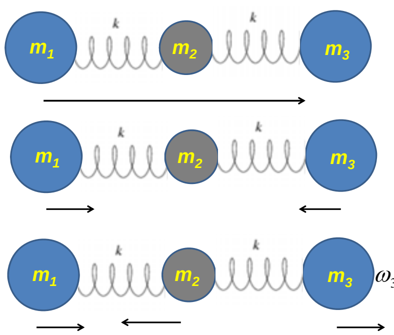
$$\begin{pmatrix} \kappa_{OO} & -\kappa_{OC} & 0 \\ -\kappa_{OC} & 2\kappa_{CC} & -\kappa_{OC} \\ 0 & -\kappa_{OC} & \kappa_{OO} \end{pmatrix}\begin{pmatrix} Y_1^\alpha \\ Y_2^\alpha \\ Y_3^\alpha \end{pmatrix} = \omega_\alpha^2 \begin{pmatrix} Y_1^\alpha \\ Y_2^\alpha \\ Y_3^\alpha \end{pmatrix}$$

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

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 $\mathbf{\Sigma}$:

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

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

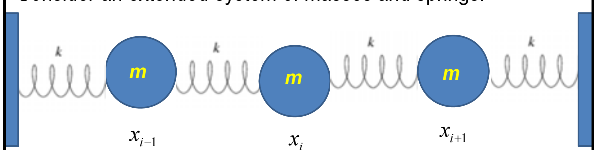
Singular value decomposition -- continued

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

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

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

Consider an extended system of masses and springs:



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

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

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

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

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

From Euler-Lagrange equations:

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

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

....

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

....

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

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 --

This example also has an algebraic solution --

From Euler - Lagrange equations:

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

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

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

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

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

From Euler-Lagrange equations -- continued:

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

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

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

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:

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

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

$$\Rightarrow B = -A$$

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

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

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

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

Summary of results:

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

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