

**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

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Course schedule

(Preliminary schedule -- subject to frequent adjustment.) (rrr)

Date	F&W Reading Topic	Assignment
1 Wed, 8/27/2014	Chap. 1 Review of basic principles	#1
2 Fri, 8/29/2014	Chap. 1 Scattering theory	#2
3 Mon, 9/01/2014	Chap. 1 Scattering theory continued	#3
4 Wed, 9/03/2014	Chap. 2 Accelerated coordinate systems	#4
5 Fri, 9/05/2014	Chap. 3 Calculus of variations	#5
6 Mon, 9/08/2014	Chap. 3 Calculus of variations	#6
7 Wed, 9/10/2014	Chap. 3 Hamilton's principle	#7
8 Fri, 9/12/2014	Chap. 3 & 6 Hamilton's principle	#8
9 Mon, 9/15/2014	Chap. 3 & 6 Lagrangians with constraints	#9
10 Wed, 9/17/2014	Chap. 3 & 6 Lagrangians and constants of motion	#10
11 Fri, 9/19/2014	Chap. 3 & 6 Hamiltonian formalism	#11
12 Mon, 9/22/2014	Chap. 3 & 6 Hamiltonian formalism	#11
13 Wed, 9/24/2014	Chap. 3 & 6 Hamiltonian Jacobi transformations	
14 Fri, 9/26/2014	Chap. 4 Small oscillations	Begin Take-Home
15 Mon, 9/29/2014	Chap. 4 Normal modes of motion	Continue Take-Home
16 Wed, 10/01/2014	Chap. 4 Normal modes of motion	Continue Take-Home
17 Fri, 10/03/2014	Chap. 4 Normal modes of motion	Take-Home due

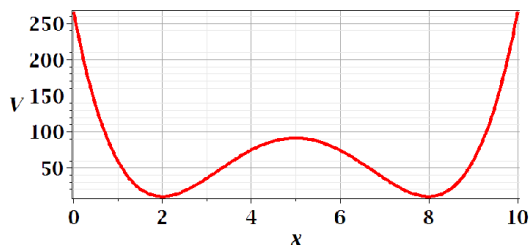
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Motivation for studying small oscillations -- many interacting systems have stable and meta-stable configurations which are well approximated by:

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



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Equations of motion for a single oscillator:

Let $k \equiv m\omega^2$

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

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

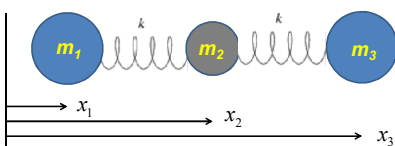
$$x(t) = A \sin(\omega t + \varphi)$$

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Example – linear molecule



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

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$$L = \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2\dot{x}_2^2 + \frac{1}{2}m_3\dot{x}_3^2$$

$$- \frac{1}{2}k(x_2 - x_1 - \ell_{12})^2 - \frac{1}{2}k(x_3 - x_2 - \ell_{23})^2$$

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

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

Coupled equations of motion :

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

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

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

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

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

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

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

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Coupled linear equations:

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

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

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

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

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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 $\mathbf{y}_\alpha^H \cdot \mathbf{y}_\beta = \delta_{\alpha\beta}$

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

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Example of transformation:

Original problem written in eigenvalue form:

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

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

Let $\mathbf{Y} \equiv \mathbf{S}\mathbf{X}$

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

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

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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 $m_2 \equiv m_c$ (CO_2)

$$\begin{pmatrix} \kappa_{oo} & -\kappa_{oc} & 0 \\ -\kappa_{oc} & 2\kappa_{cc} & -\kappa_{oc} \\ 0 & -\kappa_{oc} & \kappa_{oo} \end{pmatrix} \begin{pmatrix} Y_1^\alpha \\ Y_2^\alpha \\ Y_3^\alpha \end{pmatrix} = \omega_\alpha^2 \begin{pmatrix} Y_1^\alpha \\ Y_2^\alpha \\ Y_3^\alpha \end{pmatrix}$$

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Eigenvalues and eigenvectors :

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

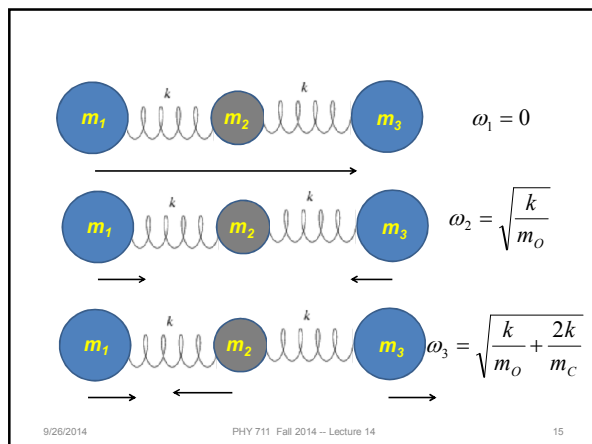
$$\omega_2^2 = \frac{k}{m_o} \quad \begin{pmatrix} Y_1^2 \\ Y_2^2 \\ Y_3^2 \end{pmatrix} = N_2 \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}, \quad \begin{pmatrix} X_1^2 \\ X_2^2 \\ X_3^2 \end{pmatrix} = N'_2 \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

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

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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

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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 $\mathbf{\Sigma}$:

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

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

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Singular value decomposition -- continued

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

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

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

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