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

Plan for Lecture 15:

Start reading Chapter 4

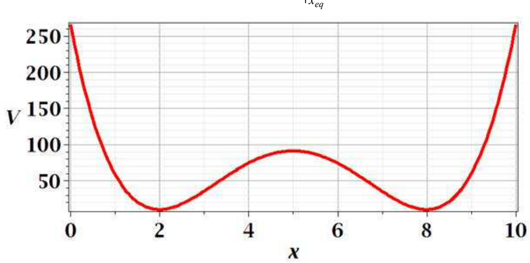
1. **Small oscillations about equilibrium**
2. **Normal modes**

	Date	F&W Reading	Topic	Assignment
1	Wed, 8/28/2013	Chap. 1	Review of basic principles;Scattering theory	#1
2	Fri, 8/30/2013	Chap. 1	Scattering theory continued	#2
3	Mon, 9/02/2013	Chap. 1	Scattering theory continued	#3
4	Wed, 9/04/2013	Chap. 2	Accelerated Coordinate Systems	#4
5	Fri, 9/06/2013	Chap. 3	Calculus of variations	#5
6	Mon, 9/09/2013	Chap. 3	Calculus of variations -- continued	
7	Wed, 9/11/2013	Chap. 3	Calculus of variations applied to Lagrangians	#6
8	Fri, 9/13/2013	Chap. 3	Lagrangian mechanics	#7
9	Mon, 9/16/2013	Chap. 3 & 6	Lagrangian mechanics	#8
10	Wed, 9/18/2013	Chap. 3 & 6	Lagrangian mechanics	#9
11	Fri, 9/20/2013	Chap. 3 & 6	Lagrangian & Hamiltonian mechanics	#10
12	Mon, 9/23/2013	Chap. 3 & 6	Hamiltonian formalism	#11
13	Wed, 9/25/2013	Chap. 3 & 6	Hamiltonian formalism	#12
14	Fri, 9/27/2013	Chap. 3 & 6	Hamiltonian formalism	#13
15	Mon, 9/30/2013	Chap. 4	Small Oscillations	#14
16	Wed, 10/02/2013	Chap. 4	Small Oscillations	

Please use this time to complete all outstanding assignments

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

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



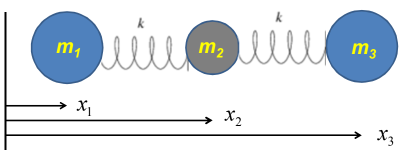
Equations of motion for a single oscillator :

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

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

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

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 :

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

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

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

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

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

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:

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

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 : $\mathbf{M}\mathbf{y}_\alpha = \lambda_\alpha \mathbf{y}_\alpha$

Transforme d 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:

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

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

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

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

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 $m_2 \equiv m_C$ (CO_2)

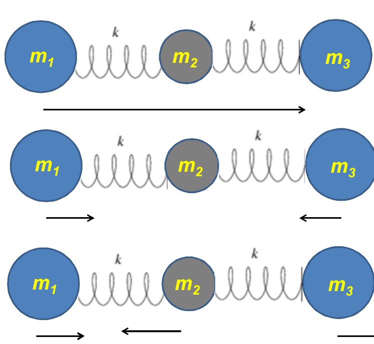
$$\begin{pmatrix} \kappa_{OO} & -\kappa_{OC} & 0 \\ -\kappa_{OC} & 2\kappa_{CC} & -\kappa_{OC} \\ 0 & -\kappa_{OC} & \kappa_{OO} \end{pmatrix}\begin{pmatrix} Y_1^\alpha \\ Y_2^\alpha \\ Y_3^\alpha \end{pmatrix} = \omega_\alpha^2 \begin{pmatrix} Y_1^\alpha \\ Y_2^\alpha \\ Y_3^\alpha \end{pmatrix}$$

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 $\mathbf{AX} = \mathbf{B}$

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

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