

PHY 711 Classical Mechanics and Mathematical Methods 9-9:50 AM MWF Olin 107

Plan for Lecture 14:

Start reading Chapter 4

1. Small oscillations about equilibrium
2. Normal modes


Course schedule

(Preliminary schedule -- subject to frequent adjustment.)

Date	F&W	Reading Topic	Assignment	Due
1 Mon, 8/28/2017	Chap. 1	Introduction	#1	9/6/2017
2 Wed, 8/30/2017	Chap. 1	Scattering theory	#2	9/6/2017
3 Fri, 9/01/2017	Chap. 1	Scattering theory		
4 Mon, 9/04/2017	Chap. 1	Scattering theory	#3	9/6/2017
5 Wed, 9/06/2017	Chap. 2	Physics in a non-inertial reference frame	#4	9/8/2017
6 Fri, 9/08/2017	Chap. 3	Calculus of variations	#5	9/11/2017
7 Mon, 9/11/2017	Chap. 3	Calculus of variations	#6	9/13/2017
8 Wed, 9/13/2017	Chap. 3	Lagrangian Mechanics	#7	9/15/2017
9 Fri, 9/15/2017	Chap. 3 and 6	Lagrangian mechanics and constraints	#8	9/20/2017
10 Mon, 9/18/2017	Chap. 3 and 6	Constants of the motion		
11 Wed, 9/20/2017	Chap. 3 and 6	Hamiltonian formalism	#9	9/27/2017
12 Fri, 9/22/2017	Chap. 3 and 6	Liouville equation		
13 Mon, 9/25/2017	Chap. 6	Canonical transformations		
14 Wed, 9/27/2017	Chap. 4	Motion from Small oscillations about equilibrium		
15 Fri, 9/29/2017	Chap. 1-4,6	Review		
Mon, 10/02/2017		Take-home exam -- No class		
Wed, 10/04/2017		Take-home exam -- No class		
16 Fri, 10/06/2017				

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Events

Colloquium: Sep. 27, 2017 at 4 PM
 WFU Physics Colloquium TITLE: "Physics, electronics, and information: QLED, OPVC, and QOP" SPEAKER: Professor Jeehan K. Noh, School of Physics and Astronomy, University of North Carolina at Chapel Hill, Chapel Hill, NC

Colloquium: Oct. 4, 2017 at 4 PM
 WFU Physics and Chemistry Colloquium TITLE: "In-situ Processing of High-Performance Fiber Carbon Nanotubes & Nanoporous Chaperone-OPVCs" SPEAKER: Professor David John Anzures, Department of Mechanical Engineering and Materials Science, Wake Forest University, Durham, NC, USA

WFU Physics Colloquium

TITLE: "Photons, electrons, and phonons; OLED, OFET, and OPV"

SPEAKER: Professor Laurie E. McNeil
Department of Physics and Astronomy
University of North Carolina at Chapel Hill, NC

ABSTRACT

TIME: Wed. Sep. 27, 2017 at 4:00

PLACE: George P. Williams, Jr. Lecture Hall (101)

First discovered at the beginning of the 20th century but still only partially understood today, organic semiconductors combine the electrical and optical properties typical of inorganic semiconductors with properties such as flexibility, low cost, and structural tunability via chemical modification. They are of significant interest due to their potential for opto-electronic applications such as displays, photosensors and solar cells. Charge transfer compounds, which are made of two or more organic molecules in which one species acts as a donor of electric charge and the other as an acceptor, could provide new properties or improved performance to increase the range of application of organic semiconductors. I will discuss how optical measurements such as resonant Raman scattering and transient absorption, when combined with numerical calculations, can elucidate the physics of the subtle interplay of interactions that is critical to applications of these materials in 21st-century opto-electronic devices.

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

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

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Equations of motion for a single oscillator:

Let $k \equiv m\omega^2$

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

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

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

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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:

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

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

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

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

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

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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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$\omega_1 = 0$

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

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

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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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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.

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

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

From Euler - Lagrange equations :

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

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

.....

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

.....

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

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From Euler - Lagrange equations :

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

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

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

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

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

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From Euler-Lagrange equations -- continued:

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

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

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

General solution:

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

Impose boundary conditions:

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

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

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Impose boundary conditions -- continued:

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

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

$$\Rightarrow B = -A$$

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

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

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

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

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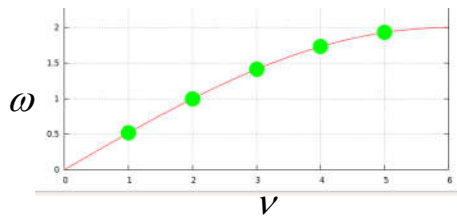
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Summary of results:

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

$$\nu = 0, 1, \dots, N$$

$$n = 1, 2, \dots, N$$



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