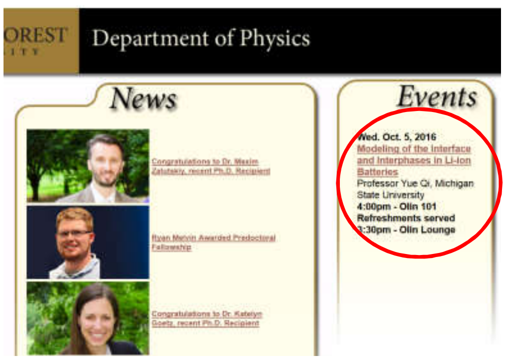
PHY 711 Classical Mechanics and Mathematical Methods
11-11:50 AM MWF Olin 107

Plan for Lecture 15:

Start reading Chapter 7

1. **Linear versus non-linear oscillators**
2. **Coupled motion of extended systems; relationship to continuum models & wave equation**



WFU Physics Colloquium

TITLE: Modeling of the Interface and Interphases in Li-ion Batteries

SPEAKER: Professor Yue Qi,

Department of Chemical Engineering and Materials Science
Michigan State University
East Lansing, Michigan

TIME: Wednesday October 5, 2016 at 4:00 PM

PLACE: Room 101 Olin Physical Laboratory

Refreshments will be served at 3:30 PM in the Olin Lounge. All interested persons are cordially invited to attend.

ABSTRACT

One of the most significant challenges for current and future lithium ion batteries is the smart structure design at the nanoscale and the control of electron and ion transport at the electrode/electrolyte interface. This issue is further complicated by the existence of ultrathin solid electrolyte interphase (SEI) covering the electrode, forming a complex heterogeneous electrode/SEI/electrolyte interface. Based on joint multi-scale modeling and experimental results, we point out that the well-known two-layer structure of SEI also exhibits two different Li^+ ion transport mechanisms. The SEI has a porous (organic) outer layer permeable to both Li^+ and anions (dissolved in electrolyte), and a dense (inorganic) inner layer facilitate only Li^+ transport. This model suggests a strategy to deconvolute the

3	Wed, 9/07/2016	Chap. 1	Scattering theory	#3	9/9/2016
4	Fri, 9/09/2016	Chap. 1 & 2	Scattering theory and rotations	#4	9/12/2016
5	Mon, 9/12/2016	Chap. 3	Calculus of variations	#5	9/14/2016
6	Wed, 9/14/2016	Chap. 3	Calculus of variations	#6	9/16/2016
7	Fri, 9/16/2016	Chap. 3	Lagrangian mechanics	#7	9/19/2016
8	Mon, 9/19/2016	Chap. 3 and 6	Lagrangian mechanics and constraints	#8	9/21/2016
9	Wed, 9/21/2016	Chap. 3 and 6	Constants of the motion	#9	9/23/2016
10	Fri, 9/23/2016	Chap. 3 and 6	Hamiltonian and canonical equations of motion	#10	9/26/2016
11	Mon, 9/26/2016	Chap. 3 and 6	Phase space	#11	9/28/2016
12	Wed, 9/28/2016	Chap. 6	Canonical transformations	#12	9/30/2016
13	Fri, 9/30/2016	Chap. 4	Small oscillations	#13	10/04/2016
14	Tue, 10/04/2016	Chap. 4	Normal modes	#14	10/07/2016
15	Wed, 10/05/2016	Chap. 7	Wave motion in one dimension	#15	10/07/2016
16	Fri, 10/07/2016	Chap. 7			
17	Mon, 10/10/2016	Chap. 7		Take-home exam	
18	Wed, 10/12/2016			Take-home exam	
19	Fri, 10/14/2016			Take-home exam	
20	Mon, 10/17/2016			Exam due	
21	Wed, 10/19/2016				
	Fri, 10/21/2016		Fall break -- no class		
22	Mon, 10/24/2016				

Linear oscillator equations (example from one dimension)

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

$$\Rightarrow \frac{1}{2}kx^2 \equiv \frac{1}{2}m\omega^2 x^2$$

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

Euler - Lagrange equations :

$$\ddot{x} = -\omega^2 x$$

Superposition :

Suppose that the functions $x_1(t)$ and $x_2(t)$ are solutions

$\Rightarrow Ax_1(t) + Bx_2(t)$ are also solutions (all A,B)

Non - linear oscillator equations (example from one dimension)

$$V(x) \approx V(x_{eq}) + \frac{1}{2}(x - x_{eq})^2 \left.\frac{d^2V}{dx^2}\right|_{x_{eq}} + \frac{1}{4!}(x - x_{eq})^4 \left.\frac{d^4V}{dx^4}\right|_{x_{eq}} + \cdots$$

$$\Rightarrow \frac{1}{2}m\omega^2\left(x^2 + \frac{1}{2}\varepsilon x^4\right)$$

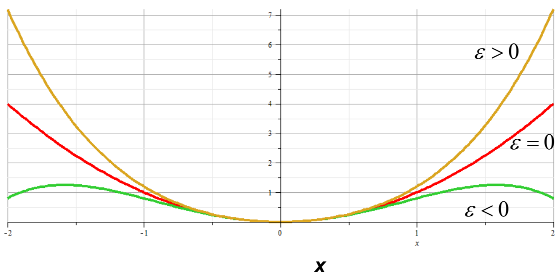
$$L(x,\dot{x}) = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2\left(x^2 + \frac{1}{2}\varepsilon x^4\right)$$

Euler - Lagrange equations :

$$\ddot{x} = -\omega^2\left(x + \varepsilon x^3\right)$$

Superposition - - no longer applies

$$V(x) \approx \frac{1}{2} m\omega^2 \left(x^2 + \varepsilon x^4\right)$$



Non - linear example - - continued

$$L(x,\dot{x}) = \frac{1}{2} m\dot{x}^2 - \frac{1}{2} m\omega^2 \left(x^2 + \frac{1}{2}\varepsilon x^4\right)$$

Euler - Lagrange equations :

$$\ddot{x} + \omega^2\left(x + \varepsilon x^3\right) = 0$$

Perturbation expansion :

$$x(t) = x_0(t) + \varepsilon x_1(t) + \ldots$$

Euler - Lagrange equations :

zero order : $\ddot{x}_0 + \omega^2 x_0 = 0$

first order : $\ddot{x}_1 + \omega^2 x_1 + \omega^2 x_0^3 = 0$

Non - linear example - - continued

$$\ddot{x} + \omega^2\left(x + \varepsilon x^3\right) = 0$$

Initial conditions :

$x(0) = X_0 \qquad \dot{x}(0) = 0$

Perturbation expansion :

$$x(t) = x_0(t) + \varepsilon x_1(t) + \ldots$$

Euler - Lagrange equations :

zero order : $\ddot{x}_0 + \omega^2 x_0 = 0 \qquad \Rightarrow x_0(t) = X_0 \cos(\omega t)$

first order : $\ddot{x}_1 + \omega^2 x_1 + \omega^2 x_0^3 = 0$

$$\Rightarrow \ddot{x}_1(t) + \omega^2 x_1(t) = -X_0^3 \cos^3(\omega t) = -\frac{X_0^3}{4}\left(3\cos(\omega t) + \cos(3\omega t)\right)$$

$$\Rightarrow x_1(t) = -\frac{X_0^3}{8\omega^2}\left\{3\omega t \sin(\omega t) + \frac{1}{4}\left[\cos(\omega t) - \cos(3\omega t)\right]\right\}$$

$$x(t) = X_0 \cos(\omega t) - \varepsilon \frac{X_0^3}{8\omega^2}\left\{3\omega t \sin(\omega t) + \frac{1}{4}\left[\cos(\omega t) - \cos(3\omega t)\right]\right\} + O(\varepsilon^2)$$

Non - linear example - - continued

$$\ddot{x} + \omega^2\left(x + \varepsilon x^3\right) = 0$$

Initial conditions :

$$x(0) = X_0 \qquad \dot{x}(0) = 0$$

Perturbation expansion :

$$x(t) = x_0(t) + \varepsilon x_1(t) + \ldots$$

Previous result (blows up at large t):

$$x(t) = X_0 \cos(\omega t) - \varepsilon \frac{X_0^3}{8\omega^2}\left\{3\omega t \sin(\omega t) + \frac{1}{4}\left[\cos(\omega t) - \cos(3\omega t)\right]\right\} + O\left(\varepsilon^2\right)$$

By rearranging terms (allowing effective frequency to vary):

$$x(t) = X_0 \cos\left(\omega\left(1 + \varepsilon\frac{3X_0^2}{8\omega}\right)t\right) - \varepsilon\frac{X_0^3}{32\omega^2}\left\{\cos(\omega t) - \cos(3\omega t)\right\} + O\left(\varepsilon^2\right)$$

Non - linear example with driving term - - Duffing equation

Georg Duffing ~ 1915

$$\ddot{x} + \omega^2\left(x + \varepsilon x^3\right) = A\cos(\Omega t)$$

Trial solution from: $x(t) \approx c_1\cos(\Omega t) + c_3\cos(3\Omega t)$

$$\left[\left(\omega^2 - \Omega^2\right)c_1 - \varepsilon\frac{3}{4}\omega^2 c_1^3[1+\cdots] - A\right]\cos(\Omega t) +$$

$$\left[\left(\omega^2 - 9\Omega^2\right)c_3 - \varepsilon\frac{1}{4}\omega^2 c_1^3[1+\cdots]\right]\cos(3\Omega t) + \cdots = 0$$

Approximate solution: (assume $\frac{c_3}{c_1} << 1$)

$$\frac{c_3}{c_1} \approx \varepsilon\frac{1}{4}c_1^2\frac{1}{1 - 9\omega^2/\Omega^2}$$

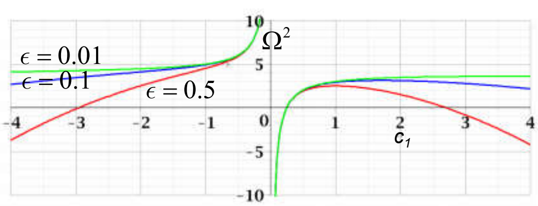
$$\left(\omega^2 - \Omega^2\right)c_1 - \varepsilon\frac{3}{4}\omega^2 c_1^3 - A = 0$$

Duffing oscillator -- continued

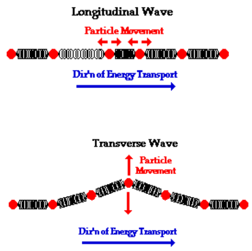
Plot for ω=2
A=1

$$\left(\omega^2 - \Omega^2\right)c_1 - \varepsilon\frac{3}{4}\omega^2 c_1^3 - A = 0$$

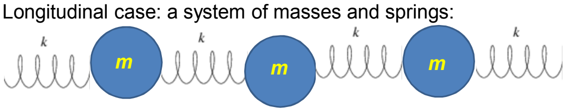
$$\Omega^2 = \omega^2 - \varepsilon\frac{3}{4}\omega^2 c_1^2 - \frac{A}{c_1}$$



Returning to linear case; continuum limit --
Longitudinal versus transverse vibrations
Images from web page:
http://www.physicsclassroom.com/class/waves/u10l1c.cfm



Longitudinal case: a system of masses and springs:



x_{i-1} $\quad x_i$ $\quad x_{i+1}$

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

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

Now imagine the continuum version of this system :

$$x_i(t) \Rightarrow \mu(x_i, t) \qquad \ddot{x}_i \Rightarrow \frac{\partial^2 \mu}{\partial t^2}$$

$$x_{i+1} - 2x_i + x_{i-1} \Rightarrow \frac{\partial^2 \mu}{\partial x^2} (\Delta x)^2$$

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

Continuum equation : $\quad m\frac{\partial^2 \mu}{\partial t^2} = k\left(\Delta x\right)^2 \frac{\partial^2 \mu}{\partial x^2}$

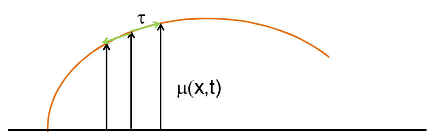
$$\frac{\partial^2 \mu}{\partial t^2} = \left(\frac{k\Delta x}{m/\Delta x}\right) \frac{\partial^2 \mu}{\partial x^2}$$

system parameter with units of (velocity)^2

For transverse oscillations on a string with tension τ and mass/length σ :

$$\left(\frac{k\Delta x}{m/\Delta x}\right) \Rightarrow \frac{\tau}{\sigma}$$

Transverse displacement:



Wave equation :

$$\frac{\partial^2 \mu}{\partial t^2} = c^2 \frac{\partial^2 \mu}{\partial x^2}$$

Lagrangian for continuous system :

Denote the generalized displacement by $\mu(x,t)$:

$$L = L\left(\mu, \frac{\partial \mu}{\partial x}, \frac{\partial \mu}{\partial t}; x, t\right)$$

Hamilton's principle :

$$\delta \int_{t_i}^{t_f} dt \int_{x_i}^{x_f} dx\, L\left(\mu, \frac{\partial \mu}{\partial x}, \frac{\partial \mu}{\partial t}; x, t\right) = 0$$

$$\Rightarrow \frac{\partial L}{\partial \mu} - \frac{\partial}{\partial x}\frac{\partial L}{\partial(\partial \mu / \partial x)} - \frac{\partial}{\partial t}\frac{\partial L}{\partial(\partial \mu / \partial t)} = 0$$

Euler - Lagrange equations for continuous system :

$$\frac{\partial L}{\partial \mu} - \frac{\partial}{\partial x}\frac{\partial L}{\partial(\partial \mu / \partial x)} - \frac{\partial}{\partial t}\frac{\partial L}{\partial(\partial \mu / \partial t)} = 0$$

Example :

$$L = \frac{\sigma}{2}\left(\frac{\partial \mu}{\partial t}\right)^2 - \frac{\tau}{2}\left(\frac{\partial \mu}{\partial x}\right)^2$$

$$\Rightarrow \sigma \frac{\partial^2 \mu}{\partial t^2} - \tau \frac{\partial^2 \mu}{\partial x^2} = 0$$

$$\frac{\partial^2 \mu}{\partial t^2} - c^2 \frac{\partial^2 \mu}{\partial x^2} = 0 \quad \text{for} \quad c^2 = \frac{\tau}{\sigma}$$

General solutions $\mu(x,t)$ to the wave equation :

$$\frac{\partial^2 \mu}{\partial t^2} - c^2 \frac{\partial^2 \mu}{\partial x^2} = 0$$

Note that for any function $f(q)$ or $g(q)$:

$$\mu(x,t) = f(x-ct) + g(x+ct)$$

satisfies the wave equation.

Initial value solutions $\mu(x,t)$ to the wave equation; attributed to D'Alembert :

$$\frac{\partial^2 \mu}{\partial t^2} - c^2 \frac{\partial^2 \mu}{\partial x^2} = 0 \qquad \text{where } \mu(x,0) = \phi(x) \text{ and } \frac{\partial \mu}{\partial t}(x,0) = \psi(x)$$

Assume :

$$\mu(x,t) = f(x-ct) + g(x+ct)$$

then : $\mu(x,0) = \phi(x) = f(x) + g(x)$

$$\frac{\partial \mu}{\partial t}(x,0) = \psi(x) = -c\left(\frac{df(x)}{dx} - \frac{dg(x)}{dx}\right)$$

$$\Rightarrow f(x) - g(x) = -\frac{1}{c}\int^{x} \psi(x')dx'$$

Solution -- continued : $\mu(x,t) = f(x-ct) + g(x+ct)$

then : $\mu(x,0) = \phi(x) = f(x) + g(x)$

$$\frac{\partial \mu}{\partial t}(x,0) = \psi(x) = -c\left(\frac{df(x)}{dx} - \frac{dg(x)}{dx}\right)$$

$$\Rightarrow f(x) - g(x) = -\frac{1}{c}\int^{x} \psi(x')dx'$$

For each x, find $f(x)$ and $g(x)$:

$$f(x) = \frac{1}{2}\left(\phi(x) - \frac{1}{c}\int^{x} \psi(x')dx'\right)$$

$$g(x) = \frac{1}{2}\left(\phi(x) + \frac{1}{c}\int^{x} \psi(x')dx'\right)$$

$$\Rightarrow \mu(x,t) = \frac{1}{2}\left(\phi(x-ct) + \phi(x+ct)\right) + \frac{1}{2c}\int_{x-ct}^{x+ct} \psi(x')dx'$$

Example:

$$\frac{\partial^2 \mu}{\partial t^2} - c^2 \frac{\partial^2 \mu}{\partial x^2} = 0 \qquad \text{where } \mu(x,0) = e^{-x^2/\sigma^2} \text{ and } \frac{\partial \mu}{\partial t}(x,0) = 0$$

$$\Rightarrow \mu(\mathrm{x},\mathrm{t}) = \frac{1}{2}\left(e^{-(x+ct)^2/\sigma^2} + e^{-(x-ct)^2/\sigma^2}\right)$$

Example:

$$\frac{\partial^2 \mu}{\partial t^2} - c^2 \frac{\partial^2 \mu}{\partial x^2} = 0 \quad \text{where } \mu(x,0) = 0 \text{ and } \frac{\partial \mu}{\partial t}(x,0) = -\frac{2x}{\sigma^2} e^{-x^2/\sigma^2}$$

$$\Rightarrow \mu(x,t) = \frac{1}{2c}\left(e^{-(x+ct)^2/\sigma^2} - e^{-(x-ct)^2/\sigma^2}\right)$$

Note that $\frac{\partial \mu(x,t)}{\partial t} = -\frac{1}{\sigma^2}\left((x+ct)e^{-(x+ct)^2/\sigma^2} + (x-ct)e^{-(x-ct)^2/\sigma^2}\right)$