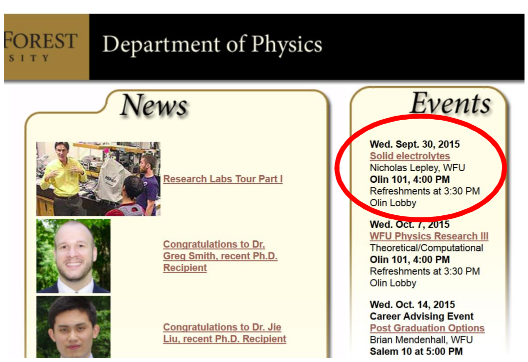
PHY 711 Classical Mechanics and Mathematical Methods
10-10:50 AM MWF Olin 103

Plan for Lecture 16:

Start reading Chapter 7

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

4	Wed, 9/02/2015	Chap. 2	Accelerated coordinate systems	#4
5	Fri, 9/04/2015	Chap. 3	Calculus of variations	#5
6	Mon, 9/07/2015	Chap. 3	Calculus of variations	#6
7	Wed, 9/09/2015	Chap. 3	Hamilton's principle	#7
8	Fri, 9/11/2015	Chap. 3 & 6	Hamilton's principle	#8
9	Mon, 9/14/2015	Chap. 3 & 6	Lagrangians with constraints	#9
10	Wed, 9/16/2015	Chap. 3 & 6	Lagrangians and constants of motion	#10
11	Fri, 9/18/2015	Chap. 3 & 6	Hamiltonian formalism	#11
12	Mon, 9/21/2015	Chap. 3 & 6	Hamiltonian formalism	#12
13	Wed, 9/23/2015	Chap. 3 & 6	Hamiltonian Jacobi transformations	#13
14	Fri, 9/25/2015	Chap. 4	Small oscillations	#14
15	Mon, 9/28/2015	Chap. 4	Normal modes of motion	#15
16	Wed, 9/30/2015	Chap. 7	Wave motion	#16
17	Fri, 10/02/2015	Chap. 7	Wave motion	
18	Mon, 10/05/2015	Chap. 7	Wave motion	
19	Wed, 10/07/2015	Chap. 7	Sturm-Liouville Equations	
20	Fri, 10/09/2015	Chap. 7	Sturm-Liouville Equations	
	Mon, 10/12/2015		No class	Take home exam
	Wed, 10/14/2015		No class	Take home exam due
	Fri, 10/16/2015		Fall break -- no class	



WFU Physics Colloquium

TITLE: Investigating Li-ion solid electrolytes using simulations based on density functional theory

SPEAKER: Nicholas D. Lepley,

Department of physics,
Wake Forest University

TIME: Wednesday September 30, 2015 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

Lithium ion batteries are used in a diverse array of applications. They power laptops and cellphones, houses and automobiles, airliners and Mars rovers. The success of Li-ion batteries has driven growing demand for batteries with higher capacity and longer lifetimes. One of the most promising paths to improving Li batteries is the development of solid electrolyte materials. This talk will briefly summarize some of my investigations of novel lithium phosphate and thiophosphate solid electrolytes, the computational quantum mechanics that enabled those investigations, as well as explaining how Li-ion batteries work and what we are doing to make them last longer.

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)

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

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

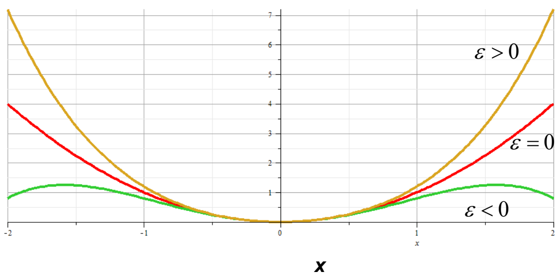
$$L(x,\dot{x}) = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2\left(x^2 + \frac{1}{2}\epsilon x^4\right)$$

Euler - Lagrange equations :

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

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 : $x(0) = X_0$ $\quad \dot{x}(0) = 0$

Perturbation expansion :

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

Euler - Lagrange equations :

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

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

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

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

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

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 $\frac{c_3}{c_1} << 1$)

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

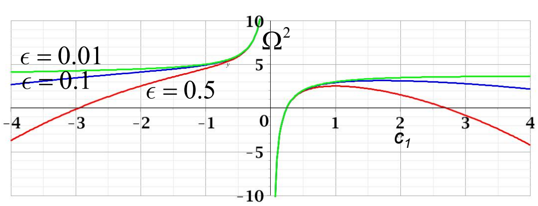
$$\left(\omega^2 - \Omega^2 \right) c_1 - \varepsilon \frac{3}{4} \omega^2 c_1^3 - A = 0$$

Duffing oscillator -- continued

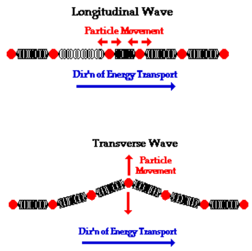
Plot for ω=2 *A*=1

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

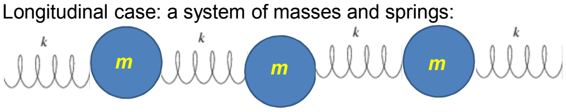
$$\Omega^2 = \omega^2 - \varepsilon \frac{3}{4} \omega^2 c_1^2 - \frac{A}{c_1}$$



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

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

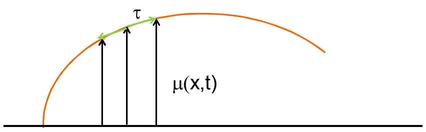
$$\frac{\partial^2 \mu}{\partial t^2} = \left(\frac{k\Delta x}{m / \Delta x} \right) \frac{\partial^2 \mu}{\partial x^2}$$

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.

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

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

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

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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 $g(x)$:

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

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

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

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Example:

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

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

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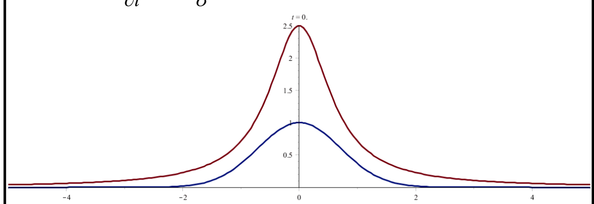
Example:

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

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

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



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