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

Plan for Lecture 16:

Continue reading Chapter 4

1. **Normal modes for extended one-dimensional systems**
2. **Normal modes for 2 and 3 dimensional systems**

	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	
17	Fri, 10/04/2013	Chap. 4	Small Oscillations	#15

WFU Physics and Computer Science Colloquium

TITLE: From chips to systems. Techniques for performing Multi Petaflop Electronic Structure Calculations on modern supercomputers.

SPEAKER: Dr. Emil Briggs,

Physics Department
North Carolina State University

TIME: Wednesday October 2, 2013 at 4:00 PM

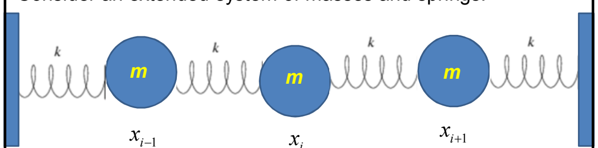
PLACE: Room 101 Olin Physical Laboratory

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

ABSTRACT

The need for higher levels of performance in HPC applications is being met today by ever increasing levels of parallel computation. This includes both chip level parallelism via GPU accelerators and multi-core CPU's and system level parallelism which utilizes hundreds or thousands of nodes linked together by high speed networking. Efficient use of such hardware resources requires new algorithms and coding methods. This talk will describe recent work with the RMG electronic structure code developed at NCSU that has enabled performance at the 6.5 PFLOP level on the latest generation of supercomputers. Challenges involved with scaling performance to the exascale level will also be described and potential solutions discussed.

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.

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

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

From Euler - Lagrange equations :

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

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

....

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

....

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

From Euler - Lagrange equations :

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

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

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

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

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

From Euler - Lagrange equations - - continued :

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

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

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

General solution :

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

Impose boundary conditions :

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

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

Impose boundary conditions - - continued :

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

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

$\Rightarrow B = -A$

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

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

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

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

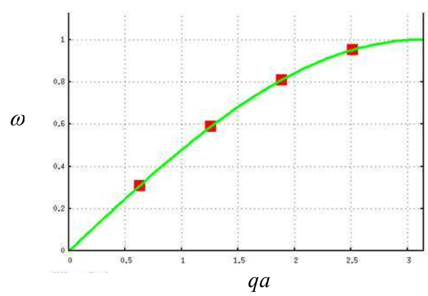
Recap -- solution for integer parameter ν

$$x_j(t) = \Re\left(2iAe^{-i\omega_\nu t}\sin\left(\frac{\nu\pi j}{N+1}\right)\right)$$

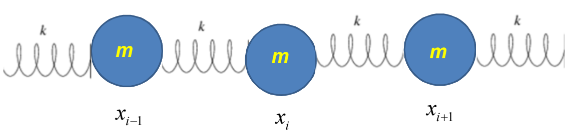
$$\omega_\nu^{\ 2} = \frac{4k}{m}\sin^2\left(\frac{\nu\pi}{2(N+1)}\right)$$

Note that non-trivial, unique values are

$$\nu = 1,2,\cdots N$$



Consider an infinite system of masses and springs:



Note: each mass coordinate is measured relative to its equilibrium position x_i^0

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

Note: In this case we have an infinite number of idential masses and springs.

In this case, the Euler - Lagrange equations all have the form:

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

Again try: $x_j(t) = Ae^{-i\omega t + iqaj}$

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

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

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

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

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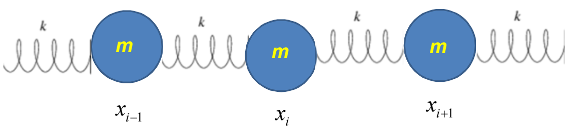
Infinite system of masses and springs -- continued



For periodic boundary conditions:

$$x_0(t) = x_{N+1}(t)$$

For $x_j(t) = Ae^{-i\omega t + iqaj}$ $\Rightarrow Ae^{-i\omega t} = Ae^{-i\omega t + iqa(N+1)}$

$$\Rightarrow qa(N+1) = 2\pi\upsilon \qquad \upsilon = 0,1,2,\cdots$$

$$q = \frac{2\pi\upsilon}{a(N+1)} \quad \text{and} \quad \omega = 2\sqrt{\frac{k}{m}}\sin\left(\frac{qa}{2}\right)$$

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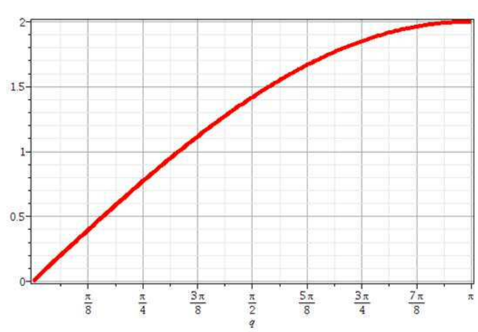

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