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

Plan for Lecture 16:

Continue reading Chapter 4

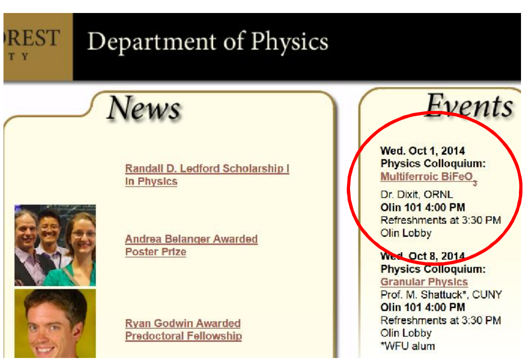
Normal modes for 2 and 3 dimensional systems

1. Finite systems
2. Periodic systems

Course schedule

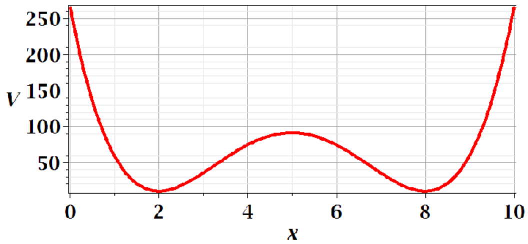
(Preliminary schedule -- subject to frequent adjustment.) rrr>

	Date	F&W Reading	Topic	Assignment
1	Wed, 8/27/2014	Chap. 1	Review of basic principles	#1
2	Fri, 8/29/2014	Chap. 1	Scattering theory	#2
3	Mon, 9/01/2014	Chap. 1	Scattering theory continued	#3
4	Wed, 9/03/2014	Chap. 2	Accelerated coordinate systems	#4
5	Fri, 9/05/2014	Chap. 3	Calculus of variations	#5
6	Mon, 9/08/2014	Chap. 3	Calculus of variations	#6
7	Wed, 9/10/2014	Chap. 3	Hamilton's principle	#7
8	Fri, 9/12/2014	Chap. 3 & 6	Hamilton's principle	#8
9	Mon, 9/15/2014	Chap. 3 & 6	Lagrangians with constraints	#9
10	Wed, 9/17/2014	Chap. 3 & 6	Lagrangians and constants of motion	#10
11	Fri, 9/19/2014	Chap. 3 & 6	Hamiltonian formalism	#11
12	Mon, 9/22/2014	Chap. 3 & 6	Hamiltonian formalism	#11
13	Wed, 9/24/2014	Chap. 3 & 6	Hamiltonian Jacobi transformations	
14	Fri, 9/26/2014	Chap. 4	Small oscillations	Begin Take-Home
15	Mon, 9/29/2014	Chap. 4	Normal modes of motion	Continue Take-Home
16	Wed, 10/01/2014	Chap. 4	Normal modes of motion	Continue Take-Home
17	Fri, 10/03/2014	Chap. 4	Normal modes of motion	Take-Home due

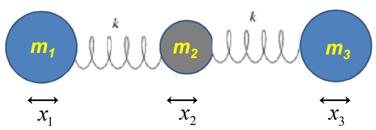


Motivation for studying small oscillations – many interacting systems have stable and meta-stable configurations which are well approximated by:

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



Example – linear molecule

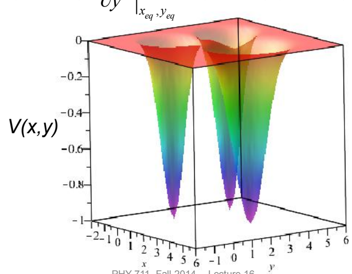


$$L = \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2\dot{x}_2^2 + \frac{1}{2}m_3\dot{x}_3^2 - \frac{1}{2}k\left(x_2 - x_1\right)^2 - \frac{1}{2}k\left(x_3 - x_2\right)^2$$

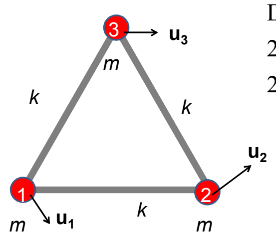
Potential in 2 and more dimensions

$$V(x,y) \approx V(x_{eq}, y_{eq}) + \tfrac{1}{2}\left(x - x_{eq}\right)^2 \left.\frac{\partial^2 V}{\partial x^2}\right|_{x_{eq}, y_{eq}}$$

$$+ \tfrac{1}{2}\left(y - y_{eq}\right)^2 \left.\frac{\partial^2 V}{\partial y^2}\right|_{x_{eq}, y_{eq}} + \left(x - x_{eq}\right)\left(y - y_{eq}\right)\left.\frac{\partial^2 V}{\partial x \partial y}\right|_{x_{eq}, y_{eq}}$$

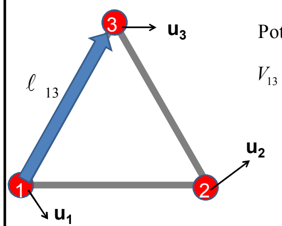


Example – normal modes of a system with the symmetry of an equilateral triangle



Degrees of freedom for 2-dimensional motion:
$2N = 6$

Example – normal modes of a system with the symmetry of an equilateral triangle -- continued



Potential contribution for spring 13:

$$V_{13} = \frac{1}{2}k\left(\left|\ell_{13} + \mathbf{u}_3 - \mathbf{u}_1\right| - \left|\ell_{13}\right|\right)^2$$

$$\approx \frac{1}{2}k\left(\frac{\ell_{13}\cdot(\mathbf{u}_3 - \mathbf{u}_1)}{\left|\ell_{13}\right|}\right)^2$$

$$\approx \frac{1}{2}k\left(\frac{1}{2}(u_{x3} - u_{x1}) + \frac{\sqrt{3}}{2}(u_{y3} - u_{y1})\right)^2$$

Example – normal modes of a system with the symmetry of an equilateral triangle -- continued

Potential contributions: $V = V_{12} + V_{13} + V_{23}$

$$\approx \frac{1}{2}k\left(\frac{\ell_{12}\cdot(\mathbf{u}_2 - \mathbf{u}_1)}{\left|\ell_{12}\right|}\right)^2 + \frac{1}{2}k\left(\frac{\ell_{13}\cdot(\mathbf{u}_3 - \mathbf{u}_1)}{\left|\ell_{13}\right|}\right)^2$$

$$+ \frac{1}{2}k\left(\frac{\ell_{23}\cdot(\mathbf{u}_3 - \mathbf{u}_2)}{\left|\ell_{23}\right|}\right)^2$$

$$\approx \frac{1}{2}k\left(u_{x2} - u_{x1}\right)^2$$

$$+ \frac{1}{2}k\left(\frac{1}{2}(u_{x3} - u_{x1}) + \frac{\sqrt{3}}{2}(u_{y3} - u_{y1})\right)^2$$

$$+ \frac{1}{2}k\left(\frac{1}{2}(u_{x2} - u_{x3}) - \frac{\sqrt{3}}{2}(u_{y2} - u_{y3})\right)^2$$

Example – normal modes of a system with the symmetry of an equilateral triangle -- continued

$$\frac{k}{m}\begin{bmatrix} \frac{5}{4} & -1 & -\frac{1}{4} & \frac{1}{4}\sqrt{3} & 0 & -\frac{1}{4}\sqrt{3} \\ -1 & \frac{5}{4} & -\frac{1}{4} & 0 & -\frac{1}{4}\sqrt{3} & \frac{1}{4}\sqrt{3} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{2} & \frac{1}{4}\sqrt{3} & \frac{1}{4}\sqrt{3} & 0 \\ \frac{1}{4}\sqrt{3} & 0 & -\frac{1}{4}\sqrt{3} & \frac{3}{4} & 0 & -\frac{3}{4} \\ 0 & -\frac{1}{4}\sqrt{3} & \frac{1}{4}\sqrt{3} & 0 & \frac{3}{4} & -\frac{3}{4} \\ \frac{1}{4}\sqrt{3} & \frac{1}{4}\sqrt{3} & 0 & \frac{3}{4} & \frac{3}{4} & \frac{3}{2} \end{bmatrix}\begin{bmatrix} u_{x1} \\ u_{x2} \\ u_{x3} \\ u_{y1} \\ u_{y2} \\ u_{y3} \end{bmatrix} = \omega^2 \begin{bmatrix} u_{x1} \\ u_{x2} \\ u_{x3} \\ u_{y1} \\ u_{y2} \\ u_{y3} \end{bmatrix}$$

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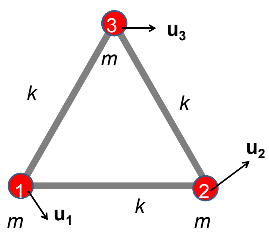
Example – normal modes of a system with the symmetry of an equilateral triangle -- continued



$$\omega^2 = \begin{bmatrix} 3 \\ \frac{3}{2} \\ \frac{3}{2} \\ 0 \\ 0 \\ 0 \end{bmatrix} \frac{k}{m}$$

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3-dimensional periodic lattices

Example – face-centered-cubic unit cell (Al or Ni)

Diagram of atom positions

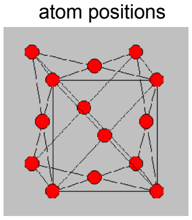
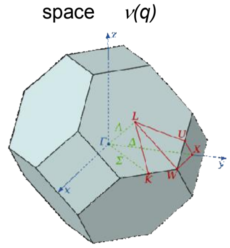


Diagram of q-space $\nu(q)$



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From: PRB **59** 3395 (1999); Mishin et. al. *ν(q)*

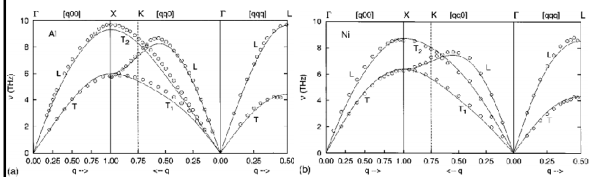
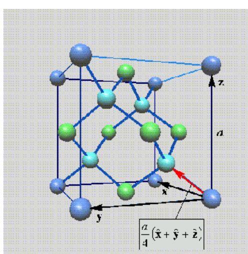


FIG. 2. Comparison of phonon-dispersion curves for Al (a) and Ni (b) predicted by the present EAM potentials, with the experimental values measured by neutron diffraction at 80 K (Al) and 298 K (Ni) (Ref. 33 for Al and Ref. 34 for Ni). The phonon frequencies at point *X* were included in the fitting database with low weight.

Lattice vibrations for 3-dimensional lattice

Example: diamond lattice



Ref: http://phycomp.technion.ac.il/~nika/diamond_structure.html

Atoms located at the positions:

$$\mathbf{R}^a = \mathbf{R}_0{}^a + \mathbf{u}^a$$

Potential energy function near equilibriu:

$$U\left(\left\{\mathbf{R}^a\right\}\right) \approx U\left(\left\{\mathbf{R}_0{}^a\right\}\right) + \frac{1}{2}\sum_{a,b}\left(\mathbf{R}^a - \mathbf{R}_0{}^a\right)\cdot \left.\frac{\partial^2 U}{\partial \mathbf{R}^a \partial \mathbf{R}^b}\right|_{\left\{\mathbf{R}_0{}^a\right\}} \cdot \left(\mathbf{R}^b - \mathbf{R}_0{}^b\right)$$

Define:

$$D_{jk}^{ab} \equiv \left.\frac{\partial^2 U}{\partial \mathbf{R}_j{}^a \partial \mathbf{R}_k{}^b}\right|_{\left\{\mathbf{R}_0{}^a\right\}}$$

so that

$$U\left(\left\{\mathbf{R}^a\right\}\right) \approx U_0 + \frac{1}{2}\sum_{a,b,j,k} u_j^a D_{jk}^{ab} u_k^b$$

$$L\left(\left\{u_j^a, \dot{u}_j^a\right\}\right) = \frac{1}{2}\sum_{a,j} m_a \left(\dot{u}_j^a\right)^2 - U_0 - \frac{1}{2}\sum_{a,b,j,k} u_j^a D_{jk}^{ab} u_k^b$$

$$L(\{u_j^a, \dot{u}_j^a\}) = \frac{1}{2}\sum_{a,j} m_a (\dot{u}_j^a)^2 - U_0 - \frac{1}{2}\sum_{a,b,j,k} u_j^a D_{jk}^{ab} u_k^b$$

Equations of motion:

$$m_a \ddot{u}_j^a = -\sum_{b,k} D_{jk}^{ab} u_k^b$$

Solution form:

$$u_j^a(t) = \frac{1}{\sqrt{m_a}} A_j^a e^{-i\omega t + i\mathbf{q}\cdot\mathbf{R}_0^a}$$

Details: $\mathbf{R}_0^a = \boldsymbol{\tau}^a + \mathbf{T}$ where $\boldsymbol{\tau}^a$ denotes unique sites and $\mathbf{T}$ denotes replicas

Define:

$$W_{jk}^{ab}(\mathbf{q}) = \sum_{\mathbf{T}} \frac{D_{jk}^{ab} e^{i\mathbf{q}\cdot(\boldsymbol{\tau}^a - \boldsymbol{\tau}^b)}}{\sqrt{m_a m_b}} e^{i\mathbf{q}\cdot\mathbf{T}}$$

Eigenvalue equations:

$$\omega^2 A_j^a = \sum_{b,k} W(\mathbf{q})_{jk}^{ab} A_k^b$$

In this equation the summation is only over unique atomic sites.

$\Rightarrow$ Find "dispersion curves" $\omega(\mathbf{q})$

B. P. Pandy and B. Dayal, J. Phys. C. Solid State Phys. **6** 2943 (1973)

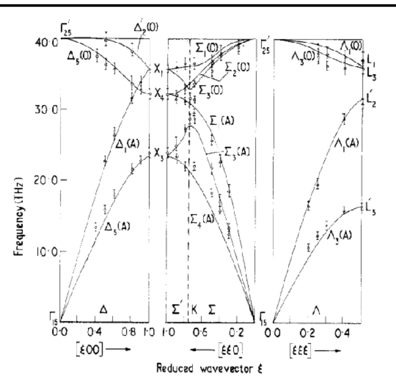


Figure 2. Phonon dispersion curves of diamond. Experimental points *et al* (1965, 1967). △ and ○ represent the longitudinal and transverse m