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

Plan for Lecture 17:

Continue reading Chapter 4

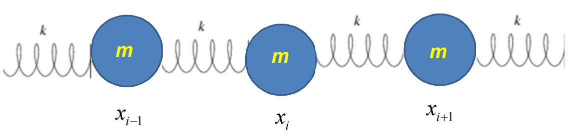
1. **Normal modes for extended one-dimensional systems**
2. **Normal modes for 2 and 3 dimensional systems**

Course schedule

(Preliminary schedule -- subject to frequent adjustment)

	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

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 :

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

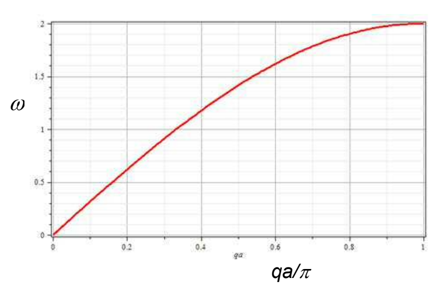
Again try : $x_j(t) = Ae^{-i\omega t + iqaj}$

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

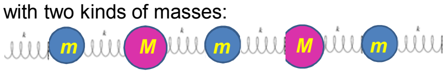
$$-\omega^2 = \frac{k}{m}\left(2\cos(qa) - 2\right)$$

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

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



Consider an infinite system of masses and springs now with two kinds of masses:



x_i y_i x_{i+1} y_{i+1} x_{i+2}

Note : each mass coordinate is measured relative to its equilibrium position $x_i^0, y_i^0, \cdots$

$$L = T - V$$

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

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

Euler - Lagrange equations :

$$m\ddot{x}_j = k\left(y_{j-1} - 2x_j + y_j\right)$$
$$M\ddot{y}_j = k\left(x_j - 2y_j + x_{j+1}\right)$$

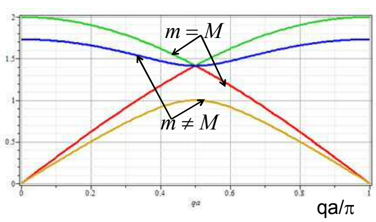
Trial solution :

$$x_j(t) = A e^{-i\omega t + i2qaj}$$
$$y_j(t) = B e^{-i\omega t + i2qaj}$$
$$\begin{pmatrix} m\omega^2 - 2k & k\left(e^{-i2qa} + 1\right) \\ k\left(e^{i2qa} + 1\right) & M\omega^2 - 2k \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = 0$$

$$\begin{pmatrix} m\omega^2 - 2k & k\left(e^{-i2qa} + 1\right) \\ k\left(e^{i2qa} + 1\right) & M\omega^2 - 2k \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = 0$$

Solutions :

$$\omega_{\pm}^2 = \frac{k}{m} + \frac{k}{M} \pm k\sqrt{\frac{1}{m^2} + \frac{1}{M^2} + \frac{2\cos(2qa)}{mM}}$$



Eigenvectors:

For $qa = 0$:

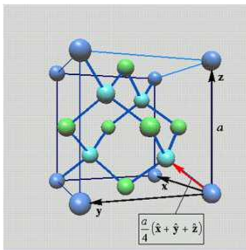
$$\omega_- = 0 \qquad \omega_+ = \sqrt{\frac{2k}{m} + \frac{2k}{M}}$$
$$\begin{pmatrix} A \\ B \end{pmatrix}_- = N\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \begin{pmatrix} A \\ B \end{pmatrix}_+ = N\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

For $qa = \frac{\pi}{2}$:

$$\omega_- = \sqrt{\frac{2k}{M}} \qquad \omega_+ = \sqrt{\frac{2k}{m}}$$
$$\begin{pmatrix} A \\ B \end{pmatrix}_- = N\begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \begin{pmatrix} A \\ B \end{pmatrix}_+ = N\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

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:

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

Define:

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

so that

$$U(\{\mathbf{R}^a\}) \approx U_0 + \frac{1}{2}\sum_{a,b,j,k} u^a_j D^{ab}_{jk} u^b_k$$

$$L(\{u^a_j, \dot{u}^a_j\}) = \frac{1}{2}\sum_{a,j} m_a(\dot{u}^a_j)^2 - U_0 - \frac{1}{2}\sum_{a,b,j,k} u^a_j D^{ab}_{jk} u^b_k$$

$$L(\{u^a_j, \dot{u}^a_j\}) = \frac{1}{2}\sum_{a,j} m_a(\dot{u}^a_j)^2 - U_0 - \frac{1}{2}\sum_{a,b,j,k} u^a_j D^{ab}_{jk} u^b_k$$

Equations of motion:

$$m_a \ddot{u}^a_j = -\sum_{b,k} D^{ab}_{jk} u^b_k$$

Solution form:

$$u^a_j(t) = \frac{1}{\sqrt{m_a}} A^a_j e^{-i\omega t + i\mathbf{q}\cdot\mathbf{R}^a_0}$$

Details: $\mathbf{R}^a_0 = \boldsymbol{\tau}^a + \mathbf{T}$ 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)

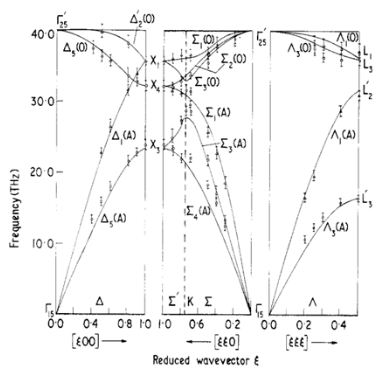
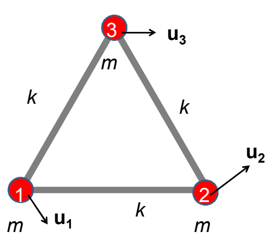


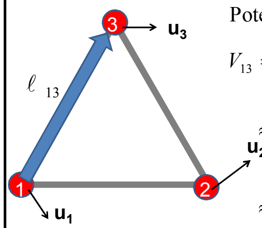
Figure 2. Phonon dispersion curves of diamond. Experimental points et al (1965, 1967). △ and ○ represent the longitudinal and transverse m

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 :

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

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

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

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

Potential contributions :

$$V = V_{12} + V_{13} + V_{23}$$

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

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

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

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

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

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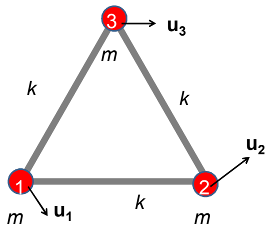
Example – normal modes of a system with the symmetry of an equilateral triangle -- continued



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