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

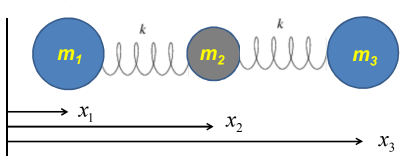
Plan for Lecture 15:

Continue reading Chapter 4

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

3	Mon, 8/31/2015	Chap. 1	Scattering theory continued	#3
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. 4	Normal modes of motion	
17	Fri, 10/02/2015	Chap. 4	Normal modes of 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	

Example – linear molecule



$$L = \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2\dot{x}_2^2 + \frac{1}{2}m_3\dot{x}_3^2$$
$$-\frac{1}{2}k\left(x_2 - x_1 - \ell_{12}\right)^2 - \frac{1}{2}k\left(x_3 - x_2 - \ell_{23}\right)^2$$

Let: $x_1 \rightarrow x_1 - x_1^0 \quad x_2 \rightarrow x_2 - x_1^0 - \ell_{12} \quad x_3 \rightarrow x_3 - x_1^0 - \ell_{12} - \ell_{23}$

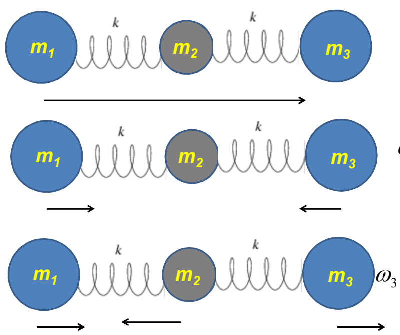
$$L = \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2\dot{x}_2^2 + \frac{1}{2}m_3\dot{x}_3^2 - \frac{1}{2}k\left(x_2 - x_1\right)^2 - \frac{1}{2}k\left(x_3 - x_2\right)^2$$

Coupled equations of motion :

$$m_1\ddot{x}_1 = k\left(x_2 - x_1\right)$$
$$m_2\ddot{x}_2 = -k\left(x_2 - x_1\right) + k\left(x_3 - x_2\right) = k\left(x_1 - 2x_2 + x_3\right)$$
$$m_3\ddot{x}_3 = -k\left(x_3 - x_2\right)$$

Let $x_i(t) = X_i^\alpha e^{-i\omega_\alpha t}$

$$-\omega_\alpha^2 m_1 X_1^\alpha = k\left(X_2^\alpha - X_1^\alpha\right)$$
$$-\omega_\alpha^2 m_2 X_2^\alpha = k\left(X_1^\alpha - 2X_2^\alpha + X_3^\alpha\right)$$
$$-\omega_\alpha^2 m_3 X_3^\alpha = -k\left(X_3^\alpha - X_2^\alpha\right)$$

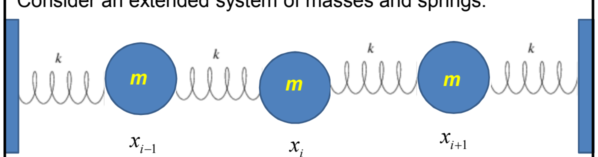


$$\omega_1 = 0$$

$$\omega_2 = \sqrt{\frac{k}{m_O}}$$

$$\omega_3 = \sqrt{\frac{k}{m_O} + \frac{2k}{m_C}}$$

Consider an extended system of masses and springs:



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

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

Note : In fact, we have N masses; x_0 and x_{N+1} will be treated using boundary conditions.

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

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

From Euler - Lagrange equations :

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

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

....

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

....

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

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

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

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 :

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

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

$$\Rightarrow B = -A$$

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

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

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

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

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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

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

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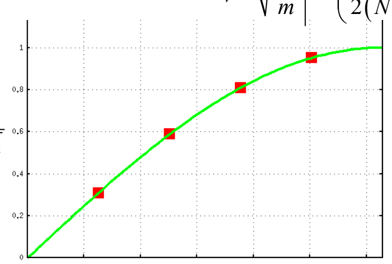
Example for *N=4*: $\omega_\nu = \sqrt{\frac{4k}{m}}\left|\sin\left(\frac{\nu\pi}{2(N+1)}\right)\right|$

$\frac{\omega_\nu}{\sqrt{4k/m}}$



qa

Note that solution form remains correct for *N*→∞

$$\omega(qa) = \sqrt{4k/m}\left|\sin(qa)\right|$$

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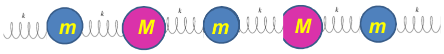
Consider an infinite system of masses and springs now with two kinds of masses:



$x_i \quad y_i \quad x_{i+1} \quad y_{i+1} \quad x_{i+2}$

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

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

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

Euler - Lagrange equations :

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

Trial solution :

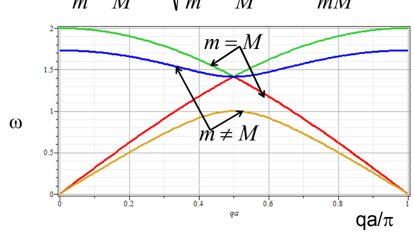
$$x_j(t) = Ae^{-i\omega t + i2qaj}$$
$$y_j(t) = Be^{-i\omega t + i2qaj}$$

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

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

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

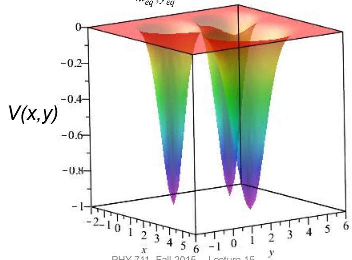
$$\omega_- = \sqrt{\frac{2k}{M}} \qquad \omega_+ = \sqrt{\frac{2k}{m}}$$

$$\begin{pmatrix} A \\ B \end{pmatrix}_- = N \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \begin{pmatrix} A \\ B \end{pmatrix}_+ = N \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

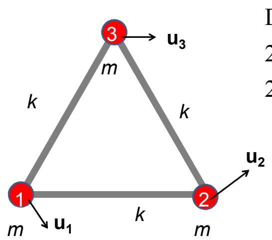
Potential in 2 and more dimensions

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

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

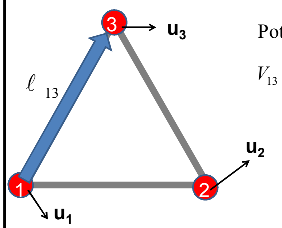


Example – normal modes of a system with the symmetry of an equilateral triangle



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

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



$$\boldsymbol{\ell}_{13} = |\boldsymbol{\ell}_{13}|\left(\frac{1}{2}\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}\hat{\mathbf{y}}\right)$$

Potential contribution for spring 13:

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

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

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

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

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

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

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

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

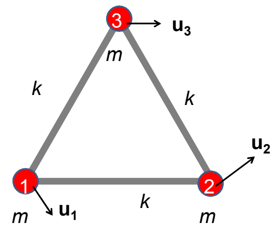
$$+\frac{1}{2}k\left(\frac{1}{2}(u_{x3} - u_{x1}) + \frac{\sqrt{3}}{2}(u_{y3} - u_{y1})\right)^2$$

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

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

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

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



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

3-dimensional periodic lattices

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

Diagram of atom positions

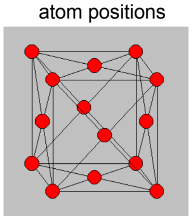
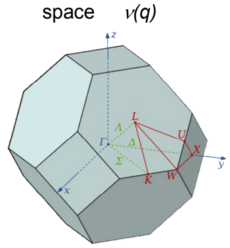


Diagram of q-space $\nu(q)$



From: PRB **59** 3395 (1999); Mishin et. al. $\nu(q)$

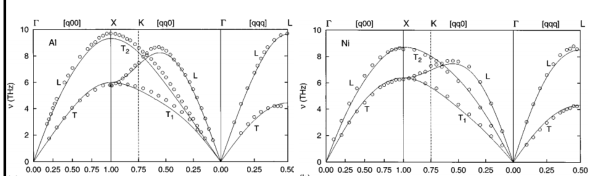
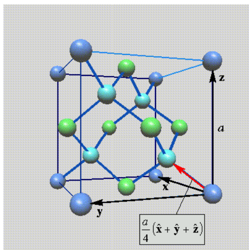


FIG. 2. Comparison of phonon-dispersion curves for Al (a) and Ni (b) predicted by the present EAM potentials, with the experimental values measured by neutron diffraction at 80 K (Al) and 298 K (Ni) (Ref. 33 for Al and Ref. 34 for Ni). The phonon frequencies at point *X* were included in the fitting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

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

Define:

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

so that

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

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

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

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)

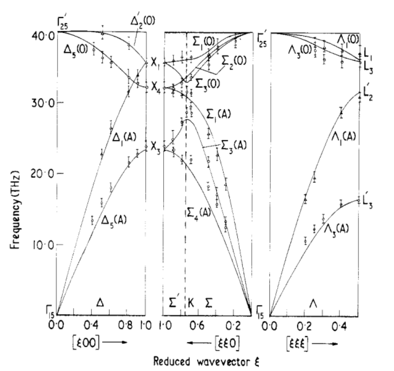


Figure 2. Phonon dispersion curves of diamond. Experimental points *et al* (1965, 1967). △ and ○ represent the longitudinal and transverse m