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

Plan for Lecture 17:

Continue reading Chapter 4

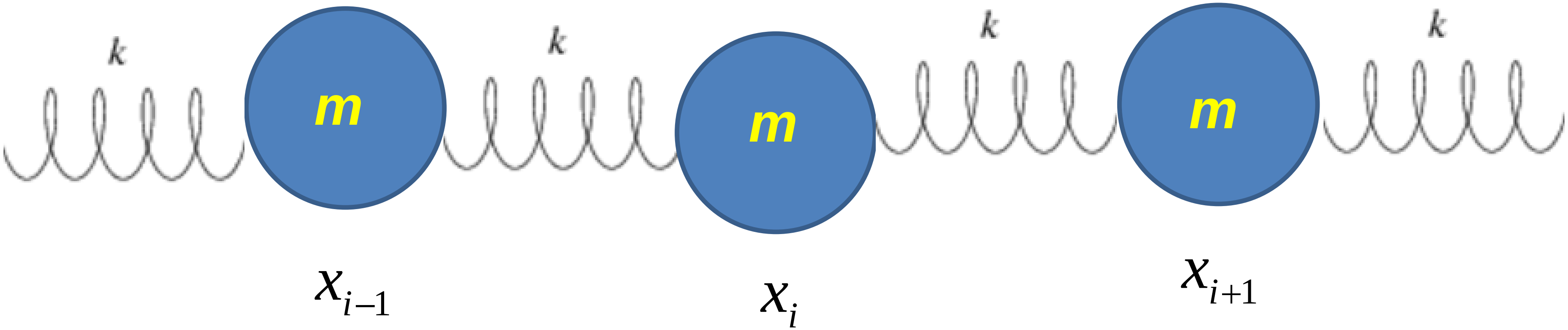
1. **Normal modes for extended one-dimensional systems**
2. **Normal modes for 2 and 3 dimensional systems**

Course schedule

(Preliminary schedule -- subject to frequent adjustment.)

	Date	F&W Reading	Topic	Assignment
1	Wed, 8/29/2012	Chap. 1	Review of basic principles;Scattering theory	#1
2	Fri, 8/31/2012	Chap. 1	Scattering theory continued	#2
3	Mon, 9/03/2012	Chap. 1	Scattering theory continued	#3
4	Wed, 9/05/2012	Chap. 1 & 2	Scattering theory/Accelerated coordinate frame	#4
5	Fri, 9/07/2012	Chap. 2	Accelerated coordinate frame	#5
6	Mon, 9/10/2012	Chap. 3	Calculus of Variation	#6
7	Wed, 9/12/2012	Chap. 3	Calculus of Variation continued	
8	Fri, 9/14/2012	Chap. 3	Lagrangian	#7
9	Mon, 9/17/2012	Chap. 3 & 6	Lagrangian	#8
10	Wed, 9/19/2012	Chap. 3 & 6	Lagrangian	#9
11	Fri, 9/21/2012	Chap. 3 & 6	Lagrangian	#10
12	Mon, 9/24/2012	Chap. 3 & 6	Lagrangian and Hamiltonian	#11
13	Wed, 9/26/2012	Chap. 6	Lagrangian and Hamiltonian	#12
14	Fri, 9/28/2012	Chap. 6	Lagrangian and Hamiltonian	#13
15	Mon, 10/01/2012	Chap. 4	Small oscillations	#14
16	Wed, 10/03/2012	Chap. 4	Small oscillations	#15
17	Fri, 10/05/2012	Chap. 4	Small oscillations	
18	Mon, 10/08/2012	Chap. 7	Wave equation	Take Home Exam
19	Wed, 10/10/2012	Chap. 7	Wave equation	Take Home Exam
20	Fri, 10/12/2012	Chap. 7	Wave equation	Take Home Exam
21	Mon, 10/15/2012	Chap. 7	Wave equation	Exam due

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:

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

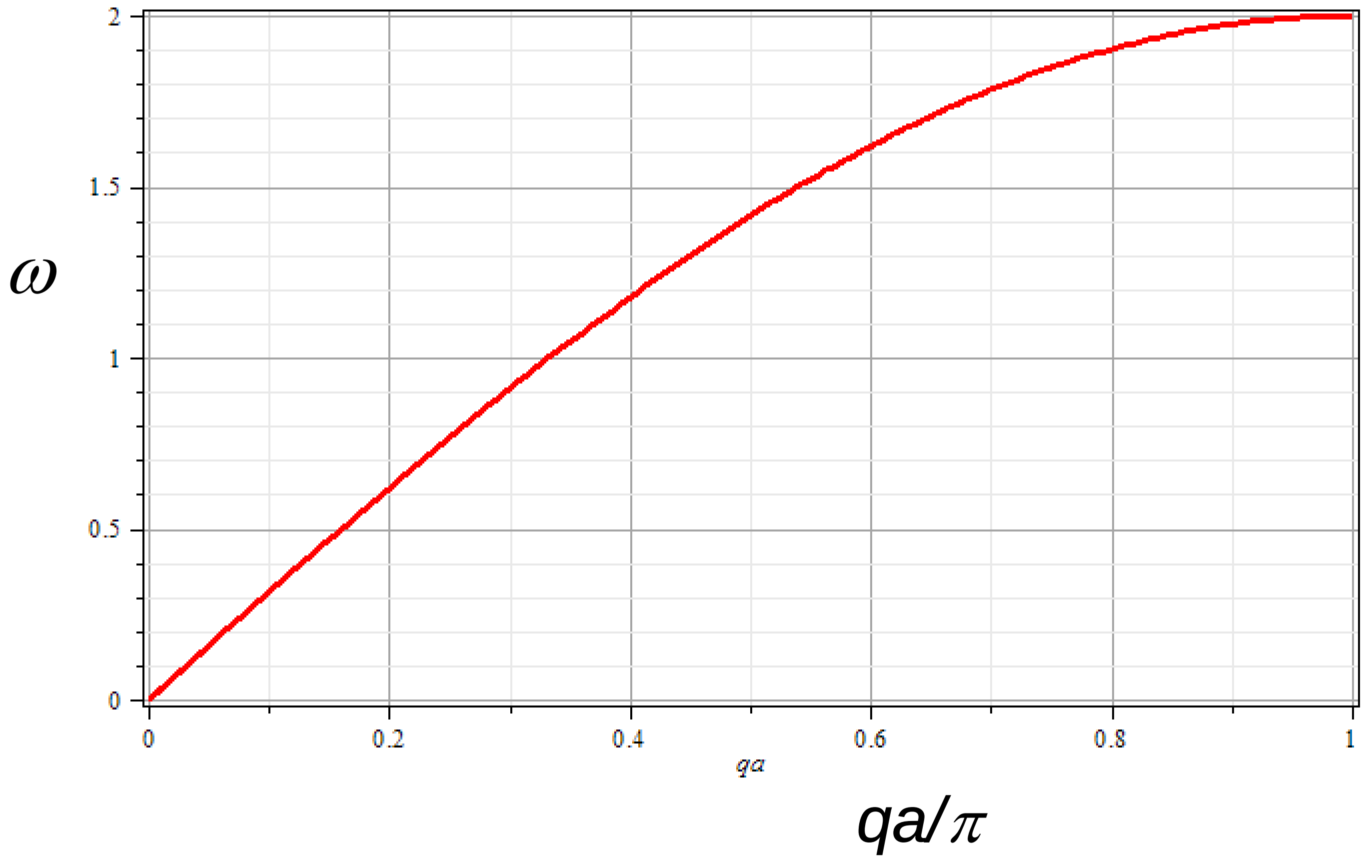
Again try: $x_j(t) = Ae^{-i\omega t + iqaj}$

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

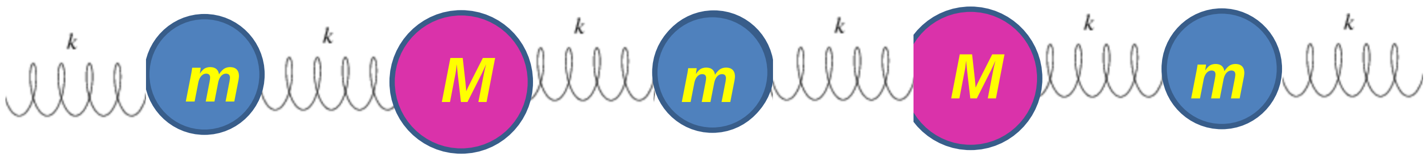
$$-\omega^2 = \frac{k}{m}\left(2\cos(qa) - 2\right)$$

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

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


2
1.5
1
0.5
0
0.2
0.4
0.6
0.8
qa
ω
qa/π

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



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

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 :

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

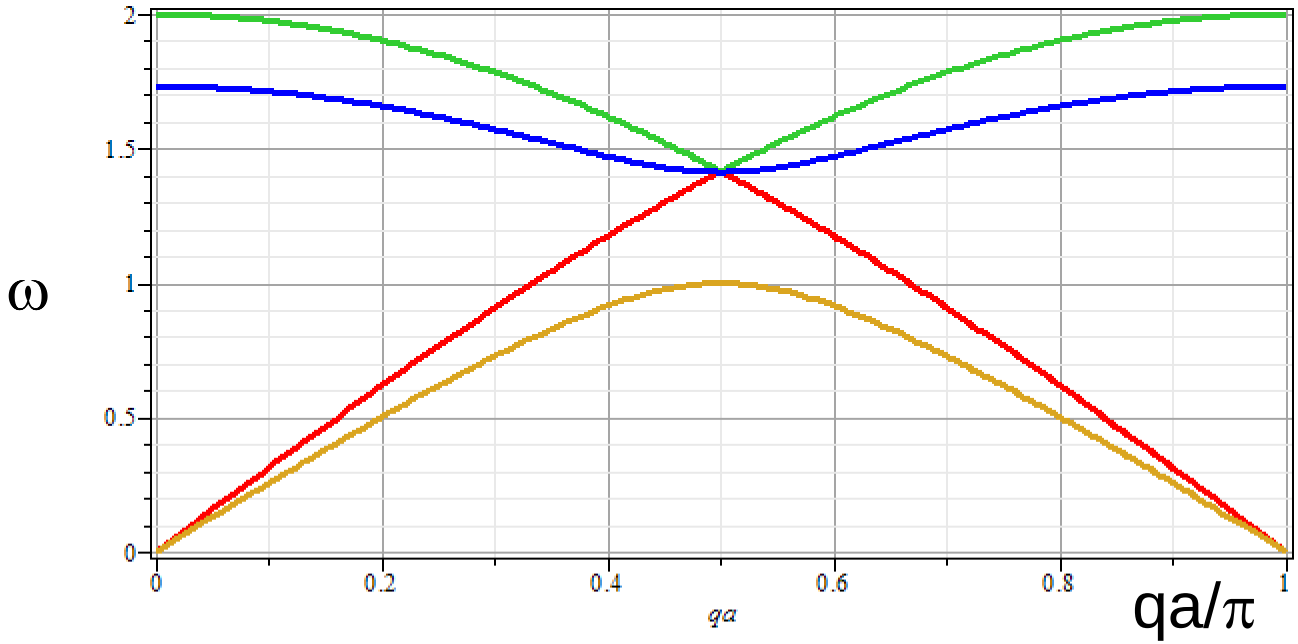
$$y_j(t) = Be^{-i\omega t + i2qaj}$$

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

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

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 $qa = 0$:

$$\omega_- = 0 \qquad \omega_+ = \sqrt{\frac{2k}{m} + \frac{2k}{M}}$$

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

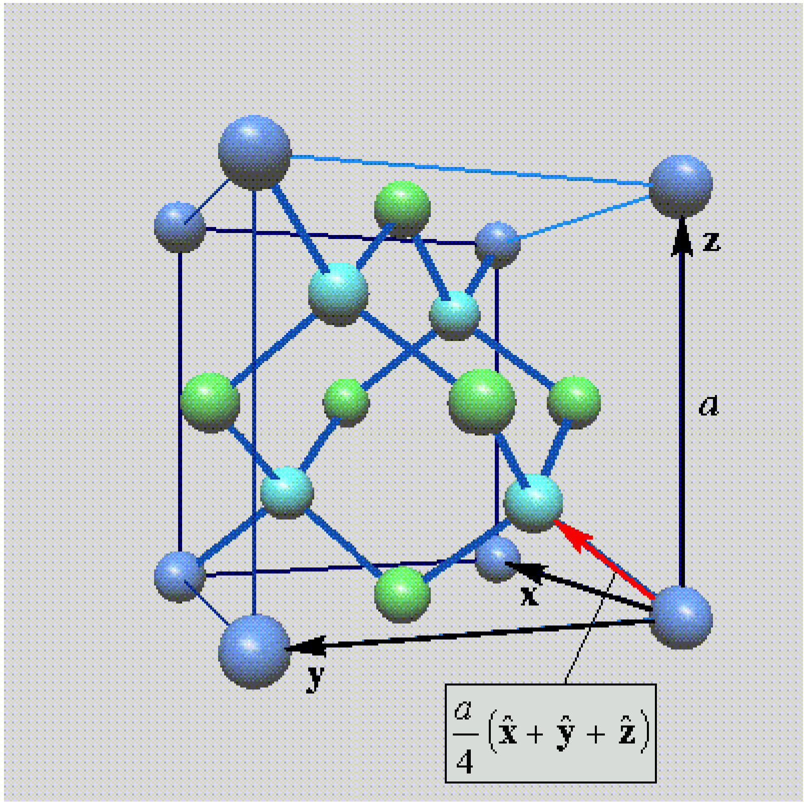
For $qa = \frac{\pi}{2}$:

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

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

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 :

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

so that

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

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

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

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:

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

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)

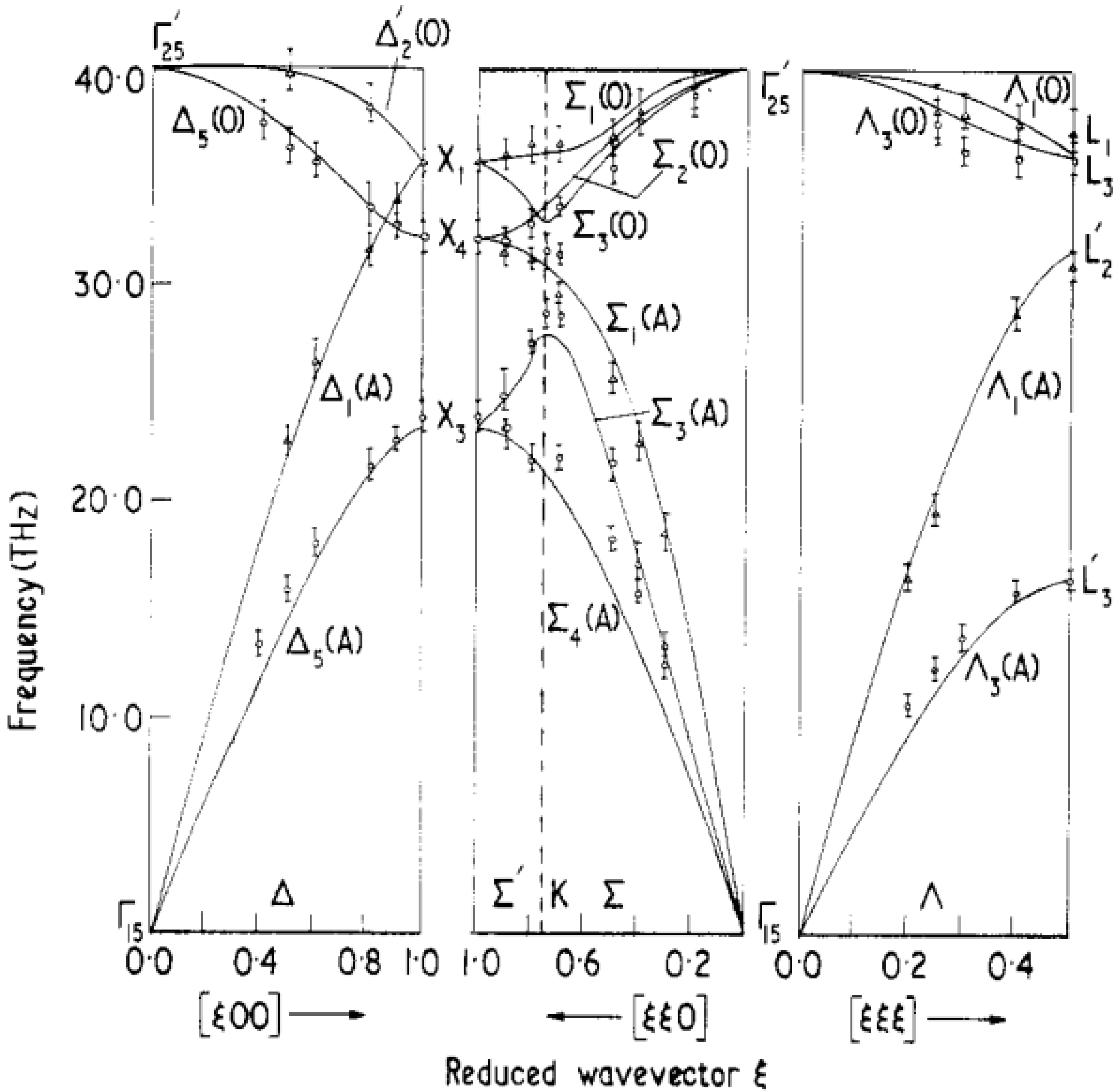


Figure 2. Phonon dispersion curves of diamond. Experimental points *et al* (1965, 1967). △ and ○ represent the longitudinal and transverse m