PHY 711 Classical Mechanics and Mathematical Methods
10-10:50 AM MWF online or (occasionally) in Olin 103

Discussion for Lecture 17: Chap. 4 (F&W)

Normal Mode Analysis

1. Short digression on singular value decomposition
2. Normal modes for extended one-dimensional systems (correcting some errors in previous slides)
3. Normal modes for 2 and 3 dimensional systems

The updated Spring 2021 undergraduate calendar is available here [PDF]. Key points include:

- Undergraduate move in will run from Jan. 23-26.
- Undergraduate classes will start Jan. 27.
- We will forgo spring break to help preserve the health of our community but will add two weekdays off during the semester.
- Exams that follow the undergraduate schedule will run from May 8-15.
- Move out will conclude May 16.
- Commencement for the Class of 2021 will be held May 17 (pending future public health guidance).
- Commencement for the Class of 2020 will be held May 22 (pending future public health guidance).

Course schedule

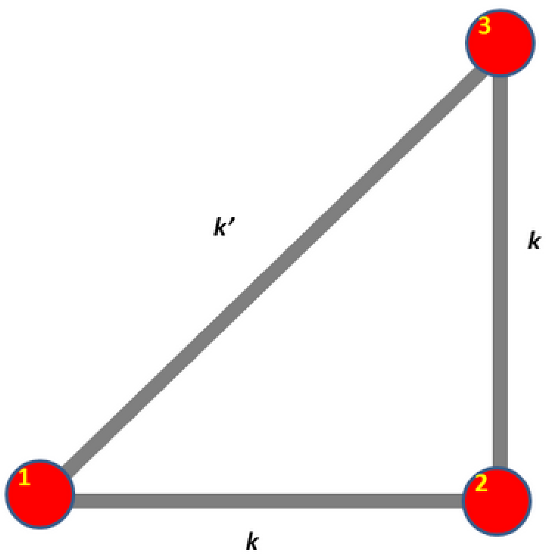
(Preliminary schedule -- subject to frequent adjustment.)

	Date	F&W Reading	Topic	Assignment	Due
1	Wed, 8/26/2020	Chap. 1	Introduction	#1	8/31/2020
2	Fri, 8/28/2020	Chap. 1	Scattering theory	#2	9/02/2020
3	Mon, 8/31/2020	Chap. 1	Scattering theory	#3	9/04/2020
4	Wed, 9/02/2020	Chap. 1	Scattering theory		
5	Fri, 9/04/2020	Chap. 1	Scattering theory	#4	9/09/2020
6	Mon, 9/07/2020	Chap. 2	Non-inertial coordinate systems		
7	Wed, 9/09/2020	Chap. 3	Calculus of Variation	#5	9/11/2020
8	Fri, 9/11/2020	Chap. 3	Calculus of Variation	#6	9/14/2020
9	Mon, 9/14/2020	Chap. 3 & 6	Lagrangian Mechanics	#7	9/18/2020
10	Wed, 9/16/2020	Chap. 3 & 6	Lagrangian & constraints	#8	9/21/2020
11	Fri, 9/18/2020	Chap. 3 & 6	Constants of the motion		
12	Mon, 9/21/2020	Chap. 3 & 6	Hamiltonian equations of motion	#9	9/23/2020
13	Wed, 9/23/2020	Chap. 3 & 6	Liouville theorm	#10	9/25/2020
14	Fri, 9/25/2020	Chap. 3 & 6	Canonical transformations		
15	Mon, 9/28/2020	Chap. 4	Small oscillations about equilibrium	#11	10/02/2020
16	Wed, 9/30/2020	Chap. 4	Normal modes of vibration	#12	10/05/2020
17	Fri, 10/02/2020	Chap. 4	Normal modes of vibration		

PHY 711 -- Assignment #12

Sept. 30, 2020

Finish reading Chapter 4 in **Fetter & Walecka**.



1. Consider the system of 3 masses (m_1=m_2=m_3=m) shown attached by elastic forces in the right triangular configuration (with angles 45, 90, 45 deg) shown above with spring constants k and k'. Find the normal modes of small oscillations for this system. For numerical evaluation, you may assume that k=k'.

Schedule for weekly one-on-one meetings

Nick – 11 AM Monday (ED/ST)
Tim – 9 AM Tuesday
Bamidele – 7 PM Tuesday
Zhi– 9 PM Tuesday
Jeanette – 11 AM Wednesday
Derek – 12 PM Friday

Your questions –
From Tim

1. Do the number of spring constants k, determine the number of normal modes of a system?
2. What is the meaning of q-space?

From Nick

1. Why can we reduce the infinite problem to 2D? Are we suggesting, since we're alternating between m and M, that the motion for any two consecutive sets of m and M is the same?
2. I think the Taylor expansion in 2-D makes sense with that cross term but what does it look like in 3-D?

Additional digression on matrix properties

Singular value decomposition

It is possible to factor any real matrix $\mathbf{A}$ into unitary matrices $\mathbf{V}$ and $\mathbf{U}$ together with positive diagonal matrix $\mathbf{\Sigma}$:

$$\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^{\mathbf{H}}$$

Note that $\mathbf{U}^H\mathbf{U} = \mathbf{I} = \mathbf{V}^H\mathbf{V}$

$$\mathbf{\Sigma} = \begin{pmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \sigma_N \end{pmatrix}$$

Singular value decomposition -- continued

Consider using SVD to solve a singular linear algebra problem $\mathbf{AX} = \mathbf{B}$

$$\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^H$$

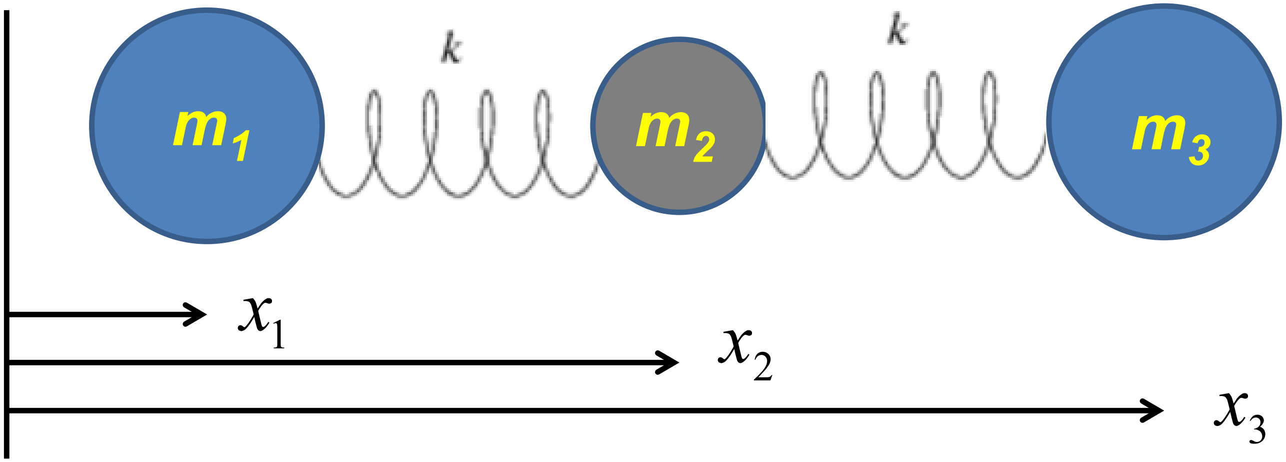
$$\mathbf{X} = \sum_{i \text{ for } \sigma_i > \varepsilon} \mathbf{v}_i \frac{\left\langle \mathbf{u}_i^H \mid \mathbf{B} \right\rangle}{\sigma_i}$$

Details are complicated ….

Your question -- what's all the fuss about singular values? What's their importance relative to eigenvalues?

Comment – I would like to see a bigger fuss. SVD is different from eigenvalue analysis and more broadly applicable. At a minimum SVD analysis identifies mathematically poorly posed problems and offers a “fix”.

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

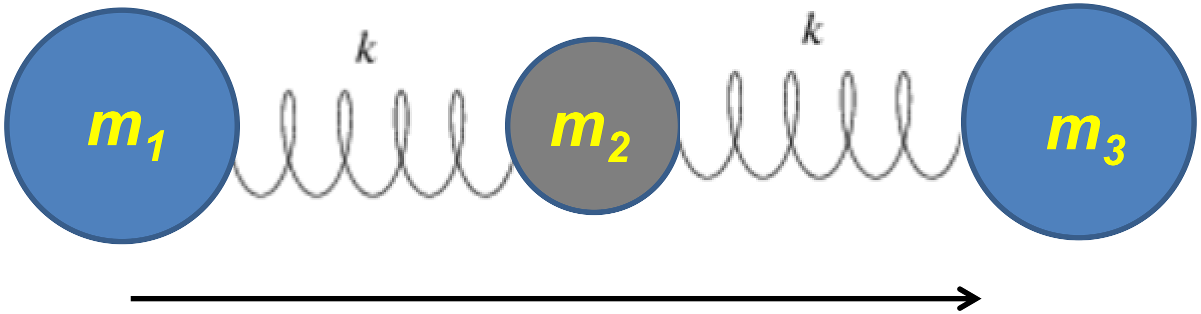
$$-\omega_\alpha^2 m_1 X_1^\alpha = k\left(X_2^\alpha - X_1^\alpha\right)$$

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

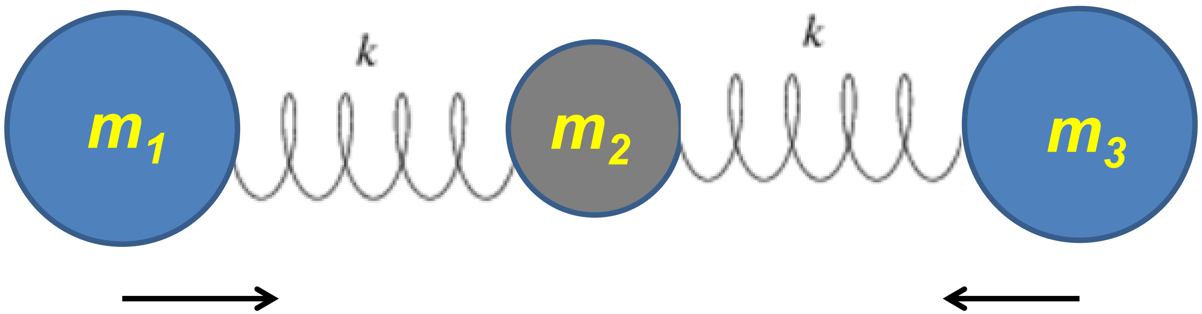
$$-\omega_\alpha^2 m_3 X_3^\alpha = -k\left(X_3^\alpha - X_2^\alpha\right)$$

For $m_1 = m_3 \equiv m_O$

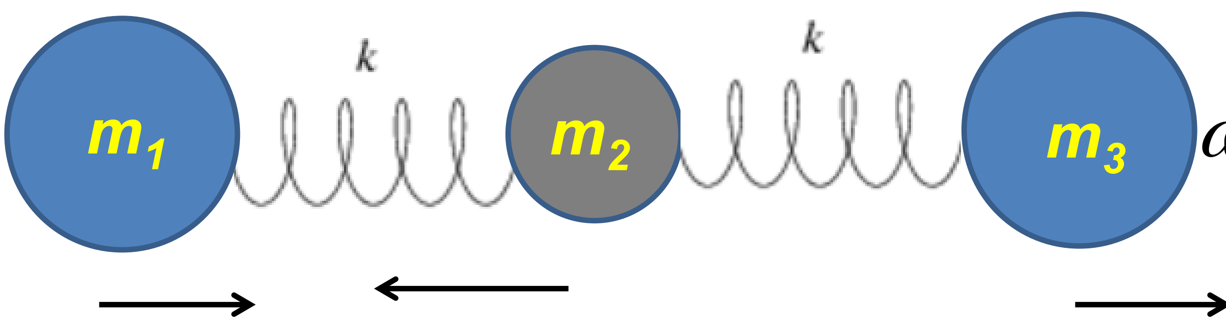
and $m_2 \equiv m_C$



$$\omega_1 = 0$$

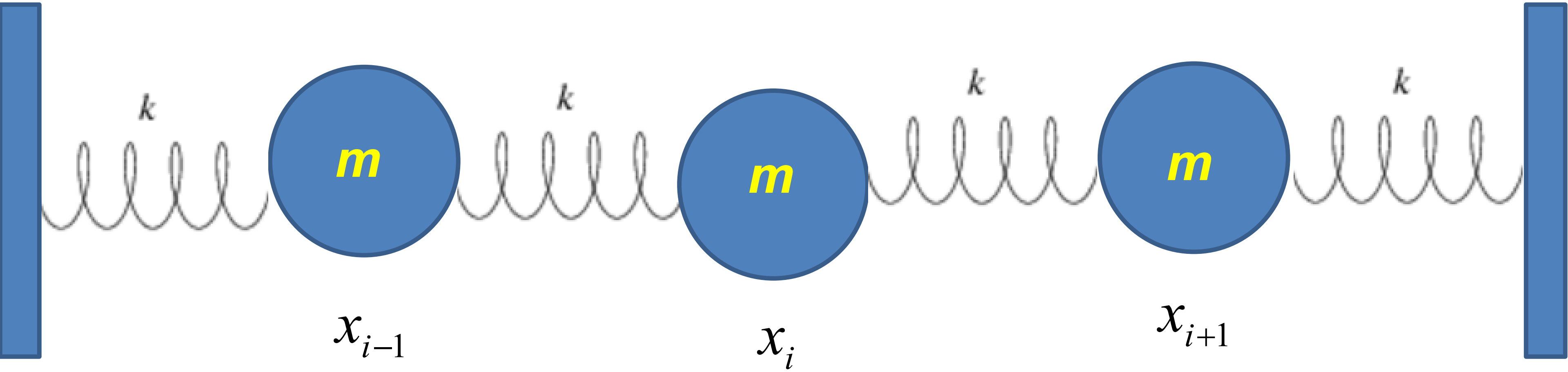


$$\omega_2 = \sqrt{\frac{k}{m_O}}$$



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

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.

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

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

From Euler - Lagrange equations :

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

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

$$\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots$$

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

$$\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots$$

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

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

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

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

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

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

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

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:

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

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

$$\Rightarrow B = \text{-}A$$

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

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

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

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

Recap -- solution for integer parameter ν

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

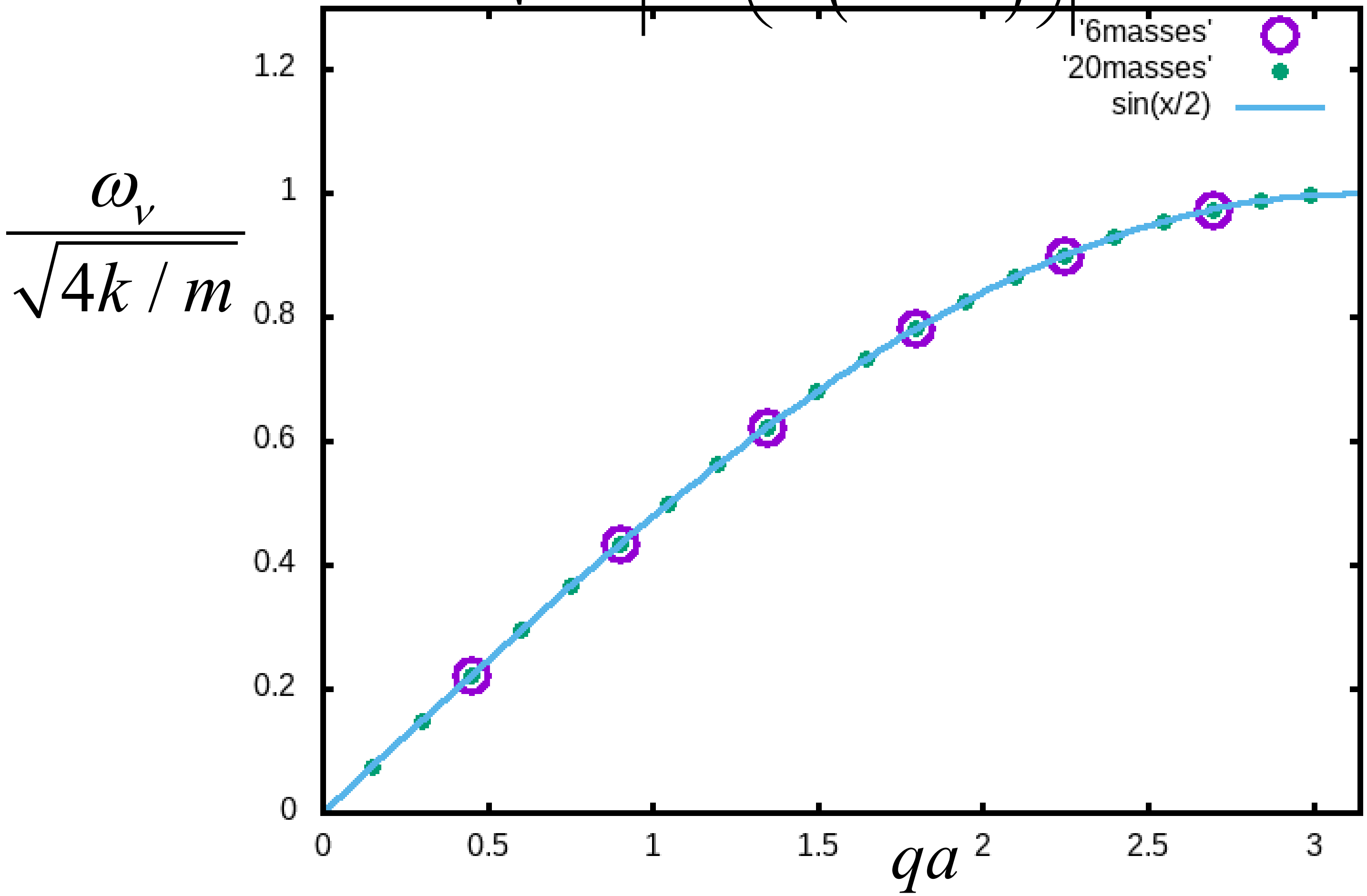
$$\omega_\nu^{\ 2} = \frac{4k}{m} \sin^2\left(\frac{\nu\pi}{2(N+1)} \right)$$

Note that non-trivial, unique values are

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

Examples

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



Note that solution form remains correct for $N \to \infty$

$$\omega(qa) = \sqrt{4k/m} \left| \sin\left(\frac{qa}{2} \right) \right|$$

Your question -- What is the meaning of q-space?

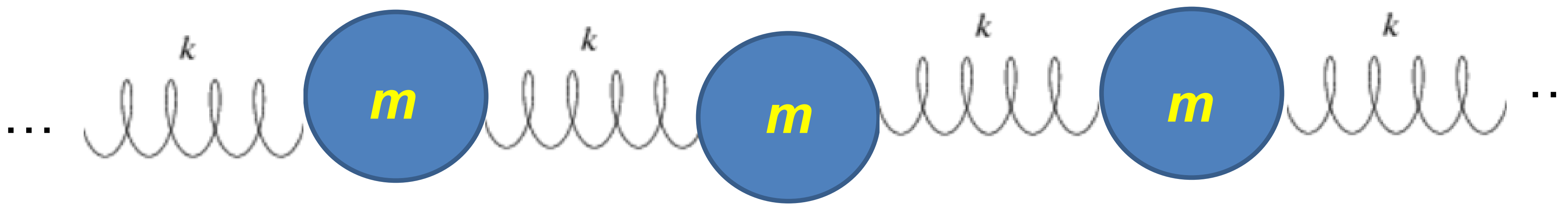
Comment – We have seen that for N masses, there are N "normal" modes. So if we imagine that N grows to infinity we should have an infinite number of modes. The parameter q allows us to "count" the infinite number of modes in a convenient way.

From previous slide – $\omega(qa) = \sqrt{4k/m}\left|\sin(qa)\right|$ remains consistent as $N \rightarrow \infty$

Your question -- Do the number of spring constants k, determine the number of normal modes of a system?

Comment – While the spring constants certainly affect the normal modes, the number of modes is typically *dN*, where d is the dimension and N is the number of masses.

For extended chain without boundaries:



$$x_{i-1} \qquad x_i \qquad x_{i+1}$$

From Euler-Lagrange equations:

$$m\ddot{x}_j = k\left(x_{j+1} - 2x_j + x_{j-1}\right) \qquad \text{for all } x_j$$

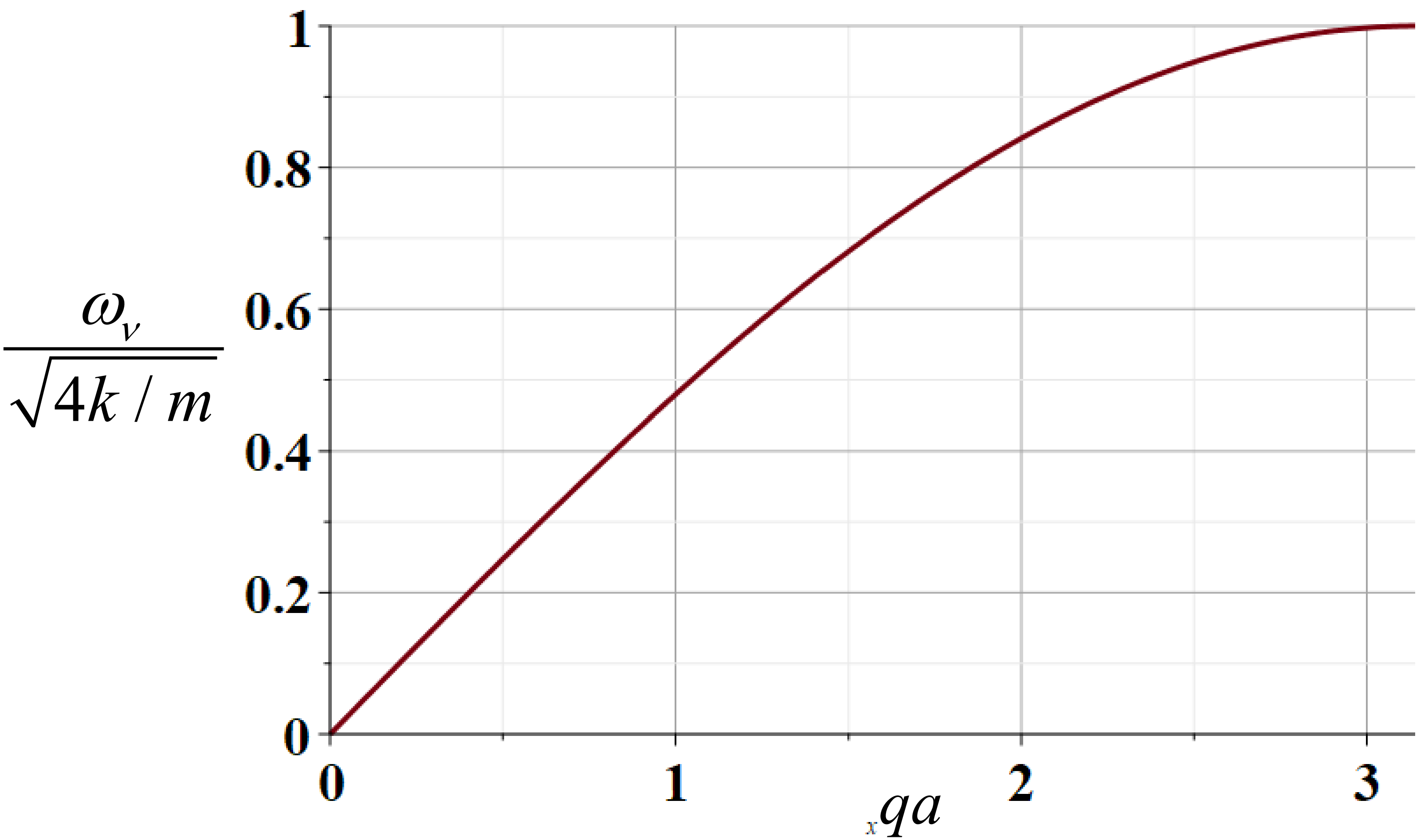
Try: $x_j(t) = Ae^{-i\omega t + iqaj}$

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

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

$$\Rightarrow \omega^2 = \frac{4k}{m}\sin^2\left(\frac{qa}{2}\right) \qquad \text{distinct values for } 0 \le qa \le \pi$$

Note that we are assuming that all masses and springs are identical here.



1
0.8
0.6
0.4
0.2
0
0
1
2
3
$\frac{\omega_\nu}{\sqrt{4k/m}}$
$_x qa$

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 $x_i^0, y_i^0, \cdots$

$$L = T - V$$

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

Because the masses are different, we cannot yet know how their displacements might be related.

$$L = T - V$$

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

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:

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

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

Note that 2qa is an unknown parameter.

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

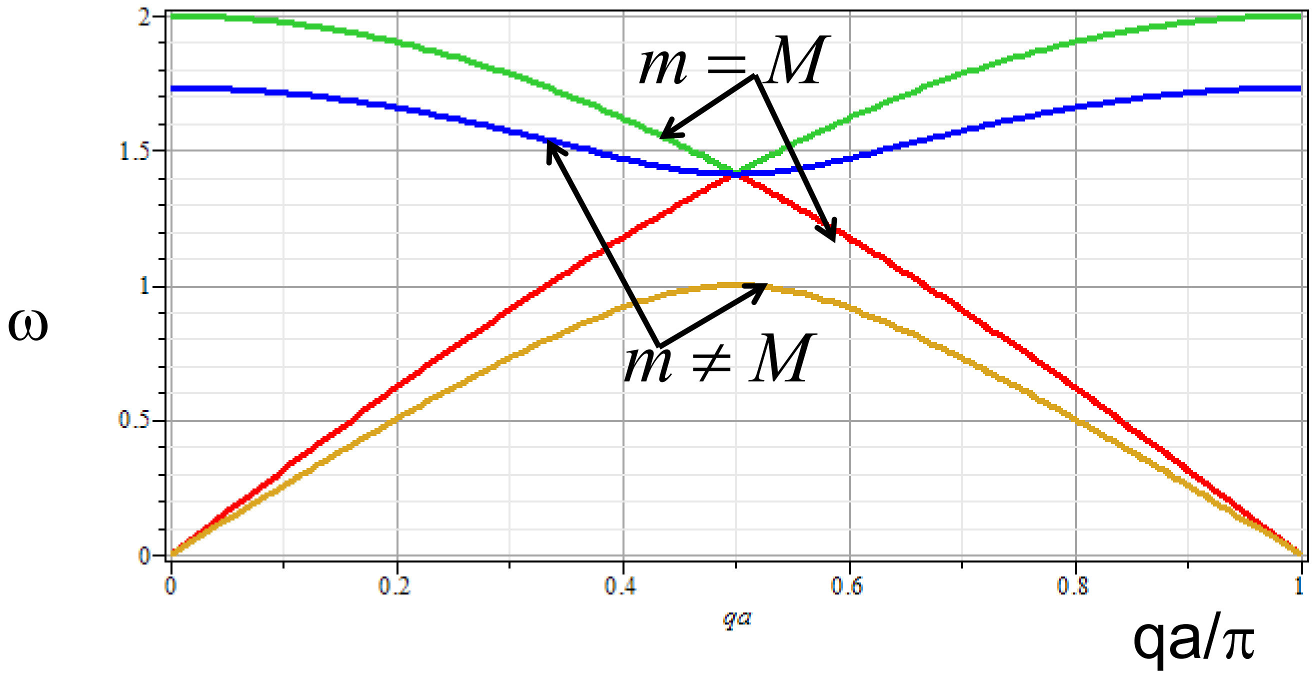
$$\begin{pmatrix} m\omega^2 - 2k & k\left(e^{-i2qa}+1\right) \\ k\left(e^{i2qa}+1\right) & M\omega^2 - 2k \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = 0$$

Solutions:

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

Note that for m=M, we obtain the same normal modes as before. Is this reassuring?

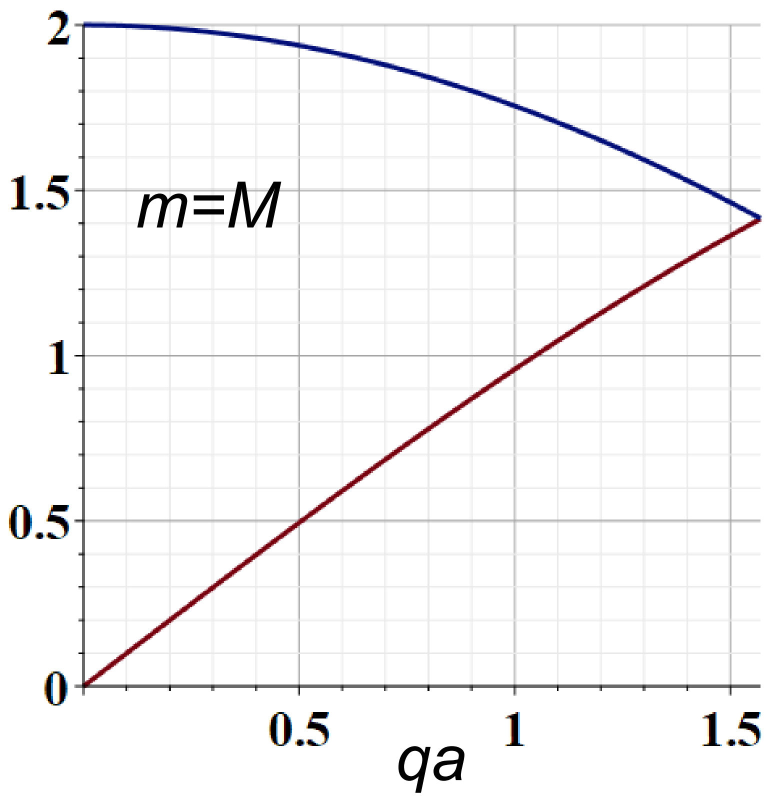
a. No
b. Yes

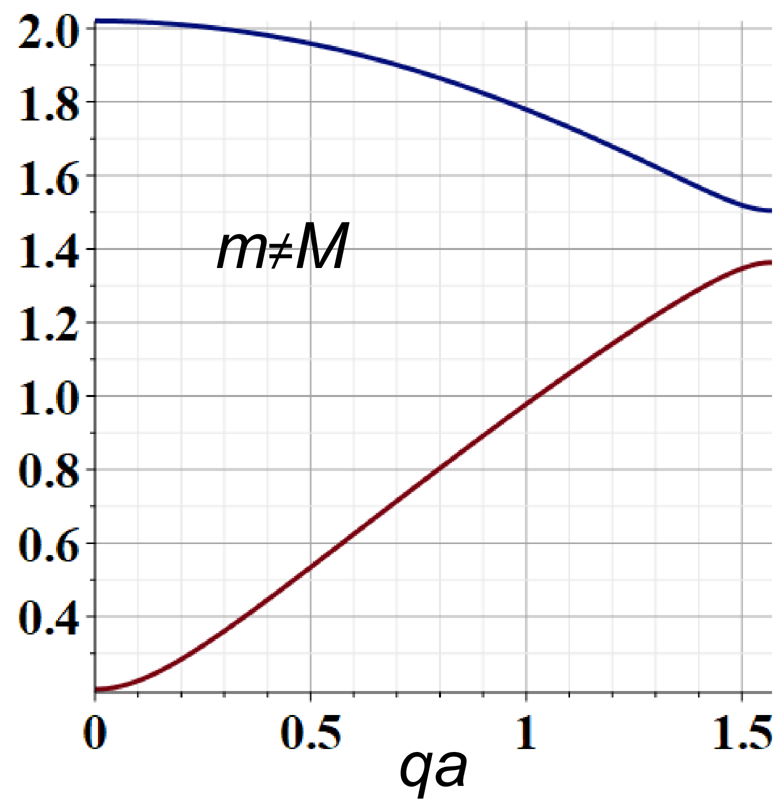


Normal mode frequencies:

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

Note that for every *qa*, there are 2 modes.





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

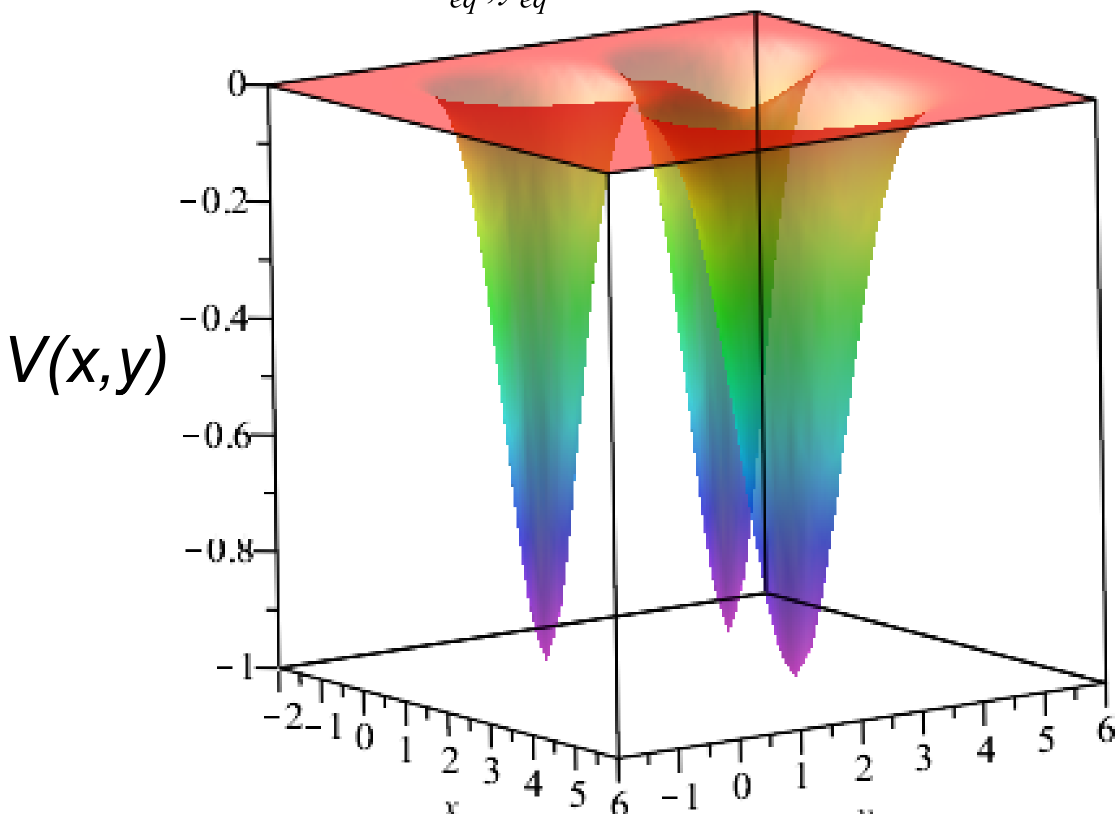
$$\omega_- = \sqrt{\frac{2k}{M}} \qquad \omega_+ = \sqrt{\frac{2k}{m}}$$

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

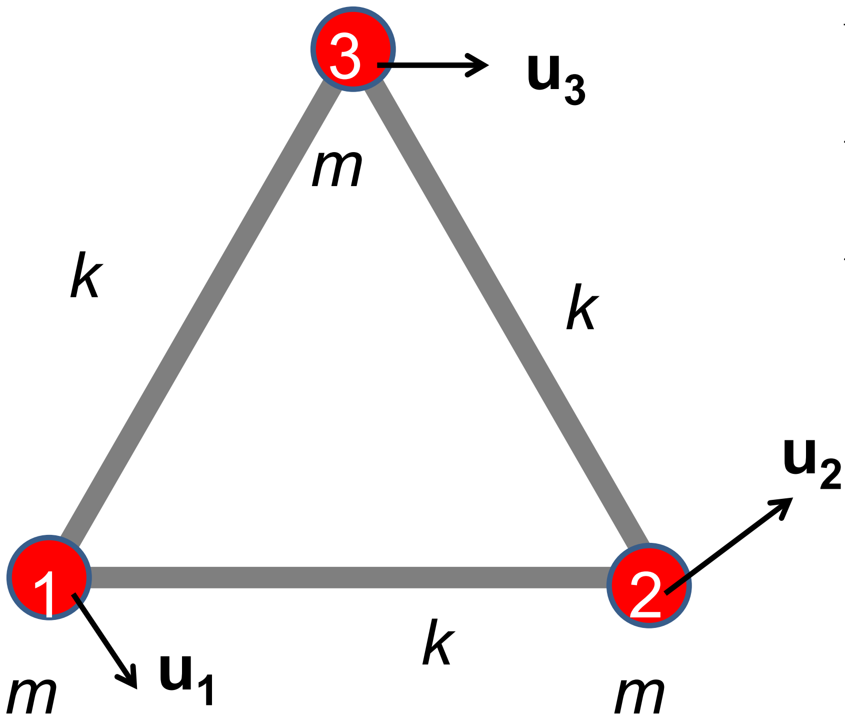
Potential in 2 and more dimensions

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

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



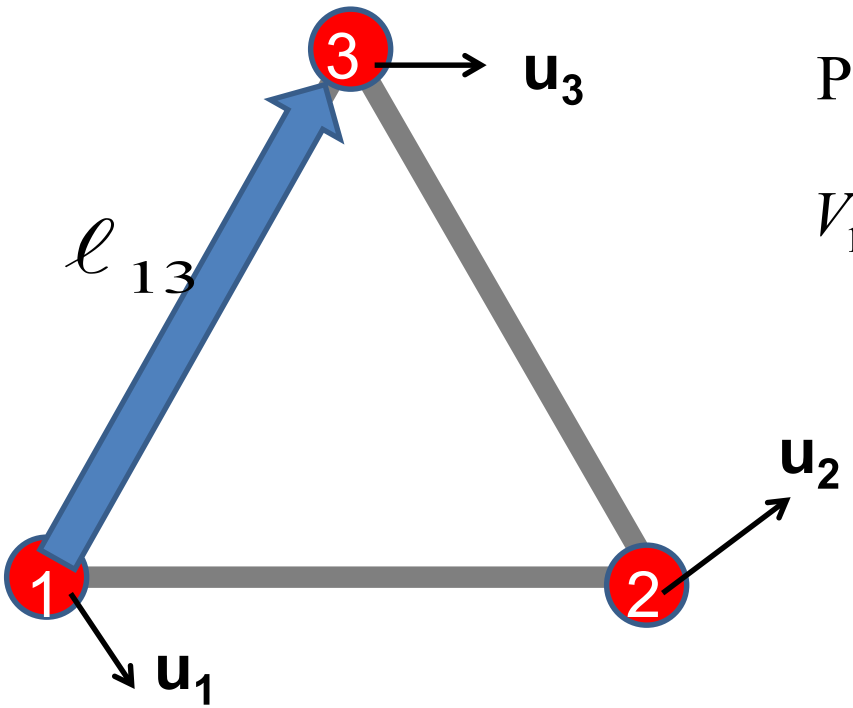
Example – normal modes of a system with the symmetry of an equilateral triangle



Degrees of freedom for 2-dimensional motion:

$$2N = 6$$

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



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

Potential contribution for spring 13:

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

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

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

Some details for spring 13:

$$\left(\left|\boldsymbol{\ell}_{13}+\mathbf{u}_3-\mathbf{u}_1\right|-\left|\boldsymbol{\ell}_{13}\right|\right)^2 \equiv \left(\left(\boldsymbol{\ell}_{13}+\mathbf{u}_{13}\right)^{1/2}-\left|\boldsymbol{\ell}_{13}\right|\right)^2$$

$$\left(\boldsymbol{\ell}_{13}+\mathbf{u}_{13}\right)^{1/2}=\left|\boldsymbol{\ell}_{13}\right|\left(1+\frac{2\boldsymbol{\ell}_{13}\cdot\mathbf{u}_{13}}{\left|\boldsymbol{\ell}_{13}\right|^2}+\frac{\left|\mathbf{u}_{13}\right|^2}{\left|\boldsymbol{\ell}_{13}\right|^2}\right)^{1/2}$$

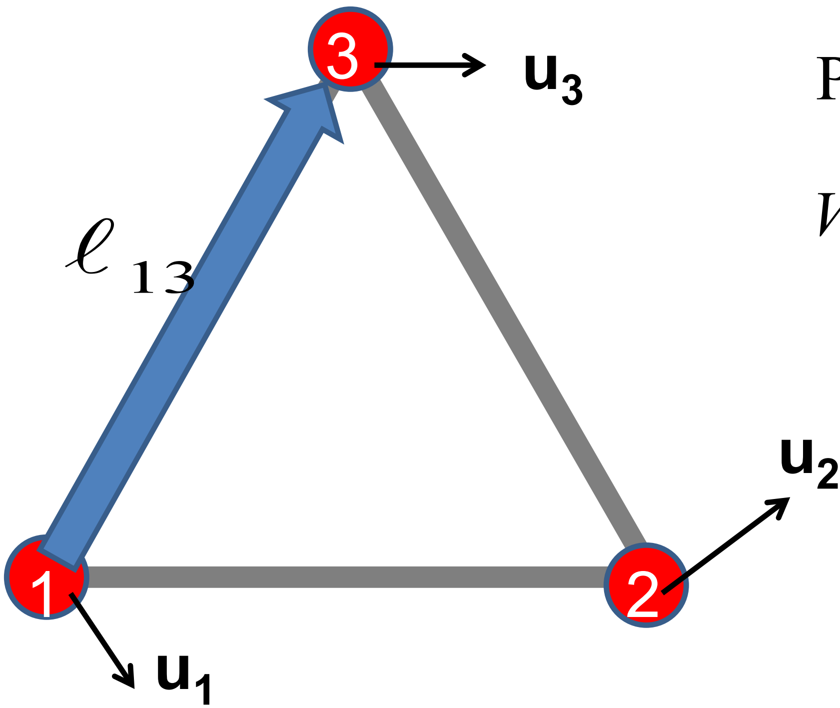
Assume $\left|\mathbf{u}_{13}\right| \ll \left|\boldsymbol{\ell}_{13}\right|$

$$\approx\left|\boldsymbol{\ell}_{13}\right|\left(1+\frac{\boldsymbol{\ell}_{13}\cdot\mathbf{u}_{13}}{\left|\boldsymbol{\ell}_{13}\right|^2}\right)=\left|\boldsymbol{\ell}_{13}\right|+\frac{\boldsymbol{\ell}_{13}\cdot\mathbf{u}_{13}}{\left|\boldsymbol{\ell}_{13}\right|}$$

$$\Rightarrow\left(\left(\boldsymbol{\ell}_{13}+\mathbf{u}_{13}\right)^{1/2}-\left|\boldsymbol{\ell}_{13}\right|\right)^2=\left(\frac{\boldsymbol{\ell}_{13}\cdot\mathbf{u}_{13}}{\left|\boldsymbol{\ell}_{13}\right|}\right)^2$$

Note that this analysis of the leading term is true in 1, 2, and 3 dimensions.

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

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

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

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

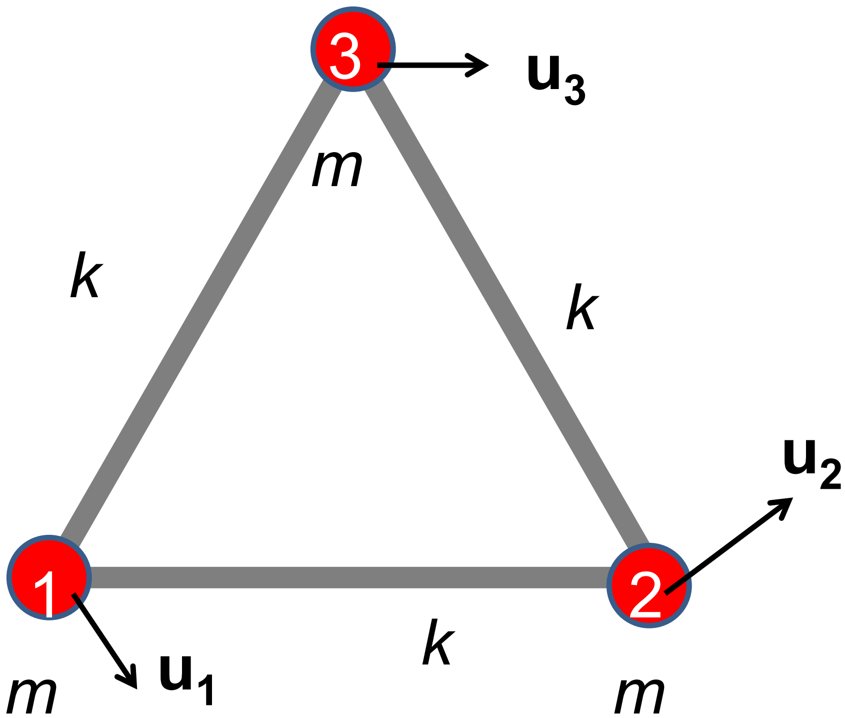
$$+\frac{1}{2}k\left(\frac{1}{2}(u_{x3}-u_{x1})+\frac{\sqrt{3}}{2}(u_{y3}-u_{y1})\right)^2$$

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

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

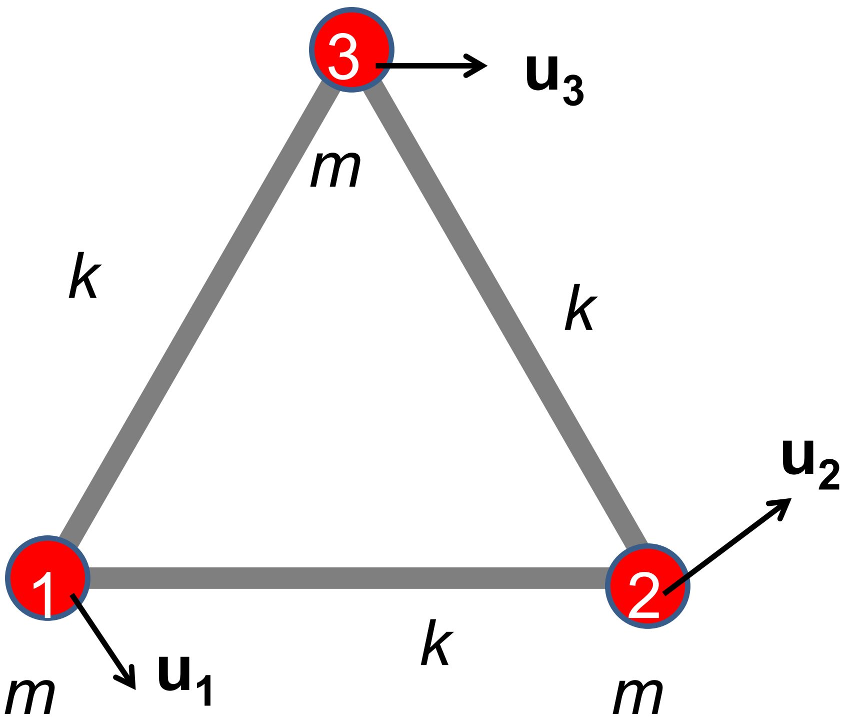
$$\frac{k}{m}\begin{bmatrix} \frac{5}{4} & -1 & -\frac{1}{4} & \frac{1}{4}\sqrt{3} & 0 & -\frac{1}{4}\sqrt{3} \\ -1 & \frac{5}{4} & -\frac{1}{4} & 0 & -\frac{1}{4}\sqrt{3} & \frac{1}{4}\sqrt{3} \\ -\frac{1}{4} & -\frac{1}{4} & \frac{1}{2} & -\frac{1}{4}\sqrt{3} & \frac{1}{4}\sqrt{3} & 0 \\ \frac{1}{4}\sqrt{3}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

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



With help from Maple

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



What can you say about the 3 zero frequency modes?

3-dimensional periodic lattices

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

Diagram of atom positions

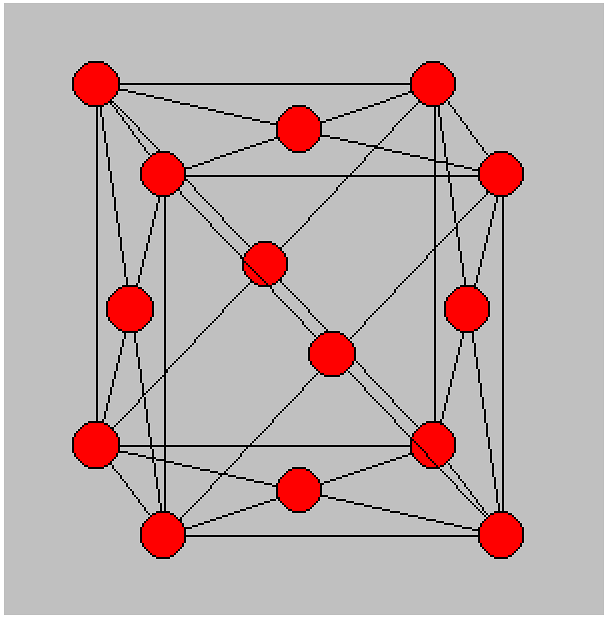
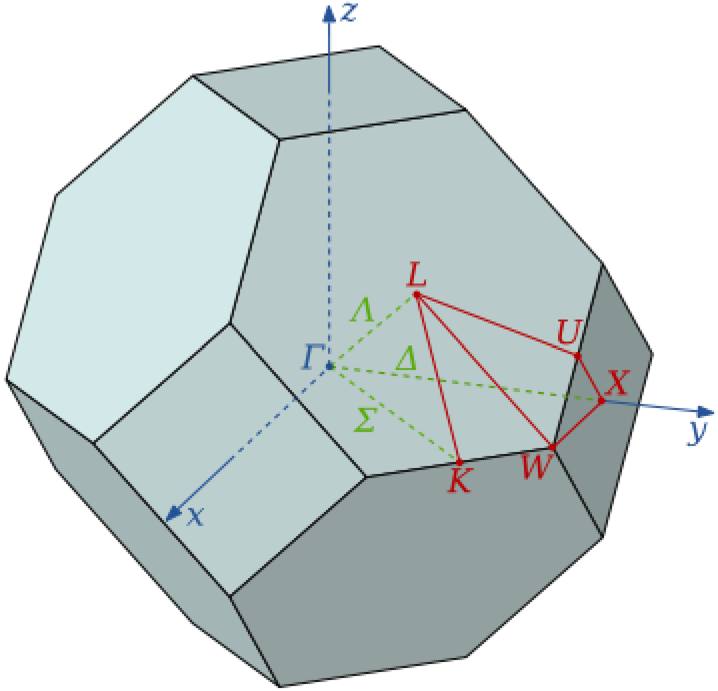


Diagram of q-space $\nu(q)$



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

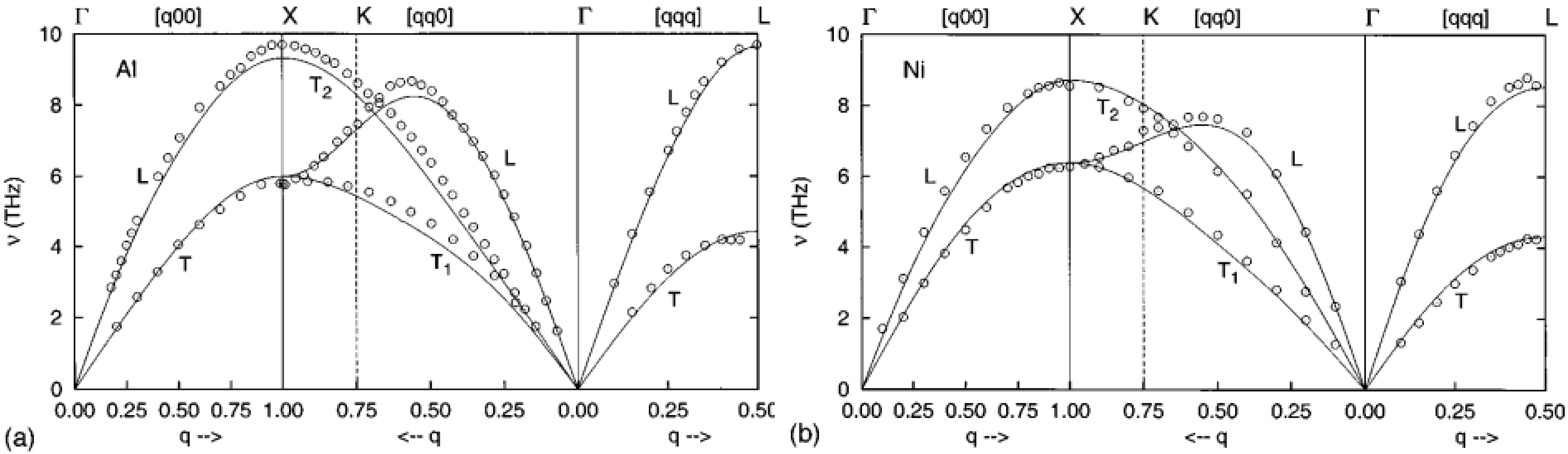
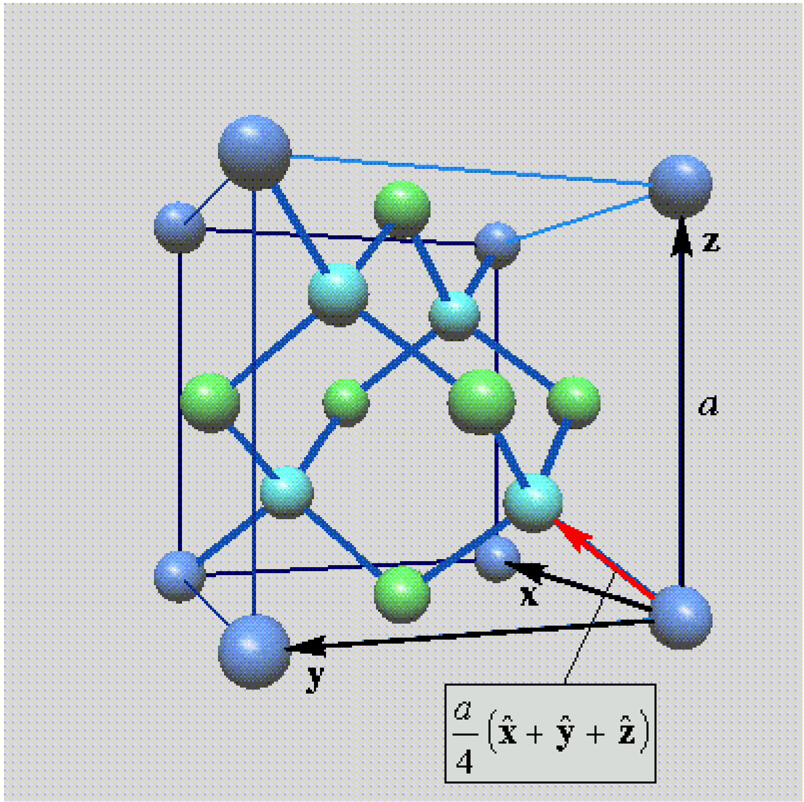


FIG. 2. Comparison of phonon-dispersion curves for Al (a) and Ni (b) predicted by the present EAM potentials, with the experimental values measured by neutron diffraction at 80 K (Al) and 298 K (Ni) (Ref. 33 for Al and Ref. 34 for Ni). The phonon frequencies at point *X* were included in the fitting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

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

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

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

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

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

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)

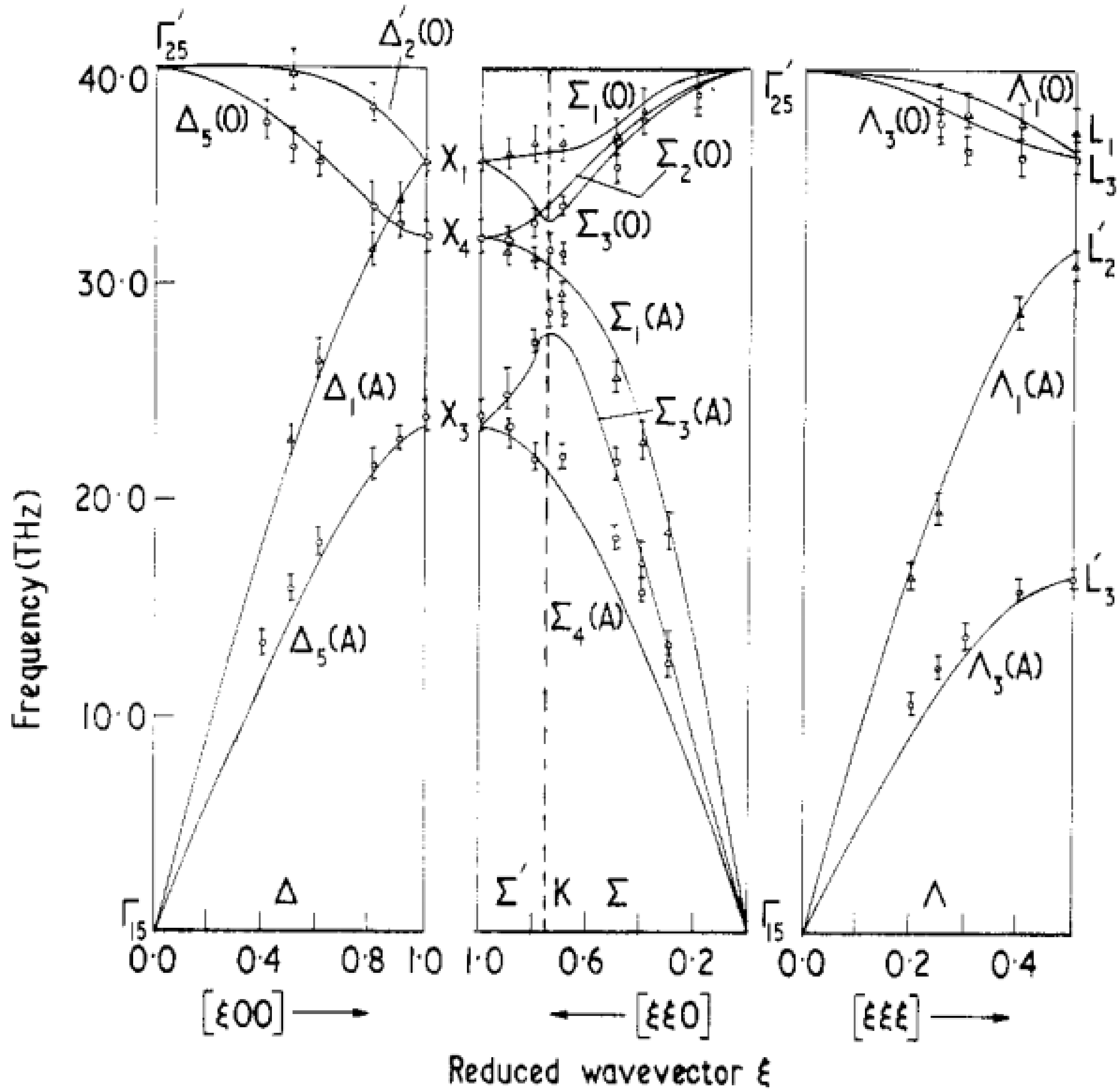


Figure 2. Phonon dispersion curves of diamond. Experimental points *et al* (1965, 1967). △ and ○ represent the longitudinal and transverse m