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

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

Normal Mode Analysis

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

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In this lecture, we will extend our normal mode analysis to more complicated systems, including infinite periodic systems and beyond one dimension.

PHYSICS COLLOQUIUM

THURSDAY • SEPTEMBER 30, 2021

Part III

Theoretical and Computational Projects

Professor Stephen Winter, representing theoretical and computational research projects in the physics department of Wake Forest University, include the focus areas of his group and that of Professor Timo Thonhauser. Research efforts by Natalie Holzwarth and William C. Kerr will also be discussed. This presentation will complete the three part snapshot of research opportunities at WFU Physics.

Discussion on Colloquium Program

This second part of the colloquium will be devoted to a discussion of the physics colloquium series, exchanging ideas with the goal of improvement and optimization. Bring your thoughts and ideas to the discussion.

Wake Forest University Physics Department Research Opportunities and Discussion on Colloquium Program

4:00 pm - Olin 101

Note: For additional information on the seminar or to obtain the video conference link, contact wfuphys@wfu.edu

Reception at 3:30pm - Olin Lounge

*We encourage all to wander outside to the front entrance or up to the Observatory Deck on the 3rd floor to enjoy their refreshments.

Course schedule

(Preliminary schedule -- subject to frequent adjustment.)

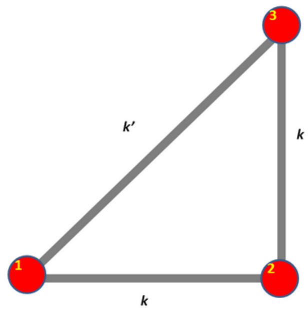
	Date	F&W Reading	Topic	Assignment	Due
1	Mon, 8/23/2021	Chap. 1	Introduction	#1	8/27/2021
2	Wed, 8/25/2021	Chap. 1	Scattering theory	#2	8/30/2021
3	Fri, 8/27/2021	Chap. 1	Scattering theory		
4	Mon, 8/30/2021	Chap. 1	Scattering theory	#3	9/01/2021
5	Wed, 9/01/2021	Chap. 1	Summary of scattering theory	#4	9/03/2021
6	Fri, 9/03/2021	Chap. 2	Non-inertial coordinate systems	#5	9/06/2021
7	Mon, 9/06/2021	Chap. 3	Calculus of Variation	#6	9/10/2021
8	Wed, 9/08/2021	Chap. 3	Calculus of Variation		
9	Fri, 9/10/2021	Chap. 3 & 6	Lagrangian Mechanics	#7	9/13/2021
10	Mon, 9/13/2021	Chap. 3 & 6	Lagrangian Mechanics	#8	9/17/2021
11	Wed, 9/15/2021	Chap. 3 & 6	Constants of the motion		
12	Fri, 9/17/2021	Chap. 3 & 6	Hamiltonian equations of motion	#9	9/20/2021
13	Mon, 9/20/2021	Chap. 3 & 6	Liouville theorm	#10	9/22/2021
14	Wed, 9/22/2021	Chap. 3 & 6	Canonical transformations		
15	Fri, 9/24/2021	Chap. 4	Small oscillations about equilibrium	#11	9/27/2021
16	Mon, 9/27/2021	Chap. 4	Normal modes of vibration	#12	9/29/2021
17	Wed, 9/29/2021	Chap. 4	Normal modes of more complicated systems	#13	10/04/2021
18	Fri, 10/01/2021	Chap. 7	Motion of strings		

This is the last lecture for Chap. 4. On Friday we will continue to discuss vibrations in extended one dimensional motion as covered in Chap. 7.

PHY 711 -- Assignment #13

Sept. 29, 2021

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'.

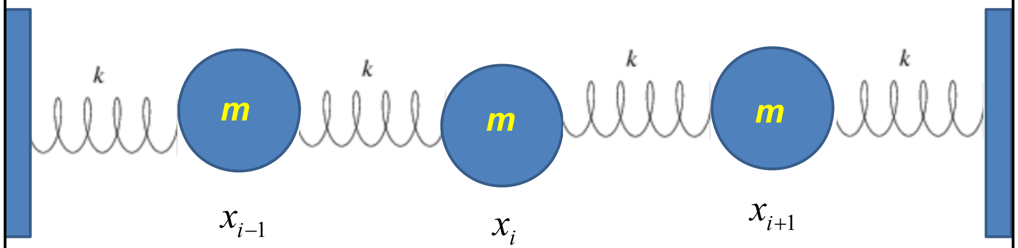
Homework due Monday.

Your questions –

From Owen -- If a spring system were undergoing chaotic motion, would the eigenvalue/eigenvector formalism we are discussing still apply? Can one know in advance whether a system will behave chaotically or not?

Comment – In the present treatment we are focusing on the linearized equations of motion. In this case, while the motion can be complicated (superposition of several modes for example), the chaotic behavior does not occur. Mathematically, chaotic behavior may occur in the presence of non-linear contributions. Physically, non-linear contributions tend to be important when the system has large deviations from equilibrium.

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.

Example of one dimensional system with fixed boundary values.

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

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

From Euler - Lagrange equations :

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

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

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

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

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

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

Review of detailed equations.

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

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

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

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

Review of solutions discussed on Wednesday.

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

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

General solution :

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

Impose boundary conditions :

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

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

Review of boundary conditions.

Impose boundary conditions -- continued:

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

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

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

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

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

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

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

Recap -- solution for integer parameter ν

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

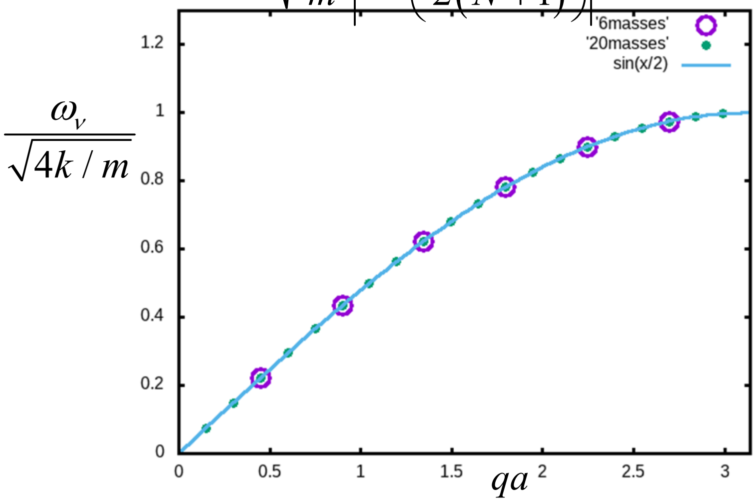
$$\omega_\nu{}^2 = \frac{4k}{m}\sin^2\left(\frac{\nu\pi}{2(N+1)}\right)$$

Note that non-trivial, unique values are

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

Review of full solution.

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

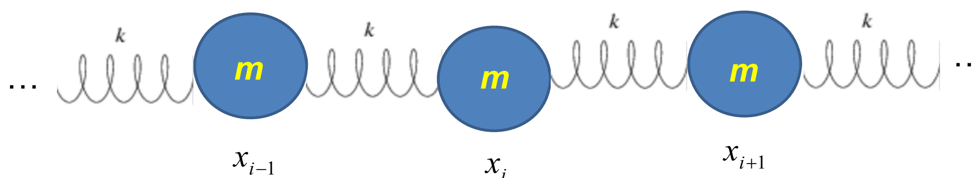


Note that solution form remains correct for $N \rightarrow \infty$

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

Plot for example. Now consider the case where N is very large.

For extended chain without boundaries:



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

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

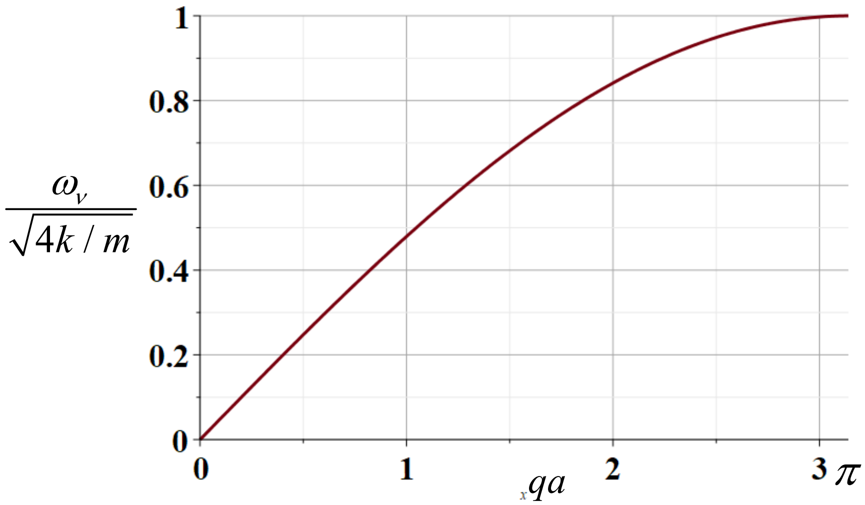
$$-\omega^2 = \frac{k}{m}\left(2\cos(qa) - 2\right)$$

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

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

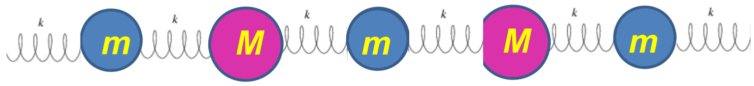
Now consider the case where N is infinite so that there are an infinite number of solutions parameterized by qa as a continuous varable.

Plot of frequencies in scaled units as a function qa



Distinct solutions occur for qa in the range of 0-pi as shown in the plot.

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

$$L = T - V$$

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

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Now consider a slight modification of the previous example where masses are alternately m and M with labels x and y.

$$L = T - V$$

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

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.

Does this form seem reasonable?

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

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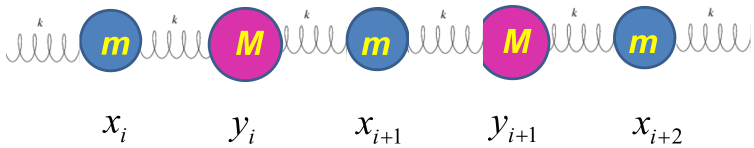
In this case, we can analyze the system by considering different amplitudes for the m and M masses. The resulting coupled equations can be written in matrix form.

Comment on notation --



Trial solution:

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

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

Using 2qa as our unknown parameter is a convenient choice so that we can easily relate our solution to the m=M case.

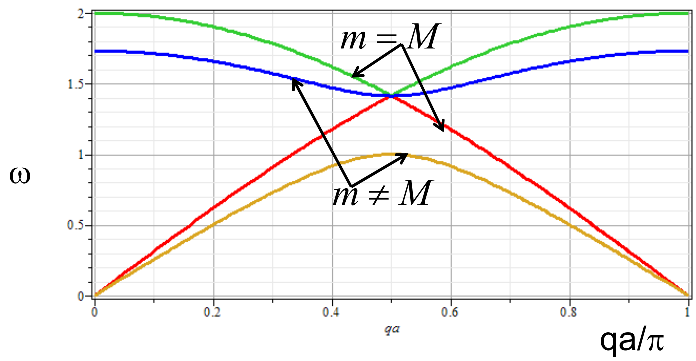
$$\begin{pmatrix} m\omega^2 - 2k & k\left(e^{-i2qa}+1\right) \\ k\left(e^{i2qa}+1\right) & M\omega^2 - 2k \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix} = 0$$

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

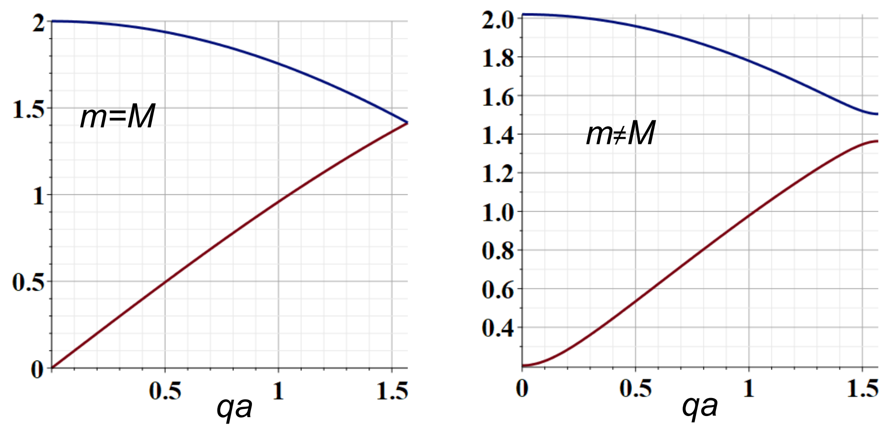


Plotting the solutions for the frequencies as a function of qa.

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.



Plotting only distinct frequencies $0 < qa < \pi/2$

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

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

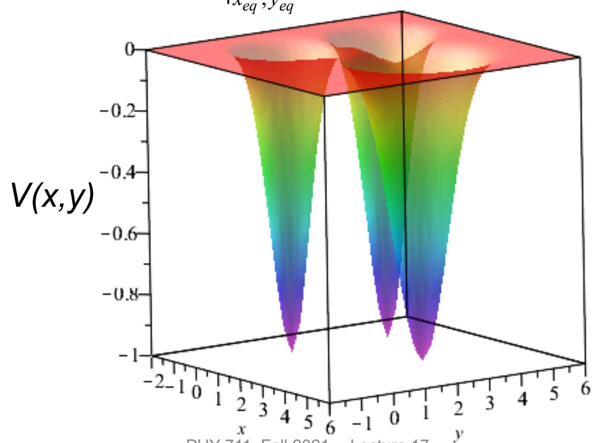
$$\begin{pmatrix} A \\ B \end{pmatrix}_- = N\begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \begin{pmatrix} A \\ B \end{pmatrix}_+ = N\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Some details about the solutions.

Potential in 2 and more dimensions

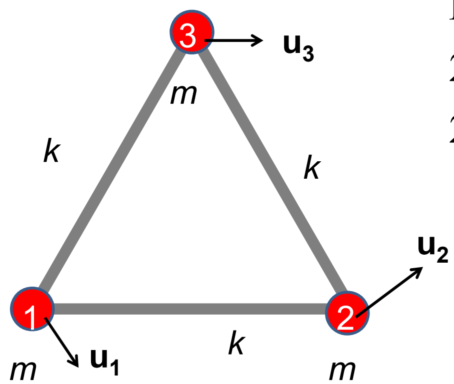
$$V(x,y) \approx V(x_{eq},y_{eq}) + \tfrac{1}{2}\left(x-x_{eq}\right)^2 \left.\frac{\partial^2 V}{\partial x^2}\right|_{x_{eq},y_{eq}}$$

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



Returning to the finite systems, consider equilibria in two dimensions as shown.

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



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

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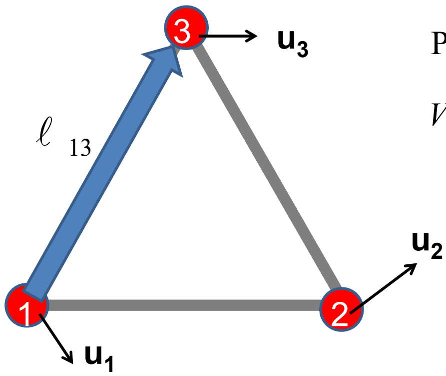
Specifically, we will consider 3 masses in an equilateral triangle configuration as shown.

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:

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

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

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

We need to consider displacements from equilibrium in the x-y plane. Keeping only linear terms in the displacements we wind up with a simple relationship to analyze.

Some details for spring 13:

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

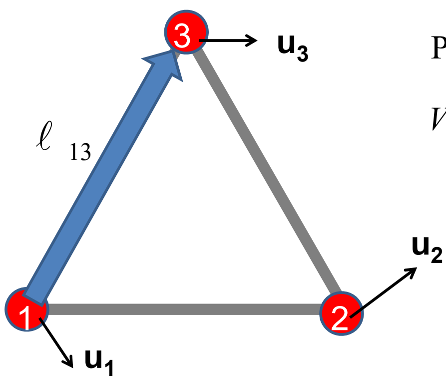
$$\left(\boldsymbol{\ell}_{13}+\mathbf{u}_{13}\right)^{1/2} = \left|\boldsymbol{\ell}_{13}\right|\left(1+\frac{2\boldsymbol{\ell}_{13}\cdot\mathbf{u}_{13}}{\left|\boldsymbol{\ell}_{13}\right|^2}+\frac{\left|\mathbf{u}_{13}\right|^2}{\left|\boldsymbol{\ell}_{13}\right|^2}\right)^{1/2} \quad \text{Assume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

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

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

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:

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

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

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

We need to consider displacements from equilibrium in the x-y plane. Keeping only linear terms in the displacements we wind up with a simple relationship to analyze.

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

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

$$\approx \frac{1}{2}k\left(\frac{\ell_{12}\cdot(\mathbf{u}_2-\mathbf{u}_1)}{|\ell_{12}|}\right)^2 + \frac{1}{2}k\left(\frac{\ell_{13}\cdot(\mathbf{u}_3-\mathbf{u}_1)}{|\ell_{13}|}\right)^2 + \frac{1}{2}k\left(\frac{\ell_{23}\cdot(\mathbf{u}_3-\mathbf{u}_2)}{|\ell_{23}|}\right)^2$$

$$\approx \frac{1}{2}k\left(u_{x2}-u_{x1}\right)^2 + \frac{1}{2}k\left(\frac{1}{2}\left(u_{x3}-u_{x1}\right)+\frac{\sqrt{3}}{2}\left(u_{y3}-u_{y1}\right)\right)^2 + \frac{1}{2}k\left(\frac{1}{2}\left(u_{x2}-u_{x3}\right)-\frac{\sqrt{3}}{2}\left(u_{y2}-u_{y3}\right)\right)^2$$

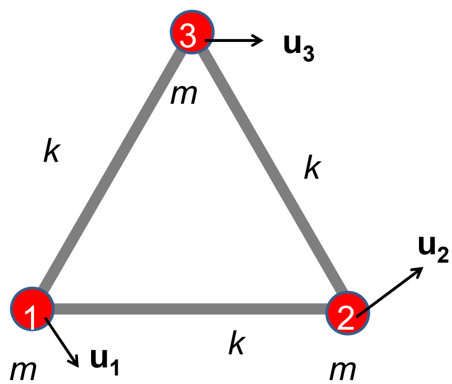
Analyzing the 3 displacements for the equilateral triangle geometry, we find these equations.

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

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

The results is a 6x6 matrix problem to find eigenvalues and eigenvectors.

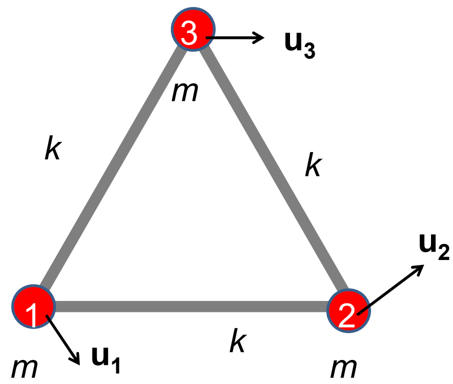
Example – normal modes of a system with the symmetry of an equilateral triangle -- continued



With help from Maple

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

Results from Maple. We have 6 eigenvalues and 3 non-zero modes for this case.



What can you say about the 3 zero frequency modes?

What can you say about the 3 non-zero frequency modes?

3-dimensional periodic lattices

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

Diagram of atom positions

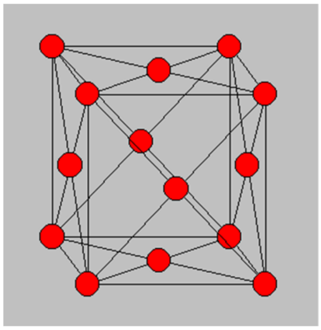
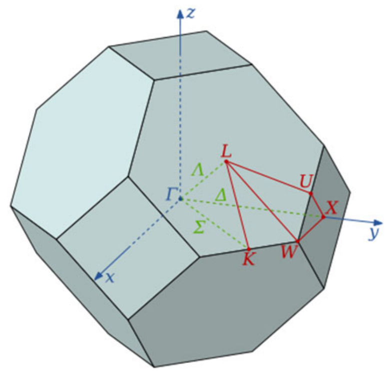


Diagram of q-space $\nu(q)$



Interesting extensions to a 3-dimensional crystalline system.

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

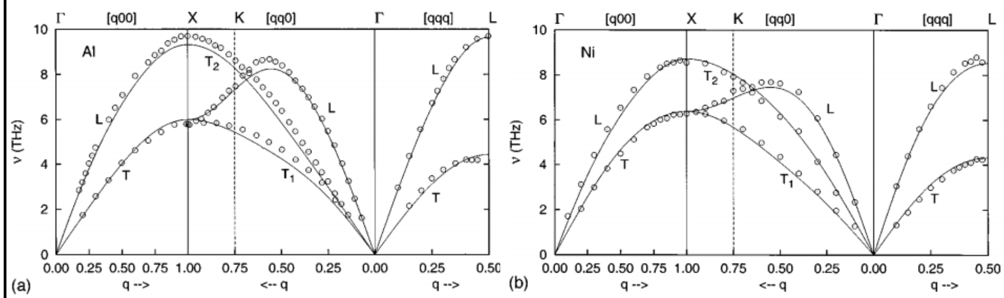


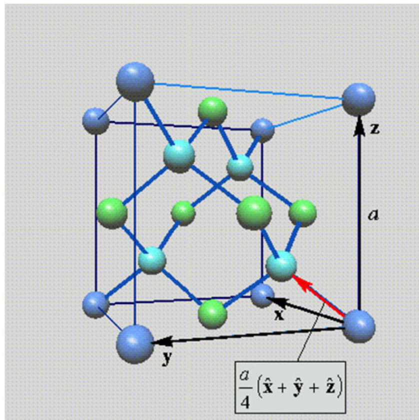
FIG. 2. Comparison of phonon-dispersion curves for Al (a) and Ni (b) predicted by the present EAM potentials, with the experimental values measured by neutron diffraction at 80 K (Al) and 298 K (Ni) (Ref. 33 for Al and Ref. 34 for Ni). The phonon frequencies at point *X* were included in the fitting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

Note that for each q, there are 3 frequencies.

Results of normal modes from experiment and simulations for face centered cubic Al (left) and Ni (right). Interestingly, the phonon frequency patterns are similar for these very different materials.

Lattice vibrations for 3-dimensional lattice

Example: diamond lattice



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

Another example – diamond.

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

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

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

Some equations for extended systems.

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

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

More euqations.

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" $\omega(\mathbf{q})$

More equations.

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

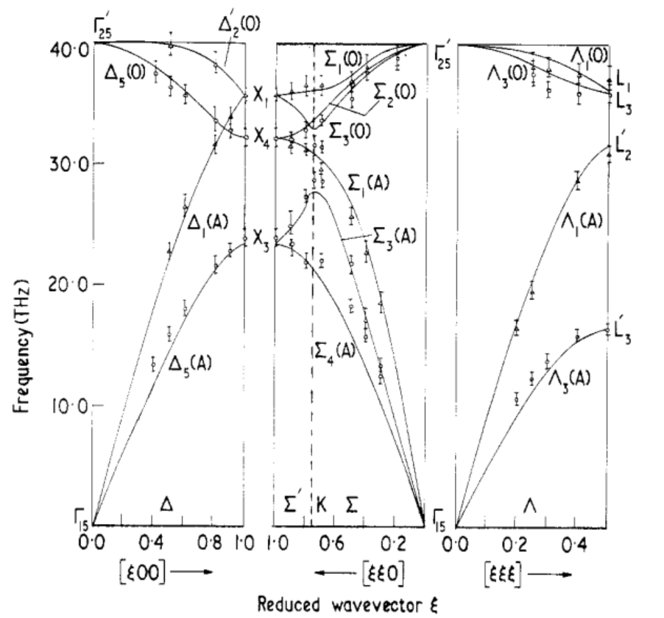


Figure 2. Phonon dispersion curves of diamond. Experimental points *et al* (1965, 1967). △ and ○ represent the longitudinal and transverse m

Results for diamond from simulation and experiment.

Examples of phonon spectra of two forms of boron nitride

Cubic structure

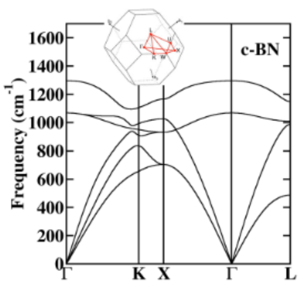


Figure 1. Phonon dispersion curves ($\omega^{\nu}(\mathbf{q})$) for cubic BN. The inset Brillouin zone diagram was reprinted from Setyawan *et al* [7], copyright (2010), with permission from Elsevier.

Hexagonal structure

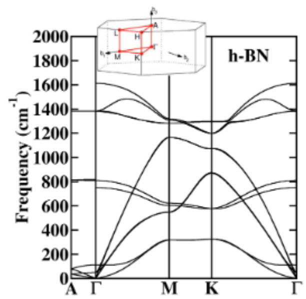


Figure 2. Phonon dispersion curves ($\omega^{\nu}(\mathbf{q})$) for hexagonal BN. The inset Brillouin zone diagram was reprinted from Setyawan *et al* [7], copyright (2010), with permission from Elsevier.