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

Plan 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**
3. **Normal modes for 2 and 3 dimensional systems**

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

Course schedule

(Preliminary schedule -- subject to frequent adjustment.)

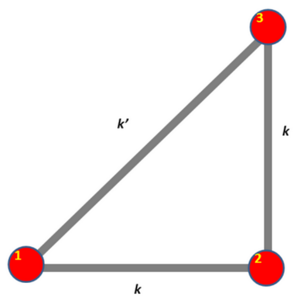
	Date	F&W Reading	Topic	Assignment	Due
1	Wed, 8/26/2020	Chap. 1	Introduction	#1	8/31/2020
2	Fri, 8/28/2020	Chap. 1	Scattering theory	#2	9/02/2020
3	Mon, 8/31/2020	Chap. 1	Scattering theory	#3	9/04/2020
4	Wed, 9/02/2020	Chap. 1	Scattering theory		
5	Fri, 9/04/2020	Chap. 1	Scattering theory	#4	9/09/2020
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		

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

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 $k=k'$.

Homework due Monday.

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 $\mathbf{\Sigma}$:

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

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

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Digression from linear algebra omitted from Wednesday's lecture.

Singular value decomposition -- continued

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

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

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

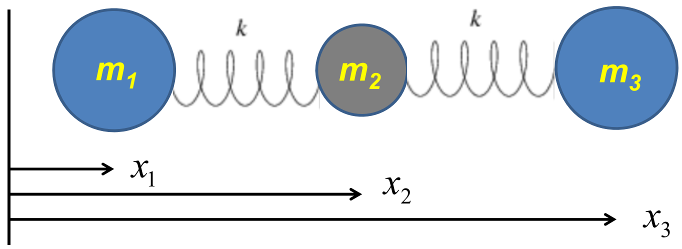
Details are complicated ….

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".

Introducing the concept of SVD without going into detail.

Example – linear molecule



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

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Back to the discussion of one-dimensional motion of masses and springs.

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

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

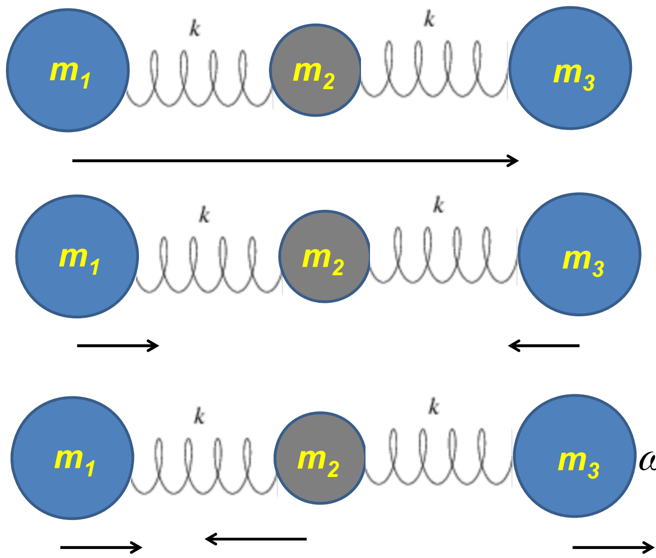
$$-\omega_\alpha^2 m_2 X_2^\alpha = k\left(X_1^\alpha - 2X_2^\alpha + X_3^\alpha\right)$$

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

More review.

For $m_1 = m_3 \equiv m_O$

and $m_2 \equiv m_C$



$$\omega_1 = 0$$

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

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

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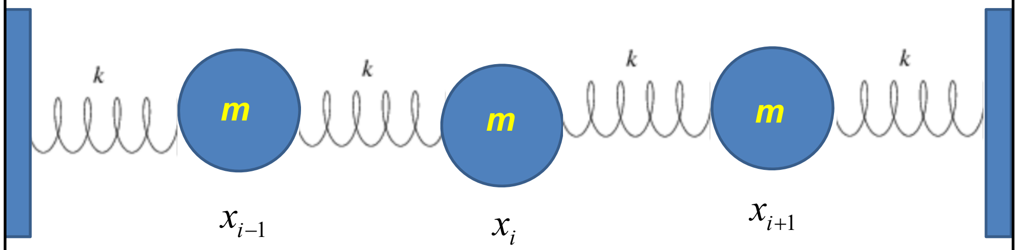
Reviewing results for example isolated molecule.

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.

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

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

From Euler - Lagrange equations :

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

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

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

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

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

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

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

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 :

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

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

Review of boundary conditions.

Impose boundary conditions -- continued:

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

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

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

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

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

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

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

Recap -- solution for integer parameter ν

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

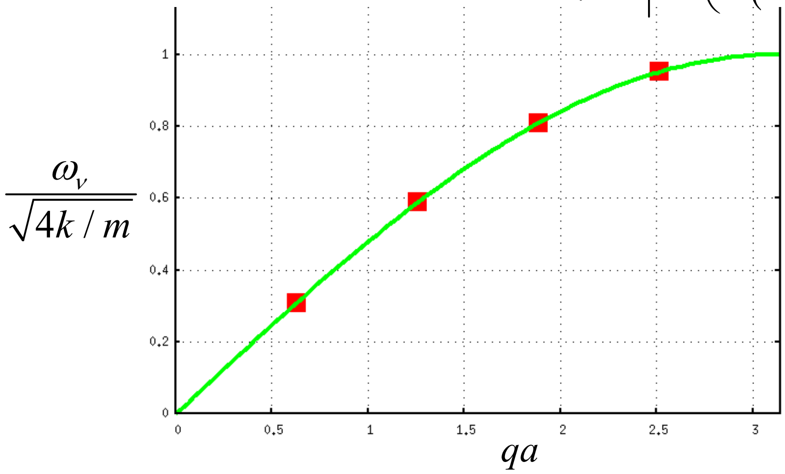
$$\omega_\nu{}^2 = \frac{4k}{m}\sin^2\left(\frac{\nu\pi}{2(N+1)}\right)$$

Note that non-trivial, unique values are

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

Review of full solution.

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

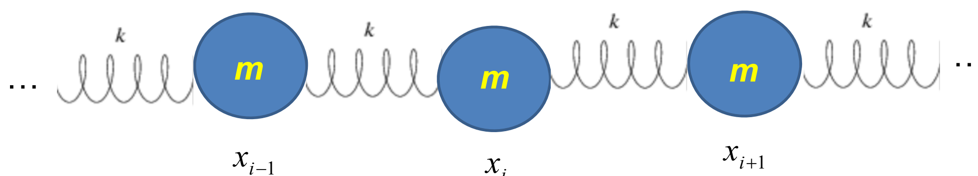


Note that solution form remains correct for $N \rightarrow \infty$

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

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

For extended chain without boundaries:



From Euler-Lagrange equations:

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

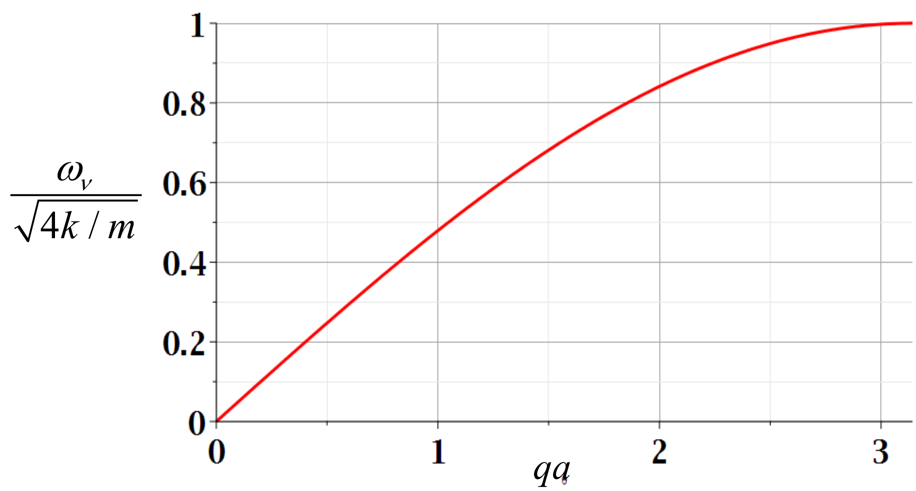
Try: $\quad x_j(t) = Ae^{-i\omega t + iqaj}$

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

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

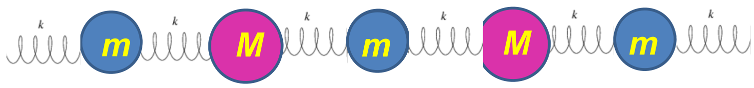
$$\Rightarrow \omega^2 = \frac{4k}{m}\sin^2\left(\frac{qa}{2}\right) \qquad \text{distinct values for } 0 \le qa \le \pi$$

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



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:



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

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

$$L = T - V$$

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

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 :

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

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

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

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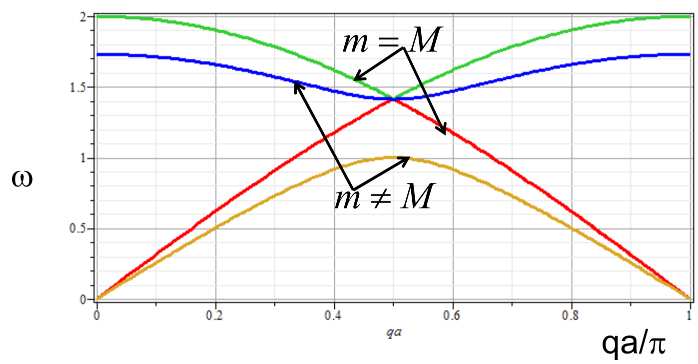
In this case, we can analyze the system by considering different amplitudes for the m and M masses. The resulting coupled equations can be written in matrix form.

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

Solutions:

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



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

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

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

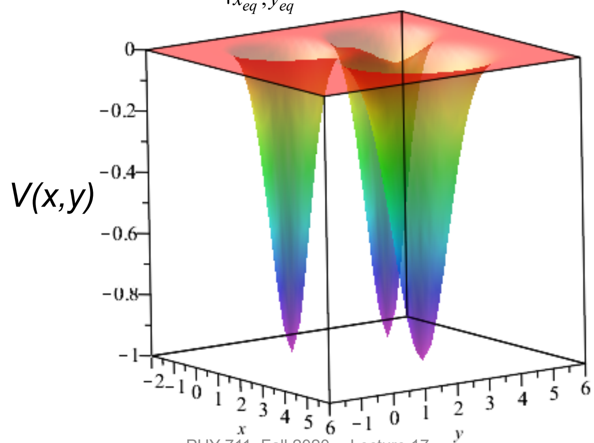
$$\begin{pmatrix} A \\ B \end{pmatrix}_- = N \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \begin{pmatrix} A \\ B \end{pmatrix}_+ = N \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Some details about the solutions.

Potential in 2 and more dimensions

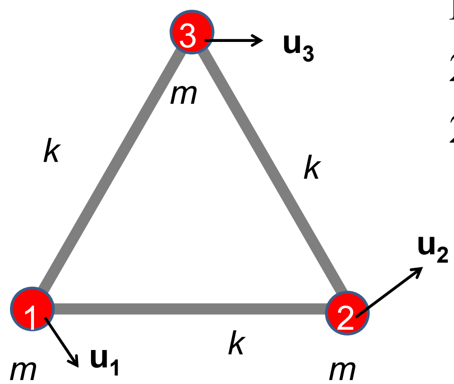
$$V(x,y) \approx V(x_{eq}, y_{eq}) + \tfrac{1}{2}\left(x - x_{eq}\right)^2 \left.\frac{\partial^2 V}{\partial x^2}\right|_{x_{eq}, y_{eq}}$$

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



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

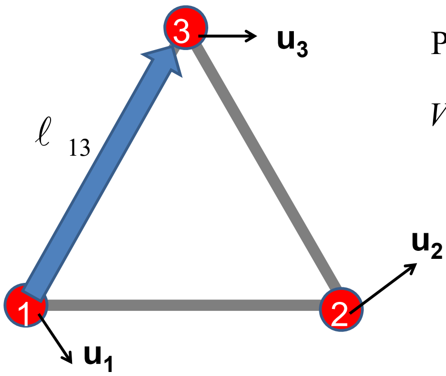


Degrees of freedom for 2-dimensional motion:

$$2N = 6$$

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.

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

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

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

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

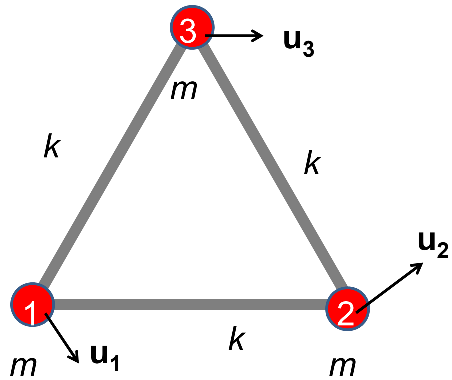
Analyzing the 3 displacements for the equilateral triangle geometry, we find these equations.

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



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

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

3-dimensional periodic lattices

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

Diagram of atom positions

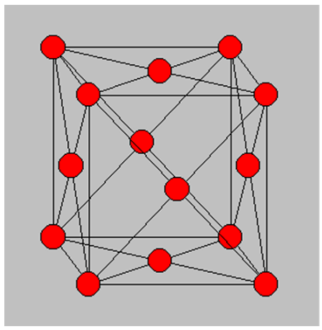
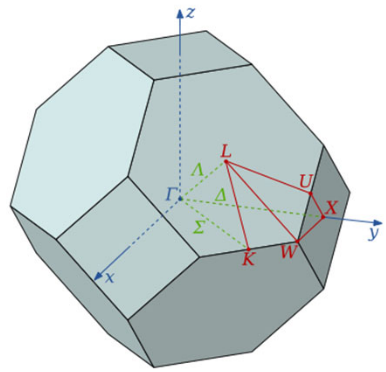


Diagram of q-space $\nu(q)$



Interesting extensions to a 3-dimensional crystalline system.

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

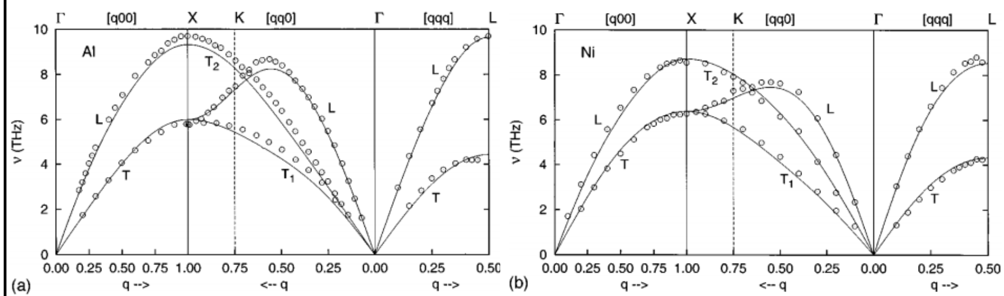
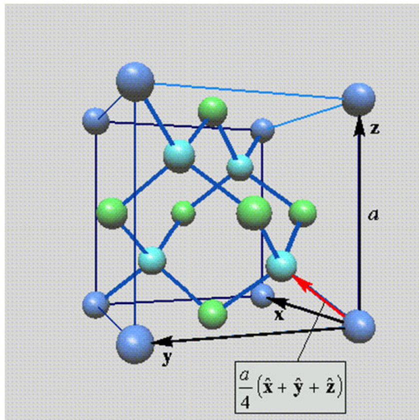


FIG. 2. Comparison of phonon-dispersion curves for Al (a) and Ni (b) predicted by the present EAM potentials, with the experimental values measured by neutron diffraction at 80 K (Al) and 298 K (Ni) (Ref. 33 for Al and Ref. 34 for Ni). The phonon frequencies at point *X* were included in the fitting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

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:

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

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

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

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

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:

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

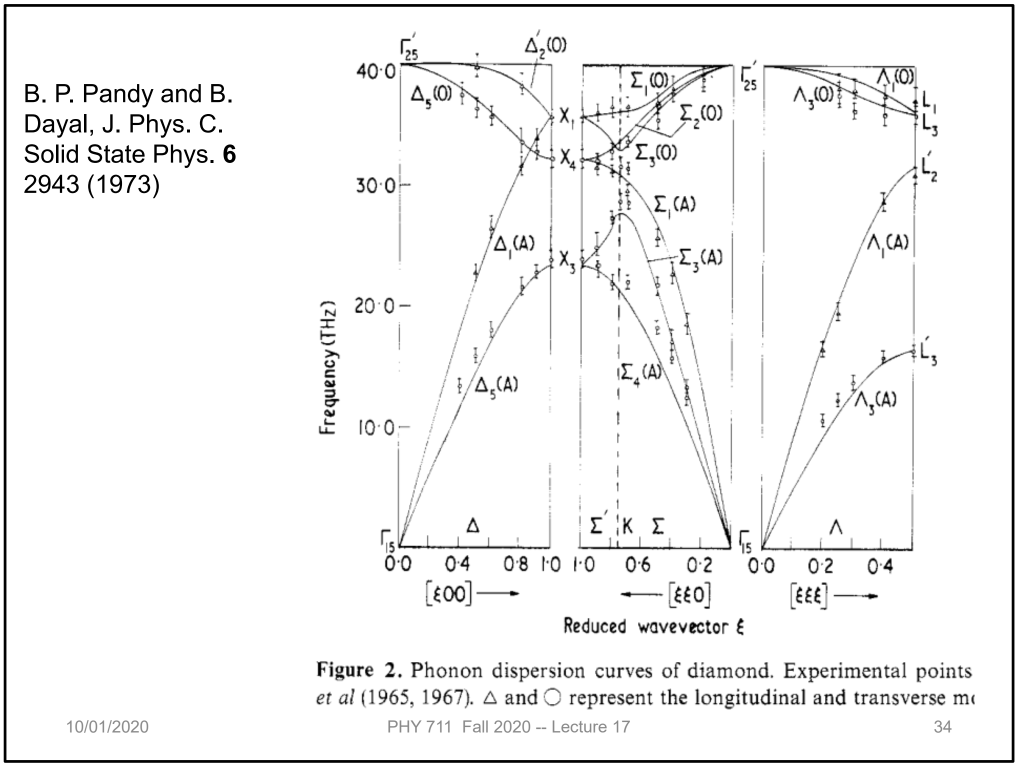
Eigenvalue equations:

$$\omega^2 A_j^a = \sum_{b,k} W(\mathbf{q})_{jk}^{ab} A_k^b$$

In this equation the summation is only over unique atomic sites.

$\Rightarrow$ Find "dispersion curves" $\omega(\mathbf{q})$

More equations.



Results for diamond from simulation and experiment.