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 finite 2 and 3 dimensional systems
2. Normal modes for extended systems

Opportunities for Physics Research Part IV

Theoretical/Computational
Biophysics and Gravitational Physics

Featuring the groups of Fred Salsbury and Sam Cho, Greg Cook, Paul Anderson, and Eric Carlson

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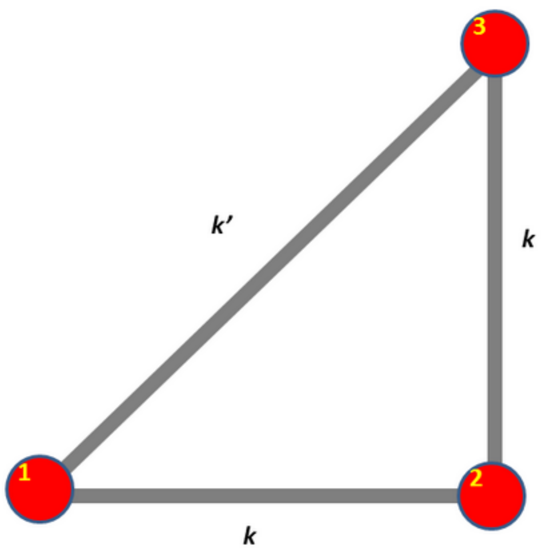
September 29, 2022 at 4 PM in Olin 101

12	Fri, 9/16/2022	Chap. 3 & 6	Hamiltonian equations of motion		
13	Mon, 9/19/2022	Chap. 3 & 6	Liouville theorm	#10	9/21/2022
14	Wed, 9/21/2022	Chap. 3 & 6	Canonical transformations	#11	9/23/2022
15	Fri, 9/23/2022	Chap. 4	Small oscillations about equilibrium	#12	9/26/2022
16	Mon, 9/26/2022	Chap. 4	Normal modes of vibration	#13	9/28/2022
17	Wed, 9/28/2022	Chap. 4	Normal modes of more complicated systems	#14	10/03/2022
18	Fri, 9/30/2022	Chap. 7	Motion of strings		
19	Mon, 10/03/2022	Chap. 7	Sturm-Liouville equations		
20	Wed, 10/05/2022	Chap. 7	Sturm-Liouville equations		
21	Fri, 10/07/2022	Chap. 1-4,6-7	Review		
	Mon, 10/10/2022	No class	Take home exam		
	Wed, 10/12/2022	No class	Take home exam		
	Fri, 10/14/2022	No class	Fall break		
22	Mon, 10/17/2022	Chap. 7	Class resumes		

PHY 711 -- Assignment #14

Sept. 28, 2022

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



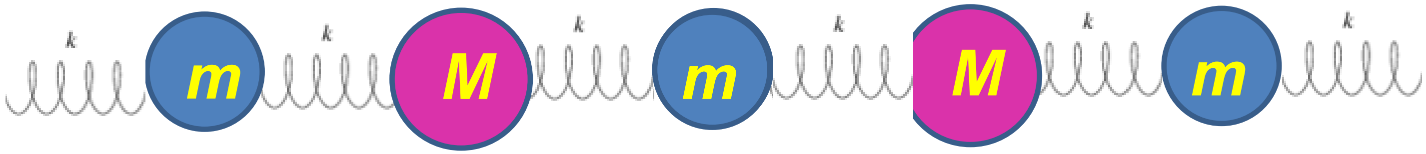
1. Consider the system of 3 masses (m_1=m_2=m_3=m) shown attached by elastic forces in the right triangular configuration (with angles 45, 90, 45 deg) shown above with spring constants k and k'. Find the normal modes of small oscillations for this system. For numerical evaluation, you may assume that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

Your questions –

From Sam -- How to think about normal modes other than their mathematical formulation. They seem to form simple patterns such as all moving in sync, but is there more to it? Or is it that the normal modes form a kind of periodic motion that repeats itself, rather than become chaotic?

Recap from previous lecture --

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

$$L = T - V$$

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

$$L = T - V$$

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

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?

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

Comment on notation --

x_i y_i x_{i+1} y_{i+1} x_{i+2}

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.

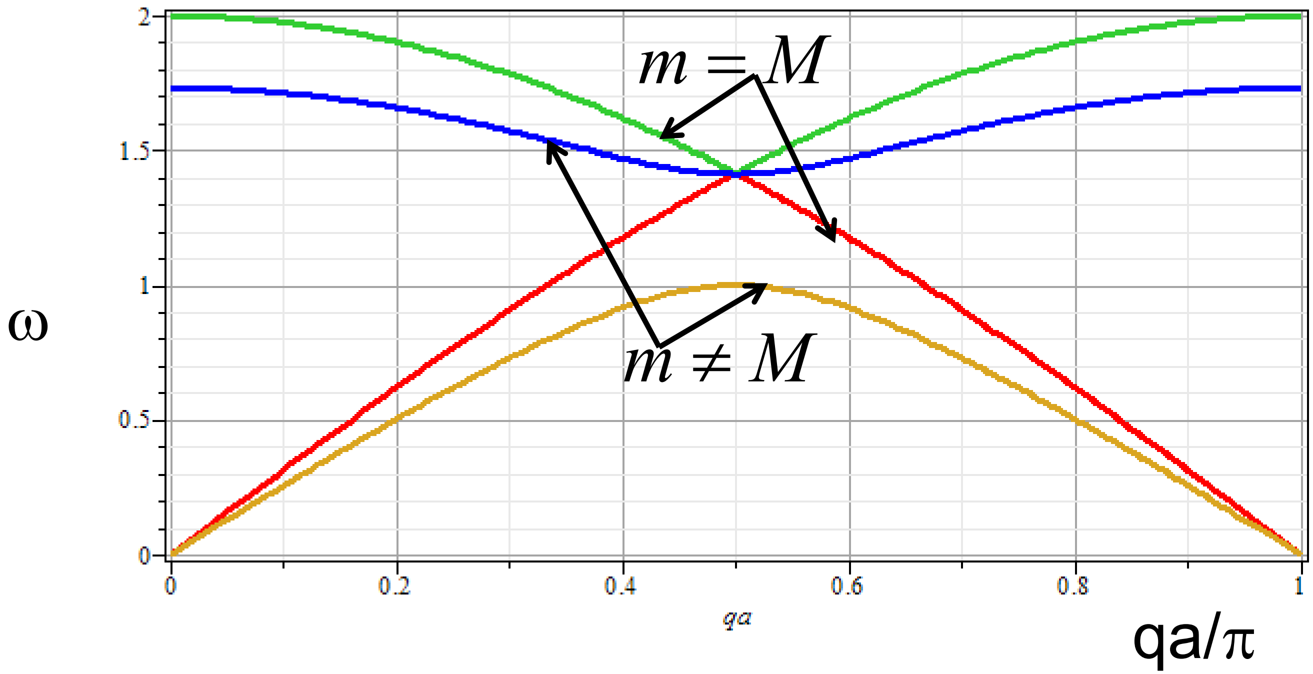
$$\begin{pmatrix} m\omega^2 - 2k & k\left(e^{-i2qa}+1\right) \\ k\left(e^{i2qa}+1\right) & M\omega^2 - 2k \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix} = 0$$

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?

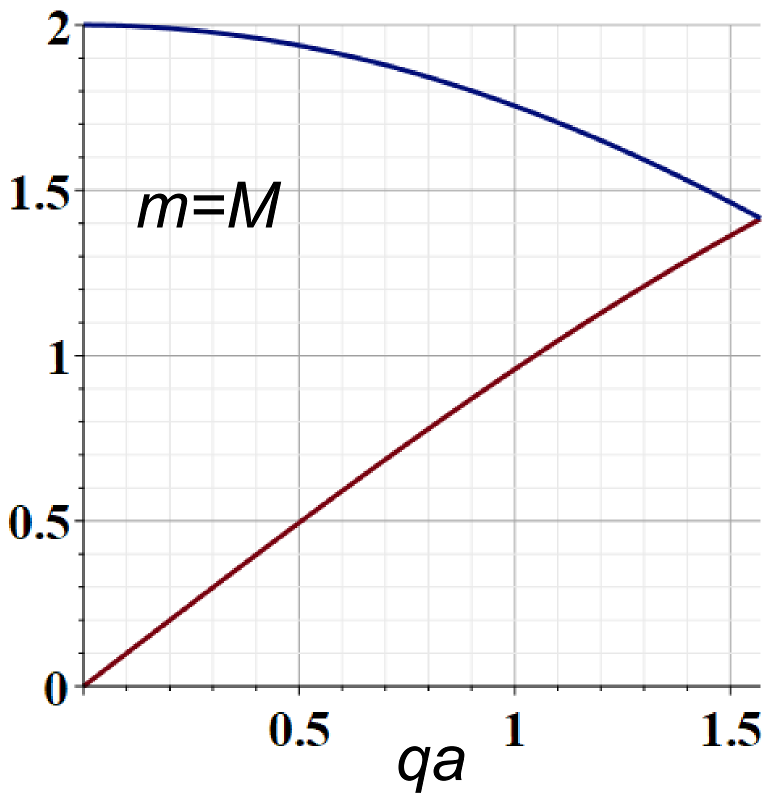
a. No
b. Yes

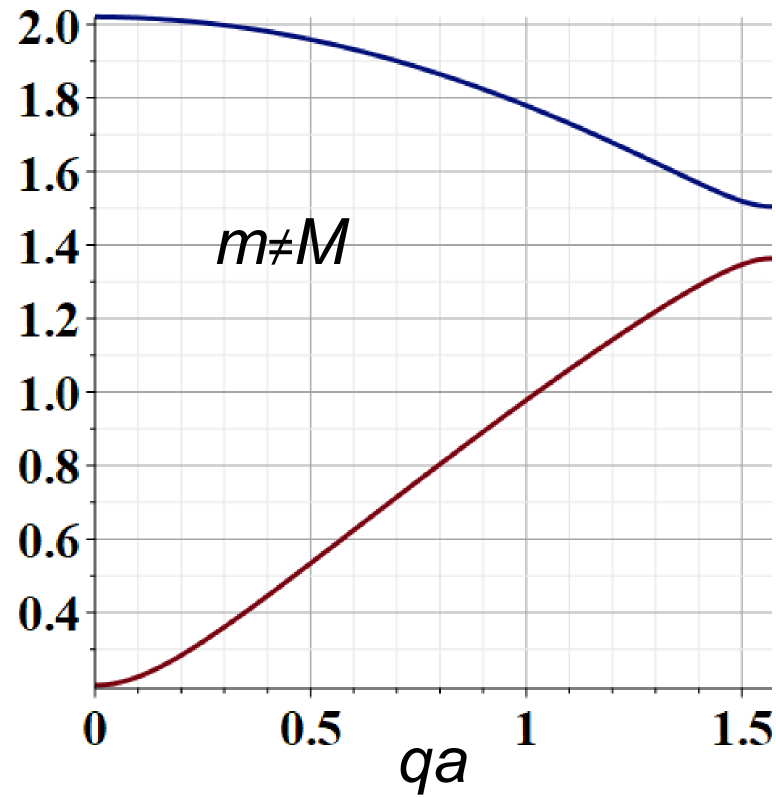


Normal mode frequencies:

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

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

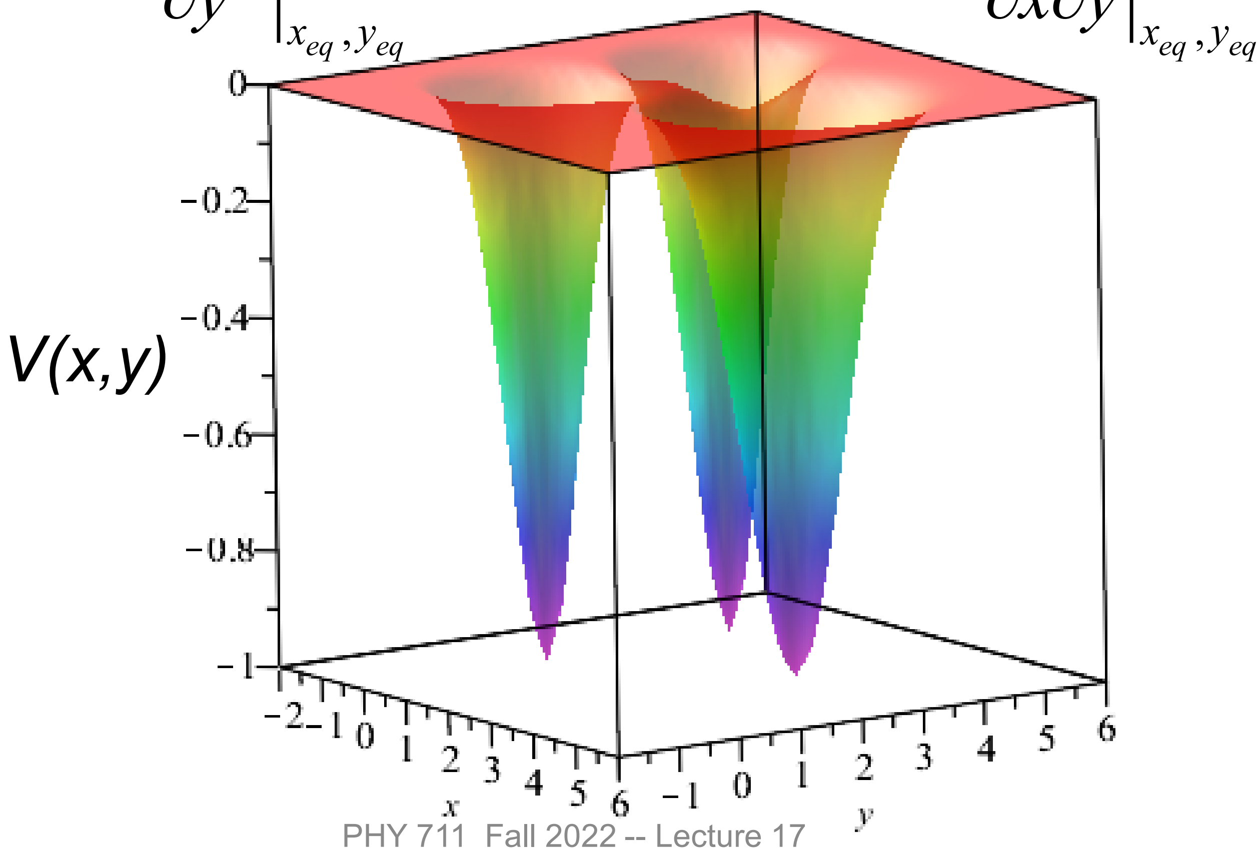
$$\omega_- = \sqrt{\frac{2k}{M}} \qquad \omega_+ = \sqrt{\frac{2k}{m}}$$

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

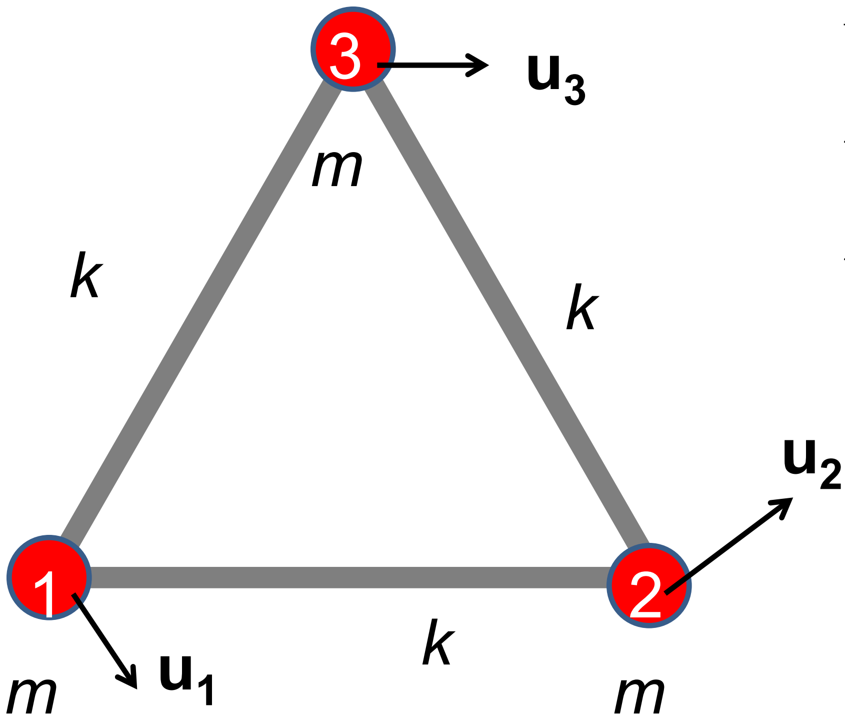
Now consider a potential system in 2 dimensions near its equilibrium point --

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

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



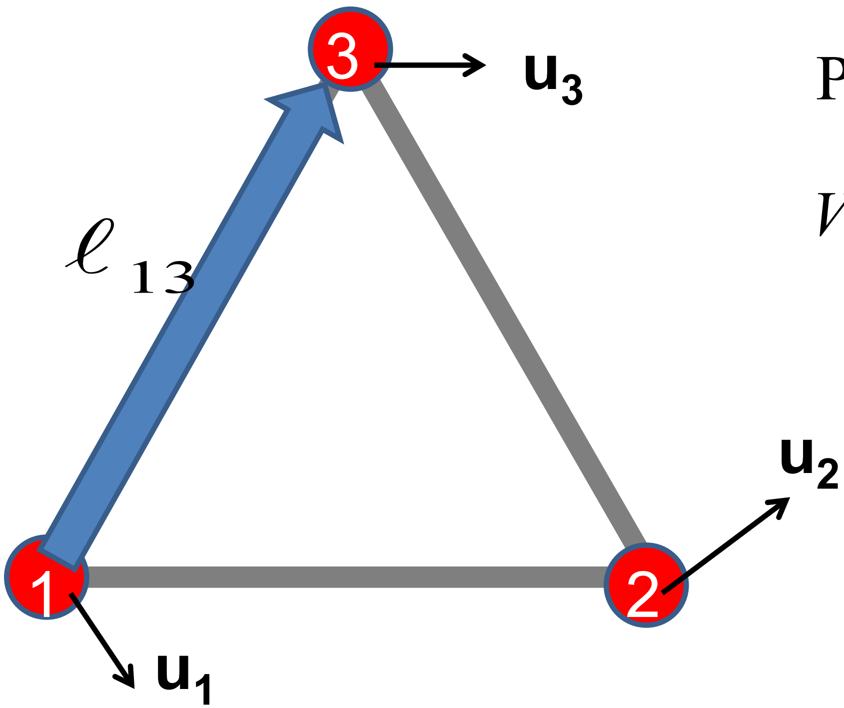
Example – normal modes of a system with the symmetry of an equilateral triangle



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:

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

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

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

Some details for spring 13:

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

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

negligible

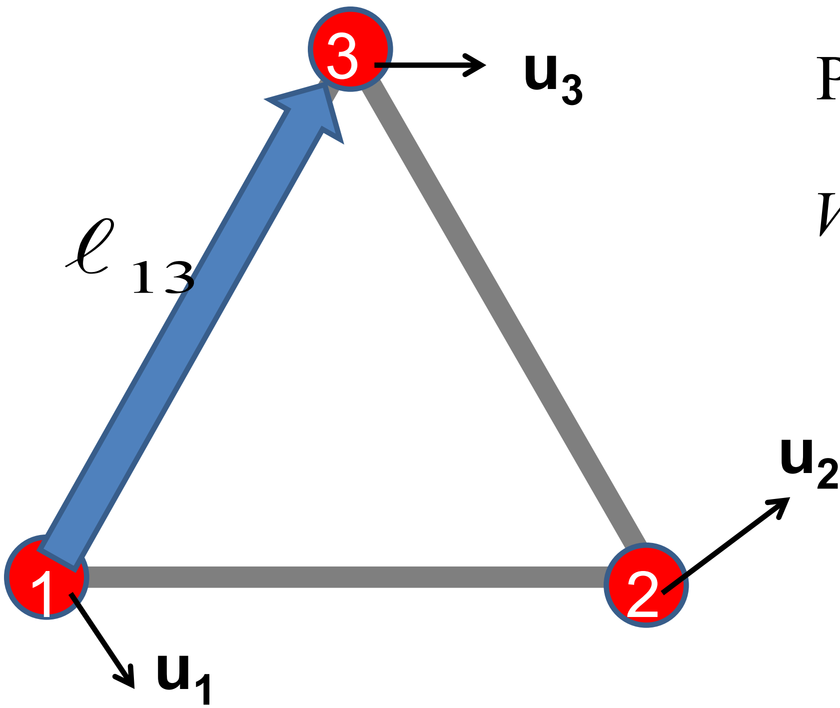
Assume $\left|\mathbf{u}_{13}\right| \ll \left|\boldsymbol{\ell}_{13}\right|$

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

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

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

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

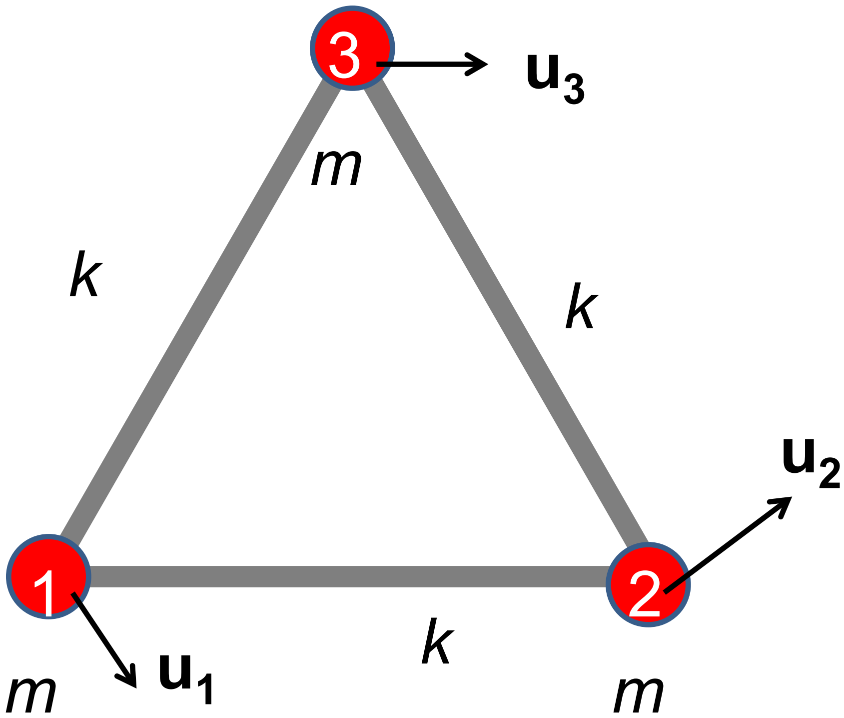
$$+\frac{1}{2}k\left(\frac{\ell_{23}\cdot(\mathbf{u}_3-\mathbf{u}_2)}{|\ell_{23}|}\right)^2$$

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

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

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

Some details for this case of the equilateral triangle --



$$\boldsymbol{\ell}_{12} = \left|\boldsymbol{\ell}_{12}\right| \hat{\mathbf{x}}$$

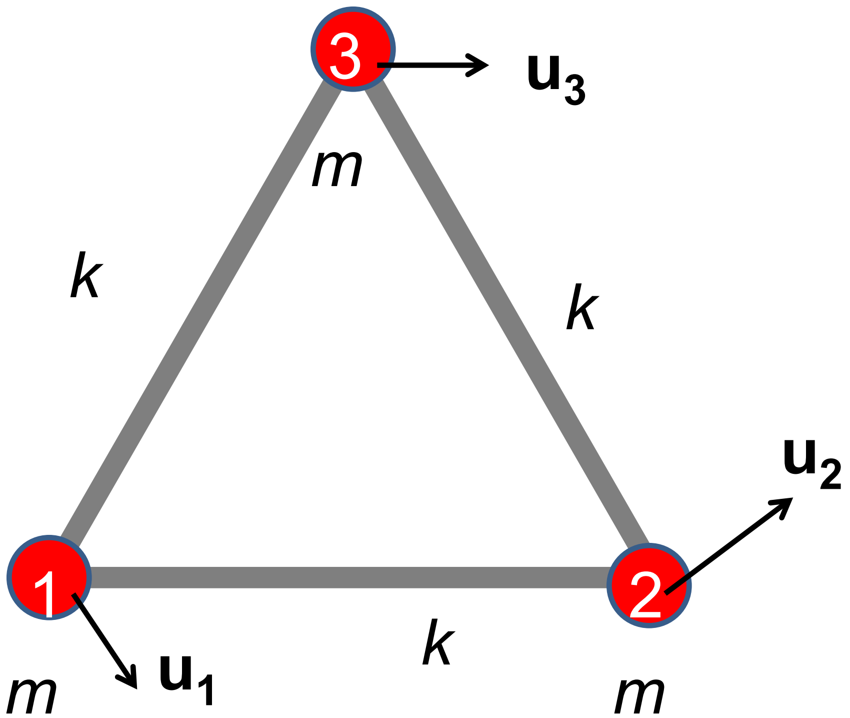
$$\boldsymbol{\ell}_{13} = \left|\boldsymbol{\ell}_{13}\right| \left(\frac{1}{2}\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}\hat{\mathbf{y}} \right)$$

$$\boldsymbol{\ell}_{23} = \left|\boldsymbol{\ell}_{23}\right| \left(-\frac{1}{2}\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}\hat{\mathbf{y}} \right)$$

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

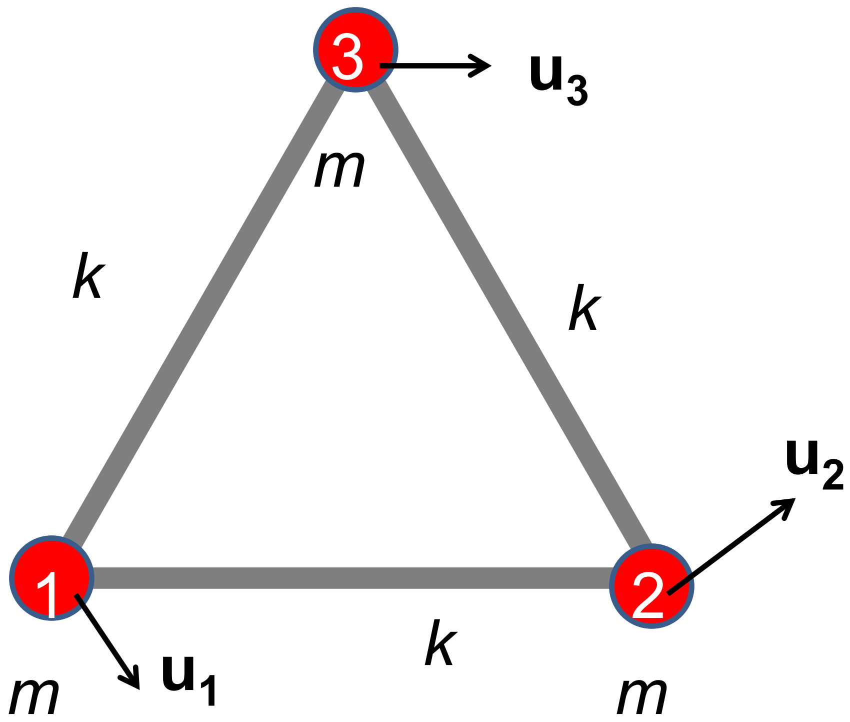
$$\frac{k}{m}\begin{bmatrix} \frac{5}{4} & -1 & -\frac{1}{4} & \frac{1}{4}\sqrt{3} & 0 & -\frac{1}{4}\sqrt{3} \\ -1 & \frac{5}{4} & -\frac{1}{4} & 0 & -\frac{1}{4}\sqrt{3} & \frac{1}{4}\sqrt{3} \\ -\frac{1}{4} & -\frac{1}{4} & \frac{1}{2} & -\frac{1}{4}\sqrt{3} & \frac{1}{4}\sqrt{3} & 0 \\ \frac{1}{4}\sqrt{3}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

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?

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

More general treatment of atomic system near equilibrium

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:

$$m_a \ddot{u}_j^a = -\sum_{b,k} D_{jk}^{ab} u_k^b$$

For a system of N atoms moving in d dimensions, we must solve a $dN \times dN$ eigenvalue problem.

Solution form:

$$u_j^a(t) = \frac{1}{\sqrt{m_a}} A_j^a e^{-i\omega t}$$

Eigenvalue problem: $$\omega^2 A_j^a = \sum_{b,k} \frac{D_{jk}^{ab}}{\sqrt{m_a m_b}} A_k^b$$

Extension of this analysis to a periodic system --

Equilibrium positions: $\mathbf{R}_0^a = \boldsymbol{\tau}^a + \mathbf{T}$

where $\boldsymbol{\tau}^a$ denotes unique sites within a unit cel

and $\mathbf{T}$ denotes all possible lattice translation ve

Solution form for the periodic extended system:

$$u_j^a(t) = \frac{1}{\sqrt{m_a}} A_j^a e^{-i\omega t + i\mathbf{q}\cdot\mathbf{R}_0^a}$$

q maps distinct configurations of periodic states.

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

3-dimensional periodic lattices

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

Diagram of atom positions

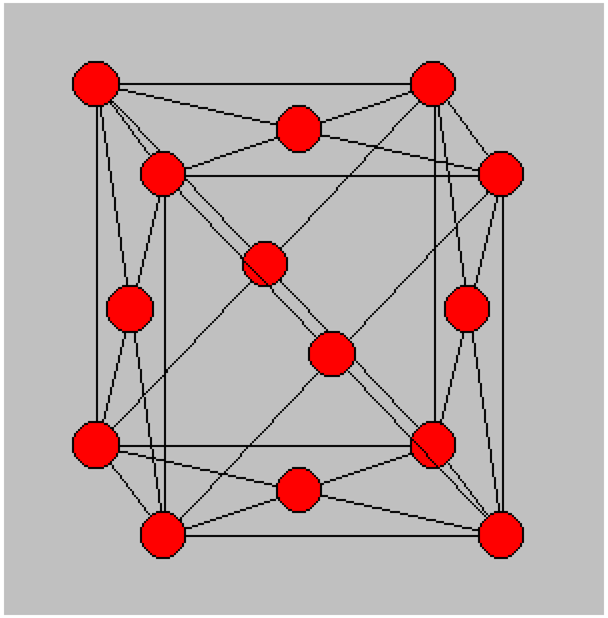
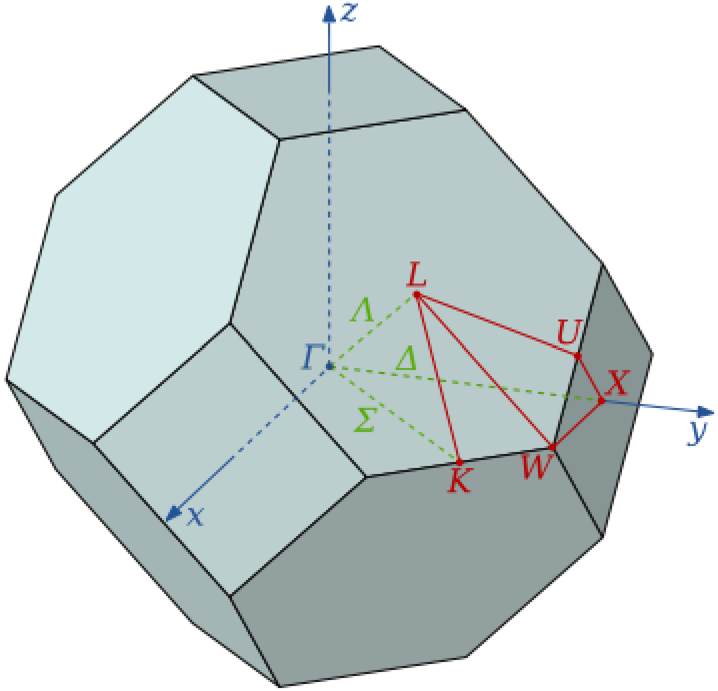


Diagram of q-space $\nu(q)$



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

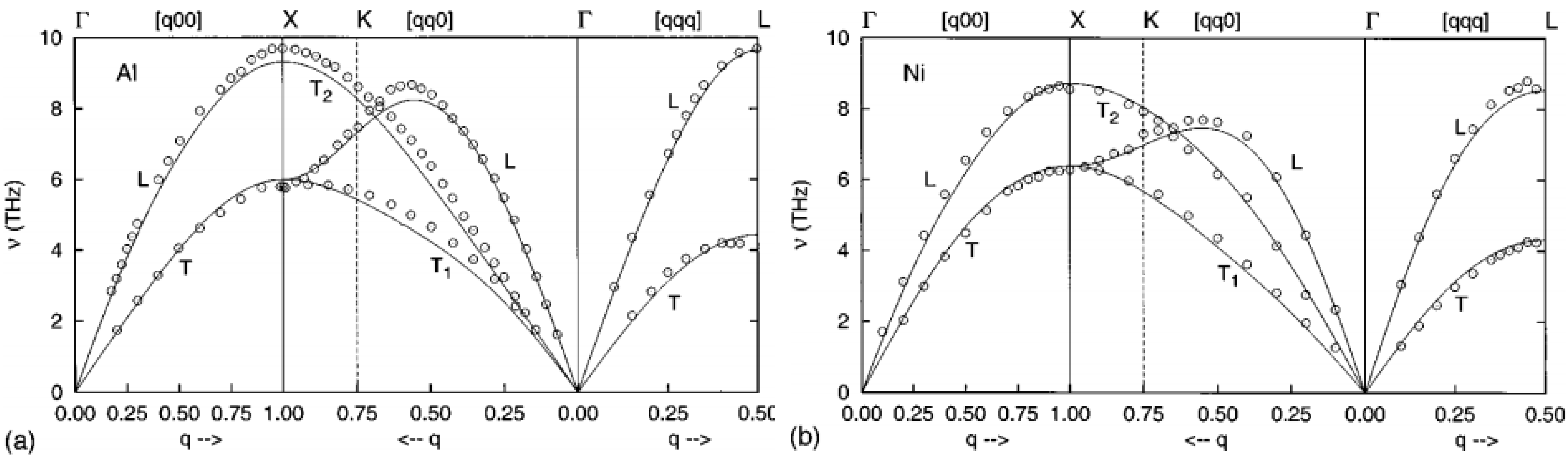
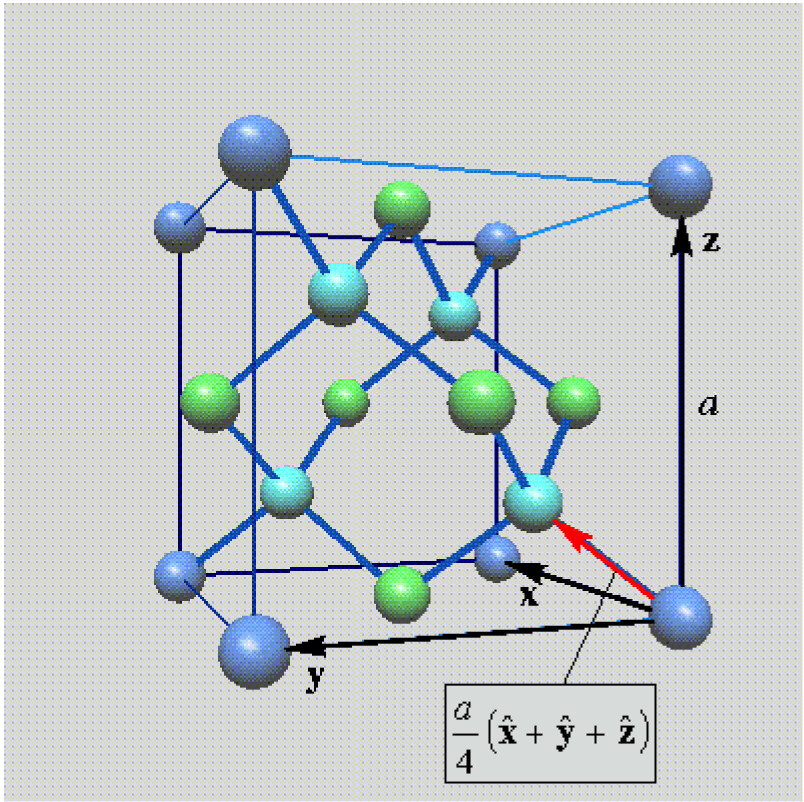


FIG. 2. Comparison of phonon-dispersion curves for Al (a) and Ni (b) predicted by the present EAM potentials, with the experimental values measured by neutron diffraction at 80 K (Al) and 298 K (Ni) (Ref. 33 for Al and Ref. 34 for Ni). The phonon frequencies at point *X* were included in the fitting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

Note that for each q, there are 3 frequencies.

Lattice vibrations for 3-dimensional lattice

Example: diamond lattice



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

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

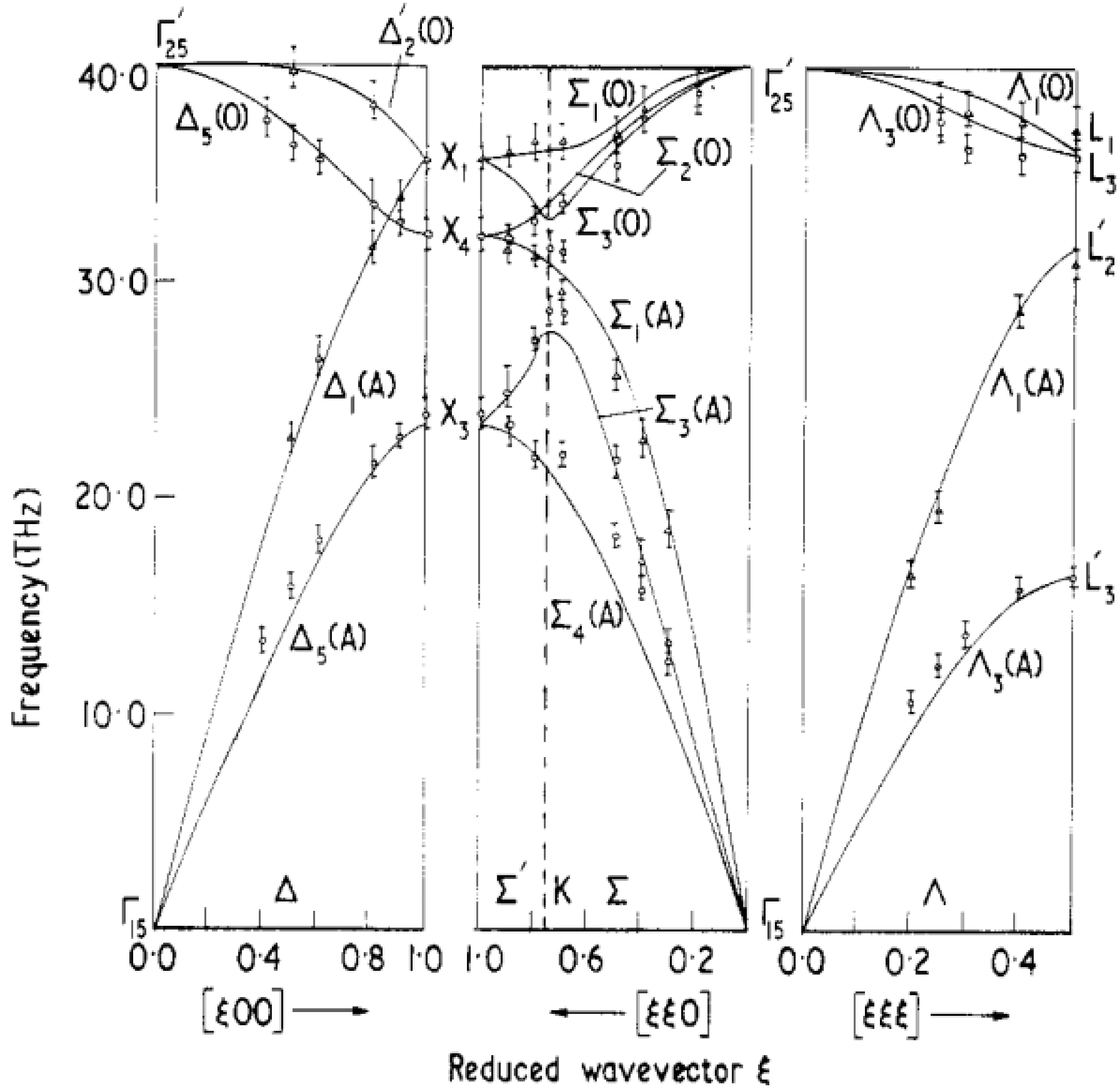


Figure 2. Phonon dispersion curves of diamond. Experimental points *et al* (1965, 1967). △ and ◯ represent the longitudinal and transverse m

Examples of phonon spectra of two forms of boron nitride

Cubic structure

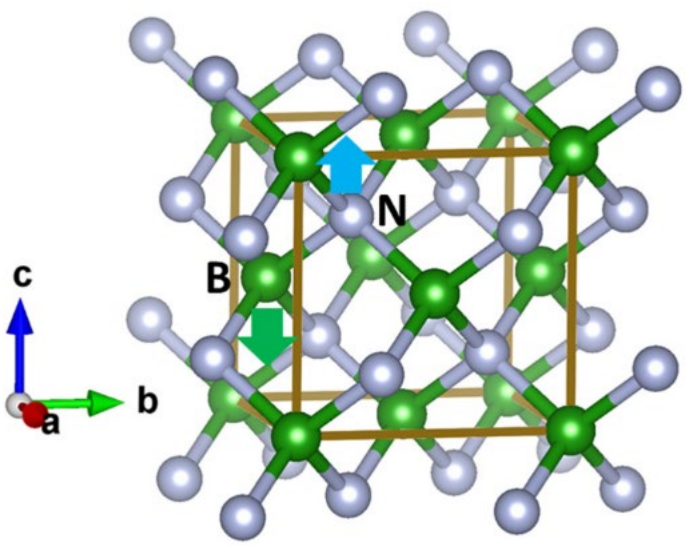


Figure 3. Ball and stick drawing of conventional unit cell of cubic BN (space group $F\bar{4}3m$ [44]) indicating one B and one N site within a primitive cell. The arrows indicate the vibrational directions of the atoms for one of the three degenerate optical modes at $\mathbf{q} = 0$ ($\mathbf{\Gamma}$ point).

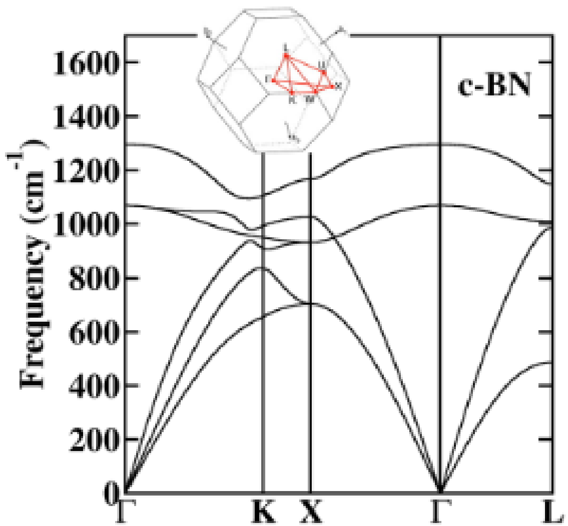


Figure 1. Phonon dispersion curves ($\omega^{\nu}(\mathbf{q})$) for cubic BN. The inset Brillouin zone diagram was reprinted from Setyawan *et al* [7], copyright (2010), with permission from Elsevier.

Examples of phonon spectra of two forms of boron nitride

Hexagonal structure

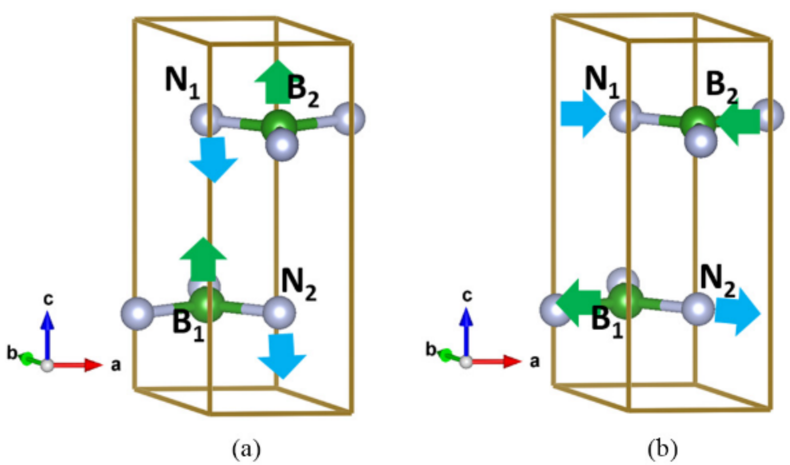


Figure 5. Ball and stick drawing of unit cell of hexagonal BN (space group $P6_3/mmc$ [44]) indicating the four B and N sites. The arrows indicate the vibrational directions of the atoms for $\mathbf{q} = 0$ (Γ point) mode # 7 (a) and for mode # 11 (b).

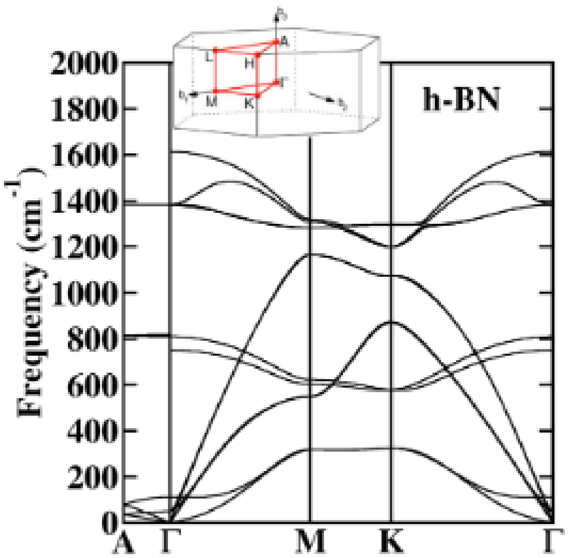


Figure 2. Phonon dispersion curves ($\omega^{\nu}(\mathbf{q})$) for hexagonal BN. The inset Brillouin zone diagram was reprinted from Setyawan *et al* [7], copyright (2010), with permission from Elsevier.

To Sam's question about the relevance of the normal modes –

1. While the classical picture gives us the normal mode frequencies and amplitudes, we must use quantum mechanics to find the real spectrum.
2. Quantum mechanically, each classical normal mode frequency ω is associated with quantum mechanical energy levels $E_n = \hbar\omega(n+\frac{1}{2}) \qquad n = 0,1,2,.....$
3. If one imagines that the vibrating system is in thermodynamic equilibrium at temperature *T*, then we can estimate its Helmholz free energy by summing up all of the spectral states and all of the normal modes --

Helmholz free energy for vibrational energy at temperature T:

$$F_{\text{vib}}(T) = \int_0^\infty d\omega\, f_{\text{vib}}(\omega, T),$$

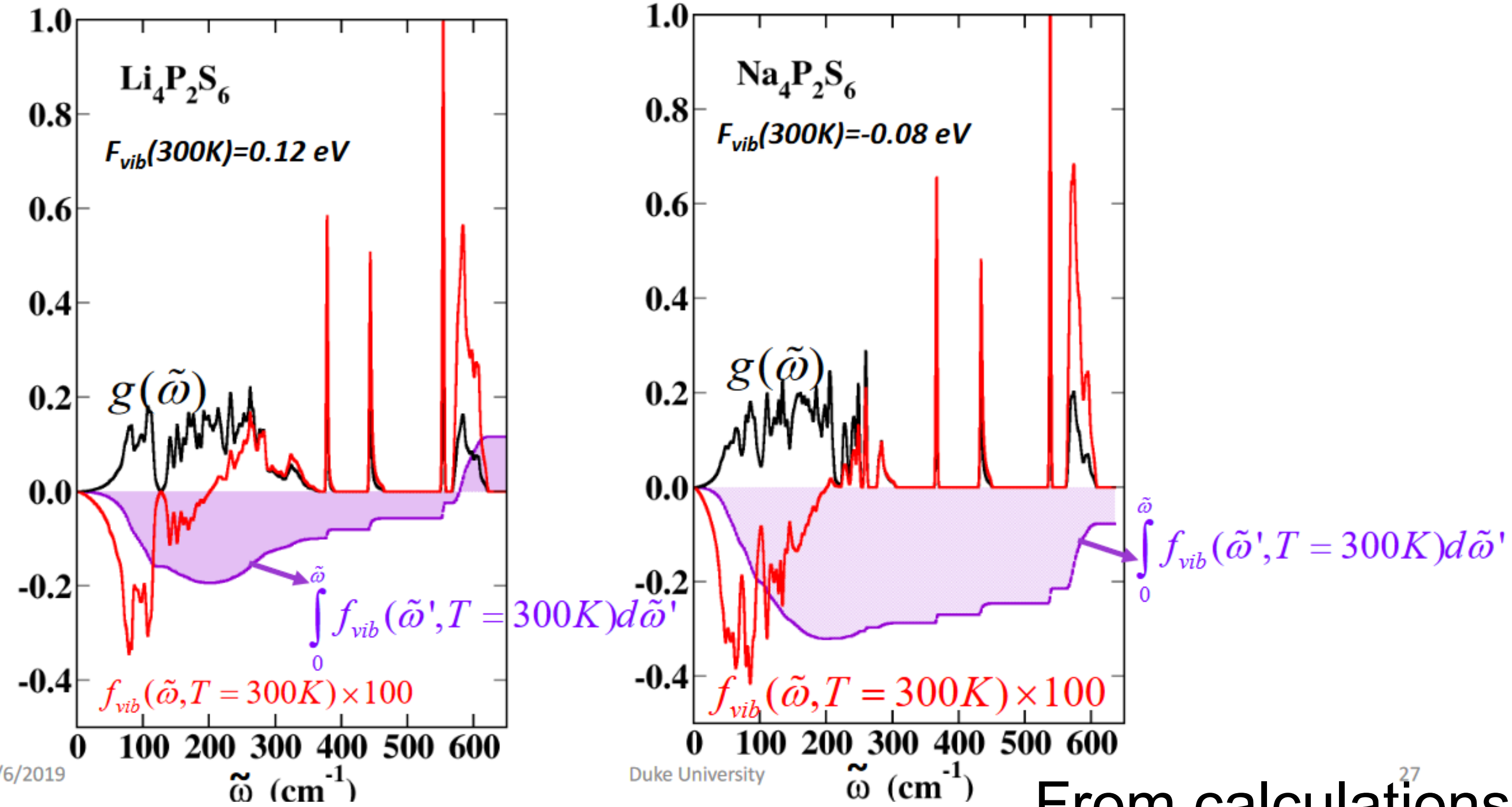
$$f_{\text{vib}}(\omega, T) = k_B T\ \ln\left[2\ \sinh\left(\frac{\hbar\omega}{2k_B T}\right)\right] g(\omega).$$

Phonon density of states:

$$g(\omega) = \frac{V}{(2\pi)^3} \int d^3q \sum_{\nu=1}^{3N} \delta(\omega - \omega_\nu(\mathbf{q})),$$

An example of phonon analysis for two similar materials --

Some details of the vibrational stabilization at T=300K for $Li_4P_2S_6$ and $Na_4P_2S_6$ in C2/m structure



From calculations by Yan Li

Simulation of structural stability patterns -- continued

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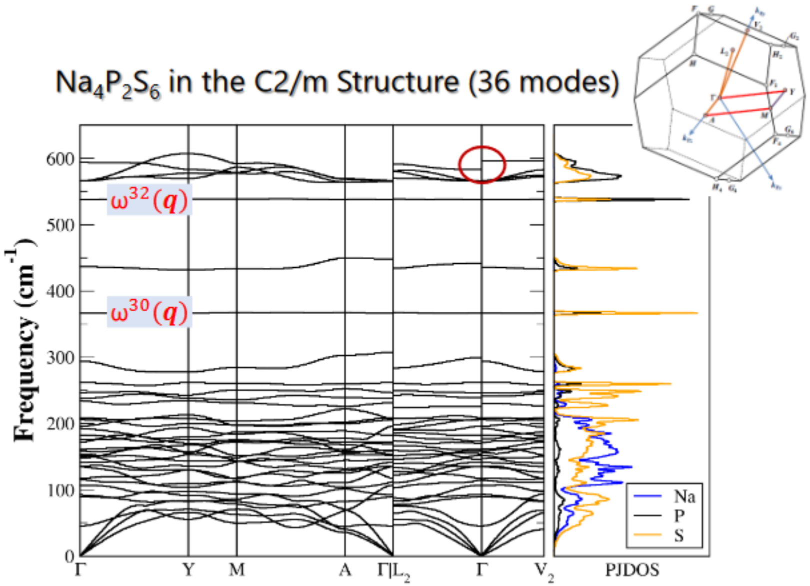
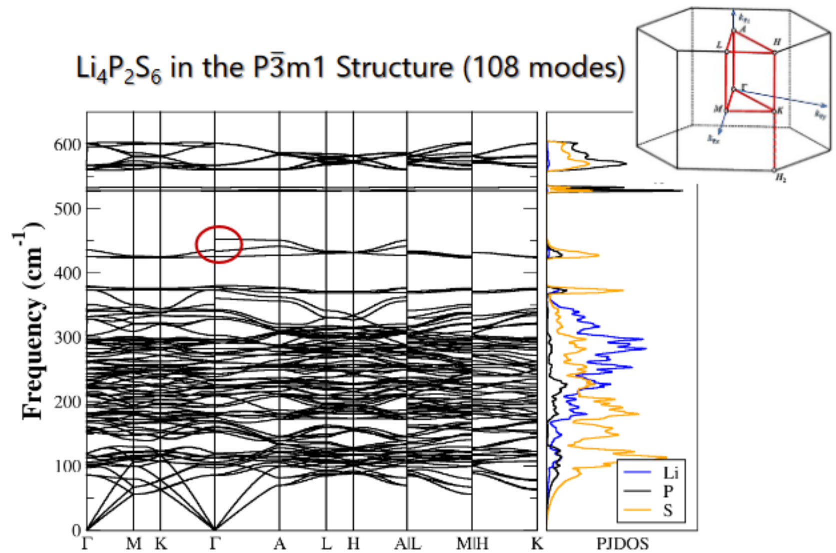
$Na_4P_2S_6$ in the C2/m Structure (36 modes)



Na^+ 0~300 cm^{-1}

$(P_2S_6)^{4-}$ 300~600 cm^{-1}

$Li_4P_2S_6$ in the P$\bar{3}$m1 Structure (108 modes)



Li^+ 0~370 cm^{-1}

$(P_2S_6)^{4-}$ 370~600 cm^{-1}

PJDOS: $$g^a(\omega) \equiv \frac{V}{(2\pi)^3}\int d^3q \sum_{\nu=1}^{3N}(\delta(\omega-\omega_\nu(\mathbf{q}))W_a^\nu(\mathbf{q}))$$

Discontinuous branches at Γ: coupling between photon and photon[2]

[1]Suggested path: Hinuma et al., *Comp. Mat. Sci.* **128**, 140-184 (2017)
[2]Li et al., *J. Phys. Condens. Matter,* **32,** 055402 (2020)

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From calculations by Yan Li