

PHY 711 Classical Mechanics and Mathematical Methods 9-9:50 AM MWF Olin 107

Plan for Lecture 16:

Continue reading Chapter 4

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

10/06/2016

PHY 711 Fall 2017 -- Lecture 16

1

Course schedule

(Preliminary schedule -- subject to frequent adjustment.)

Date	F&W Reading	Topic	Assignment	Due
1 Mon, 8/28/2017	Chap. 1	Introduction	#1	9/6/2017
2 Wed, 8/30/2017	Chap. 1	Scattering theory	#2	9/6/2017
3 Fri, 9/01/2017	Chap. 1	Scattering theory		
4 Mon, 9/04/2017	Chap. 1	Scattering theory	#3	9/8/2017
5 Wed, 9/06/2017	Chap. 2	Physics in an non-inertial reference frame	#4	9/8/2017
6 Fri, 9/08/2017	Chap. 3	Calculus of variations	#5	9/11/2017
7 Mon, 9/11/2017	Chap. 3	Calculus of variations	#6	9/13/2017
8 Wed, 9/13/2017	Chap. 3	Lagrangian Mechanics	#7	9/15/2017
9 Fri, 9/15/2017	Chap. 3 and 6	Lagrangian mechanics and constraints	#8	9/20/2017
10 Mon, 9/18/2017	Chap. 3 and 6	Constants of the motion		
11 Wed, 9/20/2017	Chap. 3 and 6	Hamiltonian formalism	#9	9/27/2017
12 Fri, 9/22/2017	Chap. 3 and 6	Louville equation		
13 Mon, 9/25/2017	Chap. 6	Canonical transformations		
14 Wed, 9/27/2017	Chap. 4	Motion from Small oscillations about equilibrium		
15 Fri, 9/29/2017	Chap. 1-4,6	Review		
Mon, 10/02/2017		Take-home exam -- No class		
Wed, 10/04/2017		Take-home exam -- No class		
16 Fri, 10/06/2017	Chap. 4	Vibrational modes		

10/06/2016

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2



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WFU Physics

WFU Physics People Events and News Undergraduate Graduate Research Resources



Events

Colloquium: Oct. 4, 2017 at 4 PM
 WFU Physics and Chemistry Colloquium
 TITLE: "Quantum Processing of High-Performance Solid-State Qubits and Technological Challenges" SPEAKER: Professor Qipeng Chen, Department of Physics and Science Data Center, Tsinghua University, Beijing, China, NO TIME ...

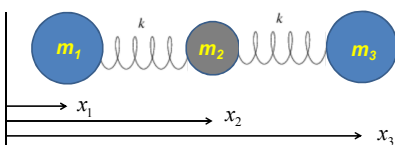
Special seminar: Oct. 6, 2017 at 3 PM
 Special WFU Physics and Chemistry Seminar
 TITLE: "Template for Energy Storage: The Determining Effect of the Interface Between Host Network and Confined Ionic Liquid" SPEAKER: Jean-Luc Dubois, Institut des ...

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3

Example – linear molecule



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

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4

Let: $x_1 \rightarrow x_1 - x_1^0$ $x_2 \rightarrow x_2 - x_1^0 - \ell_{12}$ $x_3 \rightarrow x_3 - x_1^0 - \ell_{12} - \ell_{23}$

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

Coupled equations of motion :

$$m_1 \ddot{x}_1 = k(x_2 - x_1)$$

$$m_2 \ddot{x}_2 = -k(x_2 - x_1) + k(x_3 - x_2) = k(x_1 - 2x_2 + x_3)$$

$$m_3 \ddot{x}_3 = -k(x_3 - x_2)$$

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

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

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

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

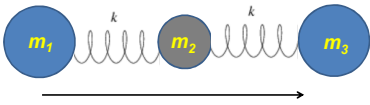
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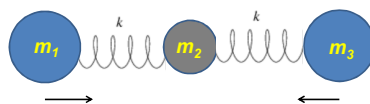
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For $m_1 = m_3 \equiv m_o$

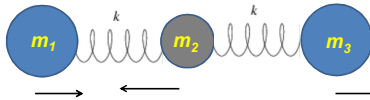
and $m_2 \equiv m_c$



$$\omega_1 = 0$$



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



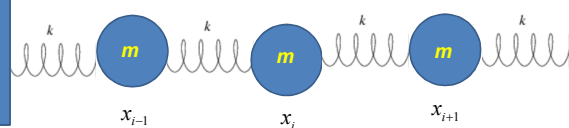
$$\omega_3 = \sqrt{\frac{k}{m_o} + \frac{2k}{m_c}}$$

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6

Consider an extended system of masses and springs:



Note: each mass coordinate is measured relative to its equilibrium position x_i^0

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

Note: In fact, we have N masses; x_0 and x_{N+1} will be treated using boundary conditions.

10/06/2016

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7

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

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

From Euler - Lagrange equations :

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

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

.....

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

.....

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

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8

From Euler - Lagrange equations :

$$m\ddot{x}_j = k(x_{j+1} - 2x_j + x_{j-1}) \quad \text{with } x_0 = 0 = x_{N+1}$$

$$\text{Try: } x_j(t) = A e^{-i\omega t + i q a j}$$

$$-\omega^2 A e^{-i\omega t + i q a j} = \frac{k}{m} (e^{i q a} - 2 + e^{-i q a}) A e^{-i\omega t + i q a j}$$

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

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

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9

From Euler - Lagrange equations -- continued :

$$m\ddot{x}_j = k(x_{j+1} - 2x_j + x_{j-1}) \quad \text{with } x_0 = 0 = x_{N+1}$$

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

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

General solution :

$$x_j(t) = \Re(Ae^{-i\omega t + iqa j} + Be^{-i\omega t - iqa j})$$

Impose boundary conditions :

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

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

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10

Impose boundary conditions -- continued :

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

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

$$\Rightarrow B = -A$$

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

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

$$\Rightarrow qa(N+1) = \nu\pi \quad \text{where } \nu = 0, 1, 2, \dots$$

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

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11

Recap -- solution for integer parameter ν

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

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

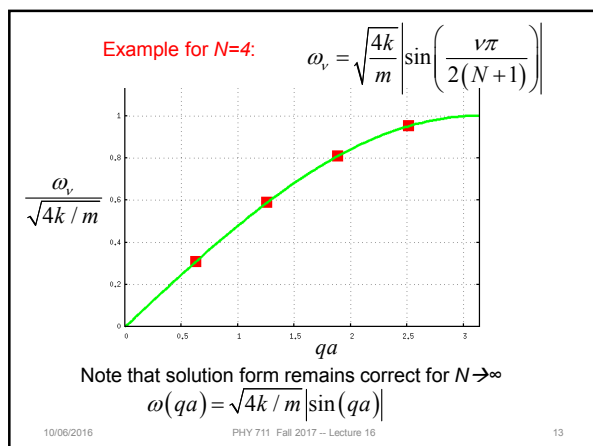
Note that non - trivial, unique values are

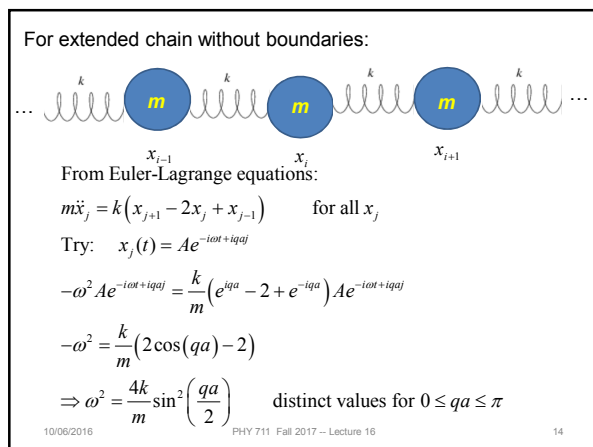
$$\nu = 1, 2, \dots, N$$

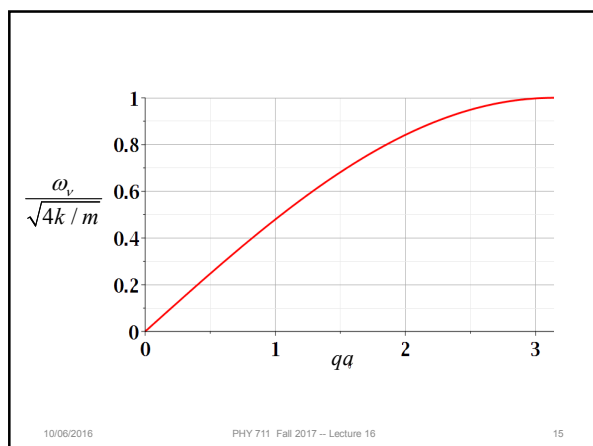
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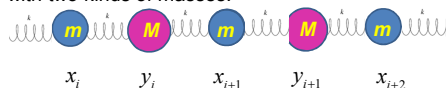
12







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



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

$$L = T - V$$

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

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16

$$L = T - V$$

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

Euler - Lagrange equations:

$$m \ddot{x}_j = k(y_{j-1} - 2x_j + y_j)$$

$$M \ddot{y}_j = k(x_j - 2y_j + x_{j+1})$$

Trial solution:

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

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

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

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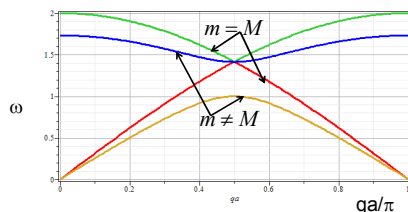
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17

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

Solutions:

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



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18

Eigenvectors:

For $qa = 0$:

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

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

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

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

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

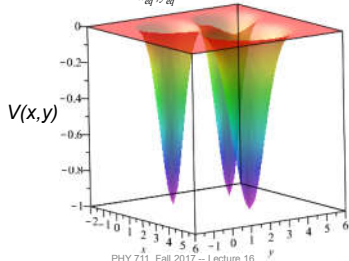
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19

Potential in 2 and more dimensions

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

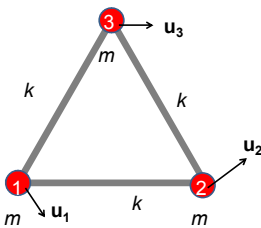


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20

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



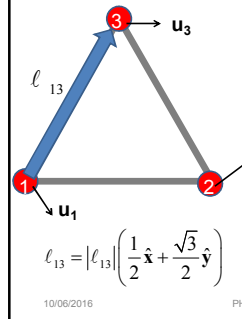
Degrees of freedom for
2-dimensional motion:
 $2N = 6$

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21

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



Potential contribution for spring 13:

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

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

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

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

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

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

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

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

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

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

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

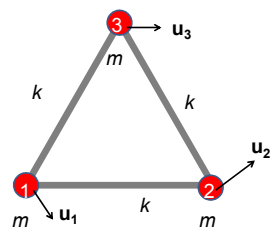
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Example – normal modes of a system with the symmetry of an equilateral triangle -- continued

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

10/06/2016 PHY 711 Fall 2017 -- Lecture 16 24

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



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

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25

3-dimensional periodic lattices

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

Diagram of
atom positions

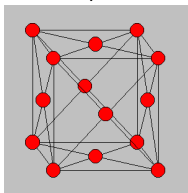
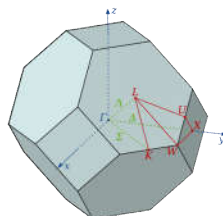


Diagram of q-
space $\nu(q)$



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26

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

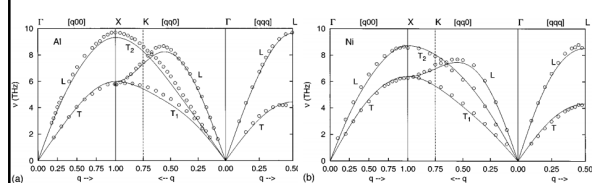


FIG. 2. Comparison of phonon-dispersion curves for Al (a) and Ni (b) predicted by the present EAM potentials, with the experimental values measured by neutron diffraction at 80 K (Al) and 298 K (Ni) (Ref. 33 for Al and Ref. 34 for Ni). The phonon frequencies at point X were included in the fitting database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

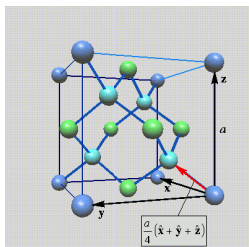
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27

Lattice vibrations for 3-dimensional lattice

Example: diamond lattice

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

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28

Atoms located at the positions :

$$\mathbf{R}^a = \mathbf{R}_0^a + \mathbf{u}^a$$

Potential energy function near equilibrium :

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

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

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

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

10/06/2016

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29

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

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: $\mathbf{R}_0^a = \mathbf{\tau}^a + \mathbf{T}$ where $\mathbf{\tau}^a$ denotes
unique sites and
 $\mathbf{T}$ denotes replicas

10/06/2016

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30

Define :

$$W_{jk}^{ab}(\mathbf{q}) = \sum_{\mathbf{r}} \frac{D_{jk}^{ab} e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')} }{\sqrt{m_a m_b}} e^{i\mathbf{q} \cdot \mathbf{r}}$$

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.

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

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31

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

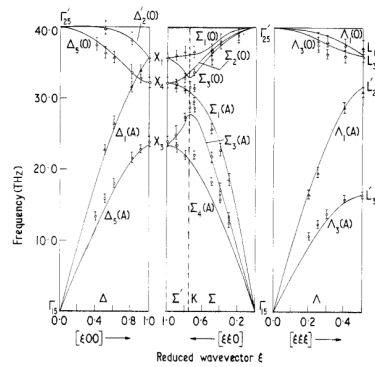


Figure 2. Phonon dispersion curves of diamond. Experimental points *et al* (1965, 1967). Δ and $\circ$ represent the longitudinal and transverse modes.

10/06/2016

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32