PHY 752 Solid State Physics
11-11:50 AM MWF Olin 103

Plan for Lecture 28: Chap. 9 of GGGPP

Lattice dynamics of crystals

1. **Normal modes of one-dimensional lattices**
2. **Normal modes of three-dimensional lattices**

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14	Fri, 9/25/2015	Chap. 5	Implementation of density functional theory	#13
15	Mon, 9/28/2015	Chap. 5	Implementation of density functional theory	#14
16	Wed, 9/30/2015	Chap. 5	First principles pseudopotential methods	#15
17	Fri, 10/02/2015	Chap. 6	Example electronic structures	#16
18	Mon, 10/05/2015	Chap. 6	Ionic and covalent crystals	#17
19	Wed, 10/07/2015	Chap. 6	More examples of electronic structures	#18
20	Fri, 10/09/2015	Chap. 1-6	Review	Start exam
	Mon, 10/12/2015		No class	Take-home exam
	Wed, 10/14/2015		No class	Exam due before 10/19/2015
	Fri, 10/16/2015		Fall break -- no class	
21	Mon, 10/19/2015	Chap. 10	X-ray and neutron diffraction	#19
22	Wed, 10/21/2015	Chap. 10	Scattering of particles by crystals	#20
23	Fri, 10/23/2015	Chap. 11	Optical and transport properties of metals	#21
24	Mon, 10/26/2015	Chap. 11	Optical and transport properties of metals	#22
25	Wed, 10/28/2015	Chap. 11	Transport in metals	#23
26	Fri, 10/30/2015	Chap. 12	Optical properties of semiconductors and insulators	
27	Mon, 11/02/2015	Chap. 7 & 12	Excitons	#24
28	Wed, 11/04/2015	Chap. 9	Lattice vibrations	#25
	Wed, 12/02/2015		Student presentations I	
	Fri, 12/04/2015		Student presentations II	
	Mon, 12/07/2015		Begin Take-home final	

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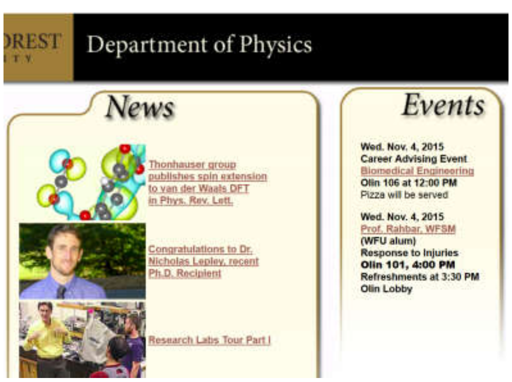

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WFU Physics Colloquium

TITLE: The response to traumatic injuries: A journey down the road less traveled

SPEAKER: Professor Elaheh Rahbar, (WFU alum)

Biomedical Engineering Center for Public Health Genomics, Wake Forest School of Medicine

TIME: Wednesday November 4, 2015 at 4:00 PM

PLACE: Room 101 Olin Physical Laboratory

Refreshments will be served at 3:30 PM in the Olin Lounge. All interested persons are cordially invited to attend.

ABSTRACT

Trauma is the leading cause of death in people under the age of 45 years in both civilian and military populations, with hemorrhagic shock accounting for nearly 50% of these fatalities. Death from hemorrhagic shock is considered potentially preventable with appropriate resuscitation. However there remains no optimal or standardized resuscitation protocol for trauma patients. In this seminar, I will present findings from various clinical prospective observational studies, pilot clinical trials and the most recent findings from the multi-site randomized clinical trial PROPPR; all which investigated the physiologic response

Thanks to the Born-Oppenheimer approximation, the nuclei of a material in equilibrium move in the potential field provided by the ground electronic state of the system

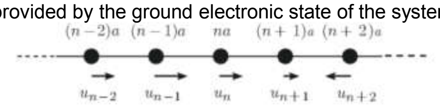
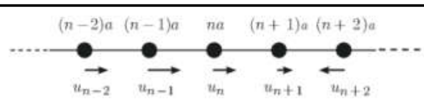


Figure 9.1 Longitudinal displacements in a one-dimensional monoatomic lattice. The equilibrium positions $t_n = na$ are indicated by circles; the displacements u_n at a given instant are indicated by arrows.

The ground electronic state depends on the nuclear positions

$E_0\left(\left\{\mathbf{R}^a\right\}\right)$ Suppose $\mathbf{R}^a = \mathbf{R}^{a0} + \mathbf{u}^a$



For one-dimensional case:

$$E_0(\{u_n\}) = E_0(0) + \frac{1}{2}\sum_{nn'}\left(\frac{\partial^2 E_0}{\partial u_n \partial u_{n'}}\right)_0 u_n u_{n'} + \frac{1}{3!}\sum_{nn'n''}\left(\frac{\partial^3 E_0}{\partial u_n \partial u_{n'} \partial u_{n''}}\right)_0 u_n u_{n'} u_{n''} + \cdots$$

$$E_0^{(\mathrm{harm})}(\{u_n\}) = E_0(0) + \frac{1}{2}\sum_{nn'} D_{nn'} u_n u_{n'}. \qquad D_{nn'} = \left(\frac{\partial^2 E_0}{\partial u_n \partial u_{n'}}\right)_0$$

Relationships:

$$D_{nn'} = D_{n'n}. \qquad D_{nn'} = D_{mm'} \quad \text{if} \quad t_n - t_{n'} = t_m - t_{m'}.$$

$$\sum_{n'} D_{nn'} = 0 \quad \text{for any} \quad n;$$

Classical equations of motion:

$$M\ddot{u}_n = -\sum_{n'} D_{nn'} u_{n'}$$

Solution

$$u_n(t) = A\, e^{i(qna-\omega t)}$$

$$-M\omega^2 A = -\sum_{n'} D_{nn'} e^{-iq(na-n'a)} A.$$

$$\boxed{M\omega^2(q) = D(q)},$$

where

$$\boxed{D(q) = \sum_{n'} D_{nn'}\, e^{-iq(na-n'a)}};$$

Analytic result for monoatomic chain with only nearest neighbor interactions

$$D_{nn} = 2C, \quad D_{n\,n+1} = D_{n-1\,n} = -C. \qquad D_{nn'} = 0 \quad \text{if } |\ n' - n| > 1$$

$$D(q) = \sum_{n'} D_{nn'} e^{iqa(n-n')} = C\left(2 - e^{iqa} - e^{-iqa}\right) = 4C\sin^2\left(qa/2\right)$$

➔ $\omega = \sqrt{\frac{4C}{M}}\left|\sin\frac{1}{2}qa\right|$

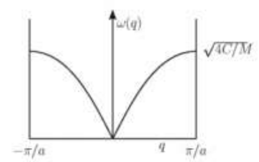


Figure 9.2 Phonon dispersion curve for a monoatomic linear lattice with nearest neighbor interactions only; the Brillouin zone is the segment between $-\pi/a$ and $+\pi/a$.

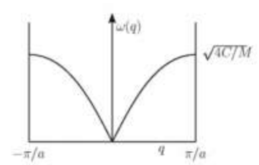


Figure 9.2 Phonon dispersion curve for a monoatomic linear lattice with nearest neighbor interactions only; the Brillouin zone is the segment between $-\pi/a$ and $+\pi/a$.

$$\omega = \sqrt{\frac{C}{M}}aq \equiv v_s q \quad (qa \ll 1);$$

velocity of sound in the material

One-dimensional diatomic lattice

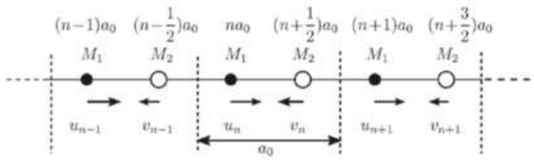


Figure 9.3 Longitudinal displacements in a one-dimensional diatomic lattice. The equilibrium positions of the two sublattices of atoms, of mass M_1 and M_2, are indicated by black and white circles, respectively; the displacements u_n and v_n at a given instant are indicated by arrows.

Equations of motion for this case:

$$M_1\ddot{u}_n = -C(2u_n - v_{n-1} - v_n)$$
$$M_2\ddot{v}_n = -C(2v_n - u_n - u_{n+1})$$

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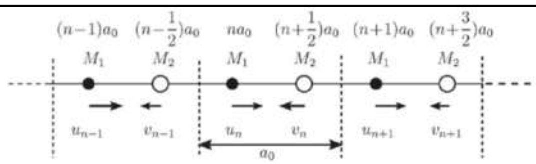

Solution: $u_n(t) = A_1\, e^{i(qna_0-\omega t)}$ and $v_n(t) = A_2\, e^{i(qna_0+qa_0/2-\omega t)}$

convenient constant

$$-M_1\omega^2 A_1 = -C(2A_1 - A_2\, e^{-iqa_0/2} - A_2\, e^{iqa_0/2}),$$
$$-M_2\omega^2 A_2 = -C(2A_2 - A_1\, e^{-iqa_0/2} - A_1\, e^{iqa_0/2}).$$

Necessary condition for non-trivial solution:

$$\begin{vmatrix} 2C - M_1\omega^2 & -2C\cos(qa_0/2) \\ -2C\cos(qa_0/2) & 2C - M_2\omega^2 \end{vmatrix} = 0.$$

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One-dimensional diatomic lattice -- continued

Normal modes

$$\omega^2 = C\left(\frac{1}{M_1}+\frac{1}{M_2}\right) \pm C\sqrt{\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2 - \frac{4\sin^2(qa_0/2)}{M_1M_2}},$$

$$\frac{A_1}{A_2} = \frac{2C\cos(qa_0/2)}{2C - M_1\omega^2},$$

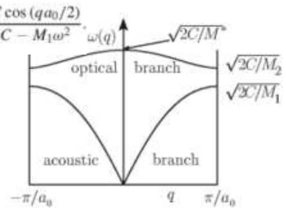

Figure 9.4 Phonon dispersion curves of a diatomic linear chain, with nearest neighbor atoms interacting with spring constant C. The masses of the atoms are M_1 and M_2 (with $M_1 > M_2$); M^* is the reduced mass.

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Lattice modes of general three-dimensional crystals

$$E_0^{(\mathrm{harm})}(\{\mathbf{u}_{n\nu}\}) = E_0(0) + \frac{1}{2}\sum_{n\nu\alpha,n'\nu'\alpha'} D_{n\nu\alpha,n'\nu'\alpha'} u_{n\nu\alpha} u_{n'\nu'\alpha'}$$

$$D_{n\nu\alpha,n'\nu'\alpha'} = \left(\frac{\partial^2 E_0}{\partial u_{n\nu\alpha}\partial u_{n'\nu'\alpha'}}\right)_0.$$

Relationships:

$$D_{n\nu\alpha,n'\nu'\alpha'} = D_{n'\nu'\alpha',n\nu\alpha}.$$

$$D_{n\nu\alpha,n'\nu'\alpha'} = D_{m\nu\alpha,m'\nu'\alpha'} \quad \text{if} \quad \mathbf{t}_n - \mathbf{t}_{n'} = \mathbf{t}_m - \mathbf{t}_{m'}$$

$$\sum_{n'\nu'} D_{n\nu\alpha,n'\nu'\alpha'} \equiv 0.$$

Lattice modes of general three-dimensional crystals -- continued

Equations of motion

$$\boxed{M_\nu \ddot{u}_{n\nu\alpha} = -\sum_{n'\nu'\alpha'} D_{n\nu\alpha,n'\nu'\alpha'} u_{n'\nu'\alpha'}}.$$

Solution

$$\mathbf{u}_{n\nu}(t) = \mathbf{A}_\nu(\mathbf{q},\omega) e^{i(\mathbf{q}\cdot\mathbf{t}_n - \omega t)}.$$

$$-M_\nu \omega^2 A_{\nu\alpha} = -\sum_{n'\nu'\alpha'} D_{n\nu\alpha,n'\nu'\alpha'} e^{-i\mathbf{q}\cdot(\mathbf{t}_n - \mathbf{t}_{n'})} A_{\nu'\alpha'}$$

$$D_{\nu\alpha,\nu'\alpha'}(\mathbf{q}) = \sum_{n'} D_{n\nu\alpha,n'\nu'\alpha'} e^{-i\mathbf{q}\cdot(\mathbf{t}_n - \mathbf{t}_{n'})}.$$

$$\boxed{\left\| D_{\nu\alpha,\nu'\alpha'}(\mathbf{q}) - M_\nu \omega^2 \delta_{\alpha\alpha'}\delta_{\nu,\nu'} \right\| = 0}.$$

Lattice modes of general three-dimensional crystals -- continued

Some special values

$$\sum_{\nu'} D_{\nu\alpha,\nu'\alpha'}(\mathbf{q}=0) \equiv 0;$$

$$\sum_{\nu'\alpha'} D_{\nu\alpha,\nu'\alpha'}(\mathbf{q}=0) A_{\alpha'} \equiv 0.$$

Orthogonality of normal modes

$$\sum_{\nu\alpha} M_\nu A^*_{\nu\alpha}(\mathbf{q},p) A_{\nu\alpha}(\mathbf{q},p') = \delta_{p,p'}.$$

Example for fcc Al lattice

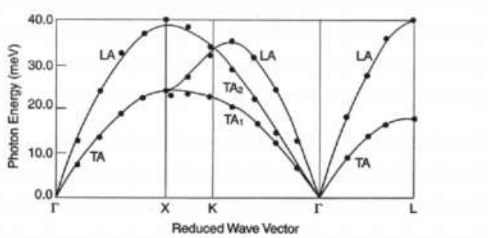

Figure 9.5 Phonon dispersion curves of aluminum along symmetry directions. The solid lines represents the calculations of Fig. 1, Phys. Rev. B *46*, 10734 (1992). Longitudinal and transverse acoustic branchesare indicated by LA and TA (or TA_1 and TA_2), respectively. The experimental points are from the papers of G. Gilat and R. M. Nicklow, Phys. Rev. *143*, 487 (1966) and R. Stedman, S. Almqvist and G. Nilsson, Phys. Rev. *162*, 549 (1967).

Example for Si and Ge lattices

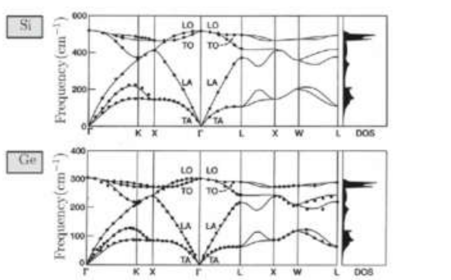

Figure 9.6 Phonon dispersion curves and density-of-states of Si and Ge calculated by Figs. 1, 2, Phys. Rev. B *43*, 7231 (1991). Longitudinal and transverse acoustic (or optical) modes are indicated by LA and TA (LO and TO), respectively. The experimental points are from G. Dolling, in "Inelastic Scattering of Neutrons in Solids and Liquids" edited by S. Ekland (IAEA, Vienna, 1963) Vol. II, p. 37; G. Nilsson and G. Nelin, Phys. Rev. B *3*, 364 (1971) and Phys. Rev. B *6*, 3777 (1972). Conversion to meV units can be done noting that $1\ cm^{-1} = 0.124$ meV.

Example for LiF

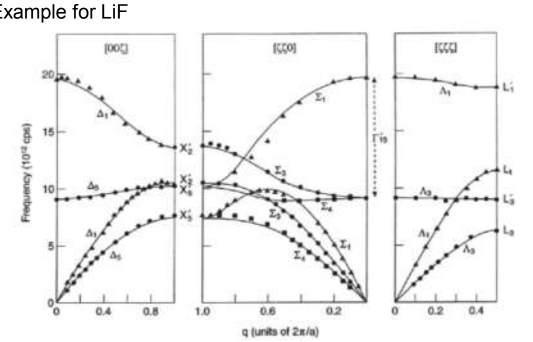

Figure 9.8 Measured phonon dispersion curves along three directions of high symmetry in LiF; the solid curves are a best least-squares fit of a parameter model [With permission from Fig. 4, Phys. Rev. *168*, 970 (1968)]. Notice that 10^{12} Hz = 4.137 meV.

Summary from various semiconductors

Table 9.2 Frequencies ω_{LO} and ω_{TO} in cm^{-1} (=0.124 meV) of longitudinal optical and transverse optical phonons for six semiconductors. The calculations are taken from P. Giannozzi, S. de Gironcoli, P. Pavone and S. Baroni, Phys. Rev. B *43*, 7231 (1991), to which we refer for further details; experimental data are in parentheses. The static and the high-frequency dielectric constants are also given; notice that the ratio $\omega_{LO}^2/\omega_{TO}^2$ equals (within experimental error) the ratio $\varepsilon_s/\varepsilon_\infty$.

	Si	**Ge**	**GaAs**	**AlAs**	**GaSb**	**AlSb**
ω_{LO}	517 (517)	306 (304)	291 (291)	400 (402)	237 (233)	334 (344)
ω_{TO}	517 (517)	306 (304)	271 (271)	363 (361)	230 (224)	316 (323)
$\omega_{LO}^2/\omega_{TO}^2$	1	1	1.15 (1.17)	1.22 (1.24)	1.06 (1.08)	1.12 (1.14)
ε_s	12.1	16.5	12.40	10.06	15.69	12.04
ε_∞	12.1	16.5	10.60	8.16	14.44	10.24
$\varepsilon_s/\varepsilon_\infty$	1	1	1.17	1.23	1.09	1.17