EEE 6212
Semiconductor Materials

Lecture 8: phonons

Outline of L8: phonons

- introduction: definitions & adiabatic approximation
- simple phonon model – harmonic oscillator
- dispersion relationship for 1D monoatomic system
- more complexity – 1D diatomic system
- 3D systems
- phonons in action – speed of sound
- quantisation
- why we *really* care about phonons….
- summary

The Hamiltonian

The Hamiltonian is a sum of operators corresponding to the potential energy and kinetic energy of the system. As energy is preserved, this is a constant:

$$\hat{T} = \frac{\hat{\mathbf{p}}\cdot\hat{\mathbf{p}}}{2m} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\nabla^2$$

$$\hat{p} = -i\hbar\nabla$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$\begin{aligned}\hat{H} &= \hat{T} + \hat{V} \\ &= \frac{\hat{\mathbf{p}}\cdot\hat{\mathbf{p}}}{2m} + V(\mathbf{r},t) \\ &= -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r},t)\end{aligned}$$

B.K. Ridley §1 p1!

lattice of nuclei

electrons

ions are ~10^4 heavier than electrons, hence move ~10^2 slower at same kinetic energy

1. Band structure of semiconductors

1.1. The crystal Hamiltonian

For an assembly of atoms the classical energy is the sum of the following:

(a) the kinetic energy of the nuclei;
(b) the potential energy of the nuclei in one another's electrostatic field;
(c) the kinetic energy of the electrons;
(d) the potential energy of the electrons in the field of the nuclei;
(e) the potential energy of the electrons in one another's field;
(f) the magnetic energy associated with the spin and the orbit.

Dividing the electrons into core and valence electrons and leaving out magnetic effects leads to the following expression for the crystal Hamiltonian:

$$H = \sum_l \frac{\mathbf{p}_l^2}{2M_l} + \sum_{l,m} U(\mathbf{R}_l - \mathbf{R}_m) + \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_{i,l} V(\mathbf{r}_i - \mathbf{R}_l) + \sum_{i,j} \frac{e^2/4\pi\epsilon_0}{|\mathbf{r}_i - \mathbf{r}_j|} \qquad (1.1)$$

where l and m label the ions, i and j label the electrons, $\mathbf{p}$ is the momentum, M is the ionic mass, m is the mass of the electron, $U(\mathbf{R}_l - \mathbf{R}_m)$ is the interionic potential, and $V(\mathbf{r}_i - \mathbf{R}_l)$ is the valence–electron–ion potential.

The Schrödinger equation determines the time-independent energies of the system:

$$H\Xi = E\Xi \qquad (1.2)$$

where H is now the Hamiltonian operator.

Brian K Ridley: Electrons and Phonons in Semiconductor Multilayers, CUP, 2nd ed., 2014

Adiabatic approximation

$$\Xi = \Psi(\mathbf{r}, \mathbf{R})\Phi(\mathbf{R})$$

electron wavefunction   ionic wavefunction

Schrödinger equation can be written as

$$\Psi(\mathbf{r}, \mathbf{R})H_L\Phi(\mathbf{R}) + \Phi(\mathbf{R})H_e\Psi(\mathbf{r}, \mathbf{R}) + H'\Psi(\mathbf{r}, \mathbf{R})\Phi(\mathbf{R}) = E\Psi(\mathbf{r}, \mathbf{R})\Phi(\mathbf{R})$$

where

$$H'\Psi(\mathbf{r}, \mathbf{R})\Phi(\mathbf{R}) = H_L\Psi(\mathbf{r}, \mathbf{R})\Phi(\mathbf{R}) - \Psi(\mathbf{r}, \mathbf{R})H_L\Phi(\mathbf{R})$$

$$H_L = \sum_l \frac{\mathbf{p}_l^2}{2M_l} + \sum_{l,m} U(\mathbf{R}_l - \mathbf{R}_m)$$

$$H_e = \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_{i,l} V(\mathbf{r}_i - \mathbf{R}_l) + \sum_{i,j} \frac{e^2/4\pi\epsilon_0}{|\mathbf{r}_i - \mathbf{r}_j|}$$

ionic equation

$$H_L\Phi(\mathbf{R}) = E_L\Phi(\mathbf{R})$$

electronic equation

$$H_e\Psi(\mathbf{r}, \mathbf{R}) = E_e\Psi(\mathbf{r}, \mathbf{R}).$$

phonon

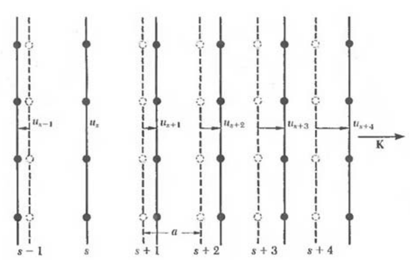
Definition: A phonon is a collective excitation in a periodic, elastic arrangement of atoms or molecules in condensed matter, such as solids and some liquids.

phonons obey Bose-Einstein statistics ('are bosons'),

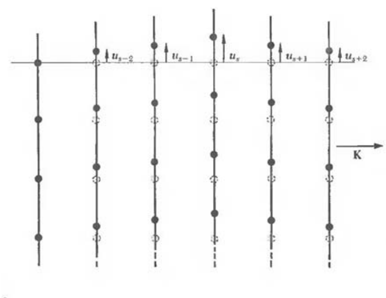
c.f. electron (fermion – two or more particles cannot occupy same state), photon (boson – two or more particles can occupy same state),…

crystal displacement

consider [hkl] crystal directions with {hkl} planes of atoms perpendicular to them

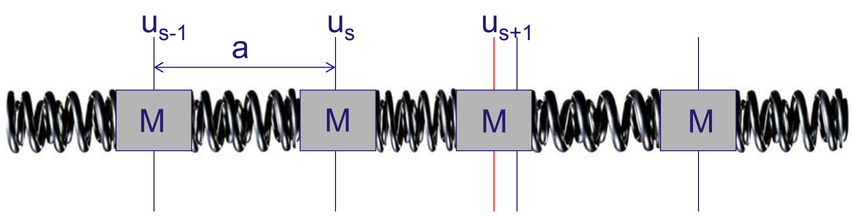


longitudinal wave



2x transverse waves
(2 degenerate polarisations)

1D monoatomic system



Assume elastic response is linear with force (Hooke's Law) – one atom per unit cell, equal distance between atoms
Force on plane s caused by displacement of plane s+p (here p=1)

$$F_s = C(u_{s+1} - u_s) + C(u_{s-1} - u_s)$$

C is force constant between nearest neighbours – different for different crystallographic directions, transverse, longitudinal waves

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Calculation of dispersion

F=Ma, (M = mass of atom) so

$$M\frac{d^2u_s}{dt^2} = C(u_{s+1} + u_{s-1} - 2u_s)$$

Want solutions with all displacements having time dependence exp(-iωt)
Then $d^2u_s/dt^2 = -\omega^2 u_s$ so:

$$-M\omega^2 u_s = C(u_{s+1} + u_{s-1} - 2u_s)$$

Solution to this differential equation has travelling wave solutions of form

$$u_{s\pm 1} = u \exp(isKa)\exp(\pm iKa)$$

K is wavevector, *a* is separation of planes – putting these two together

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Calculation of dispersion (2)

$$-\omega^2 Mu\exp(isKa) = Cu\{\exp[i(s+1)Ka] + \exp[i(s-1)Ka] - 2\exp(isKa)\}$$

Cancelling *u* exp(is*Ka*) -

$$\omega^2 M = -C[\exp(iKa) + \exp(-iKa) - 2]$$

exp(i*Ka*)=cos(*Ka*)+ i sin(*Ka*)

$$\omega^2 = (2C/M)(1 - \cos Ka)$$

Using $\sin^2(x) = \frac{1}{2}[1 - \cos(2x)]$

$$\omega^2 = (4C/M)\sin^2 \tfrac{1}{2}Ka$$

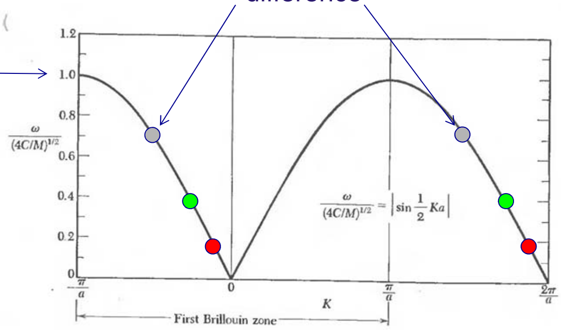
$\omega = 2\sqrt{C/M}\,\sin(\tfrac{1}{2}Ka)$

Phonon dispersion

identical
$2\pi n/a$ phase
difference

As $\exp(2\pi i n)=1$

$$u_{s\pm1} = u \exp(isKa)$$



This is a standing wave-
c.f. Bragg diffraction

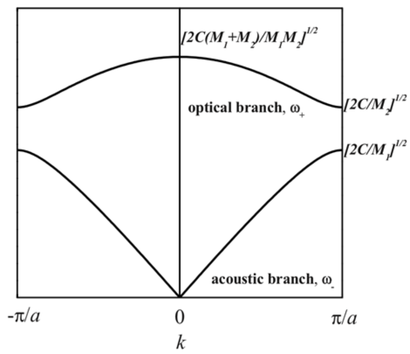
group velocity = $d\omega/dk = 0$

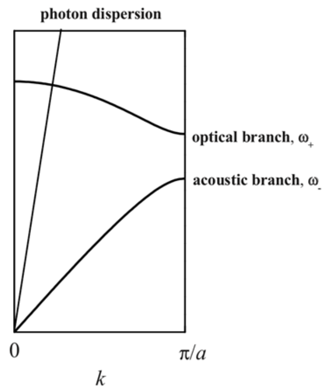
(propagation of envelope)

property of entire lattice – not single atom
Bloch waves – solutions completely described by behaviour in single Brillouin zone ➔ $K \pm \pi/a$

1D diatomic system

Previously considered 1 atom per unit cell – Derivation for 2 is provided e.g. in Kittel's textbook and lead to a new branch





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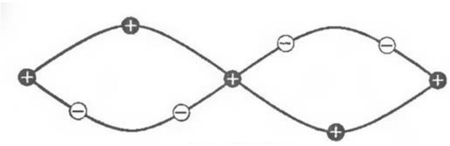
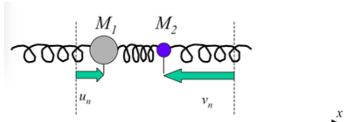
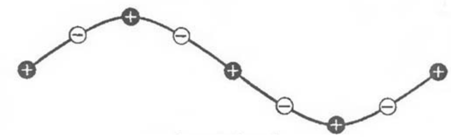
Different phonon types



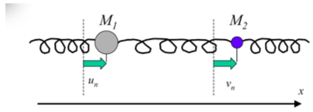
transverse optical



longitudinal optical



transverse acoustic



longitudinal acoustic

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3D systems

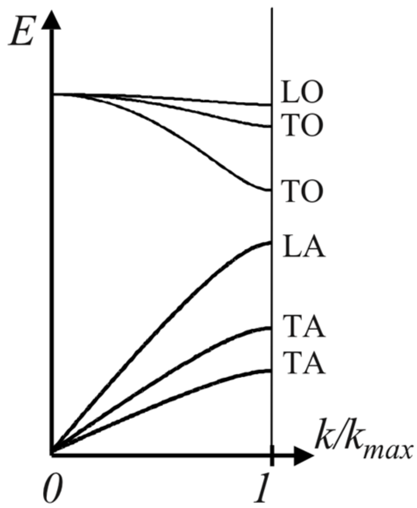
Real crystal expands and contracts in 3D

All essentials of 1D diatomic system remain

optic phonons – v(or E) is finite at k=0

acoustic phonons – v(or E) tends to zero as $k \rightarrow 0$

Differently polarised phonons non-identical- splitting of transverse phonons



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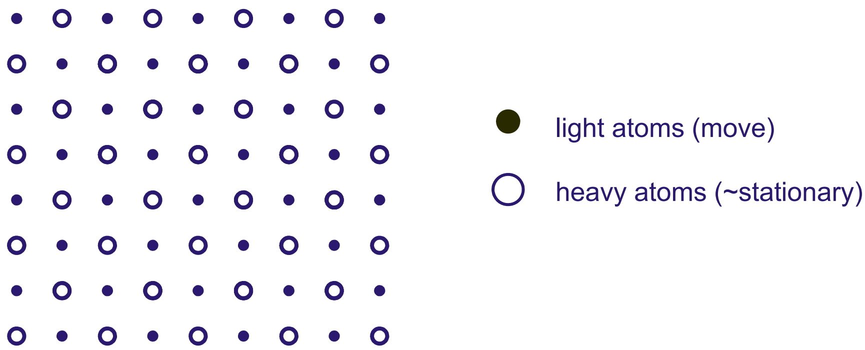
Different phonon flavours…again



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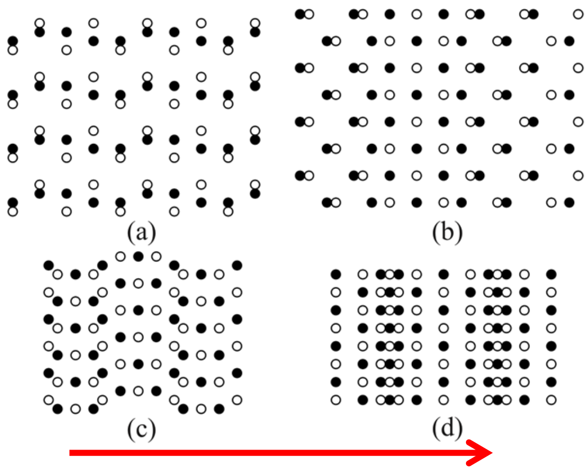
Different phonon flavours...again



(a) TO
(b) LO
(c) TA
(d) LA

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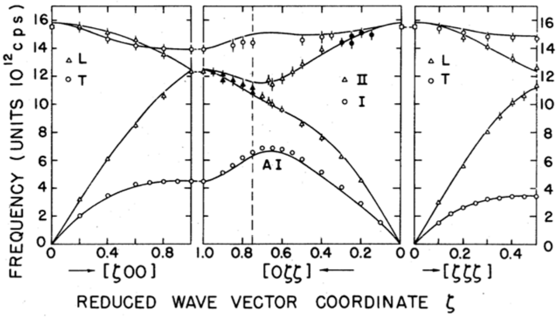
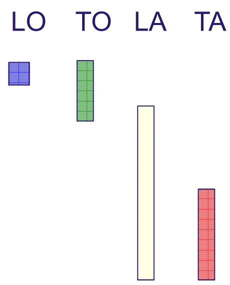
Silicon phonon pispersion





No gaps ! Can always find a phonon of particular ***v*** or ***k***
Gaps with regard to allowed ***v*** or ***k*** for optic or acoustic phonons

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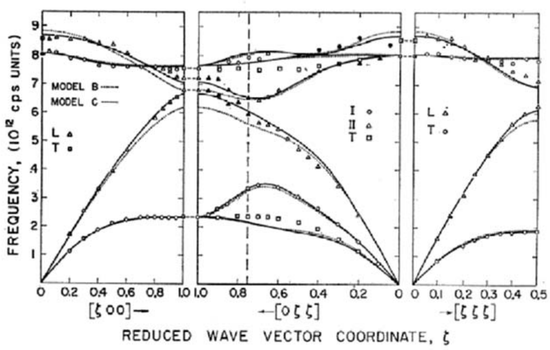
GaAs phonon dispersion



similar in form to Si

values changed - different chemistry

As (V), Ga (III)

TO and LO not degenerate at zone centre – different restoring forces for propagating LO and TO

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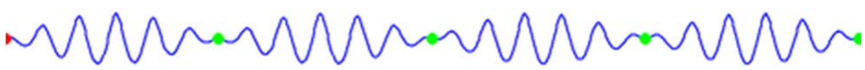
Phase and group velocity



- Phase velocity – peak
- Group velocity – envelope – energy of wave

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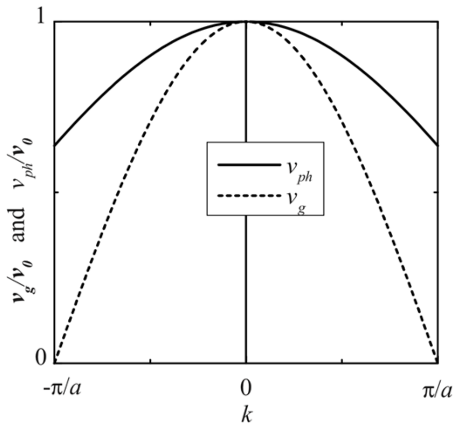
Velocity of sound (phase)

$$\omega^2 = \frac{2C}{M}(1 - \cos ka) = \frac{4C}{M}\sin^2\frac{ka}{2}$$

$$v_{\mathrm{ph}} = \frac{\omega}{k}$$

$$v_{\mathrm{ph}} = \sqrt{\frac{4C}{M}}\left|\frac{\sin\left(\frac{ka}{2}\right)}{k}\right| = a\sqrt{\frac{C}{M}}\left|\frac{\sin\left(\frac{ka}{2}\right)}{\frac{ka}{2}}\right| = v_0\left|\frac{\sin\left(\frac{ka}{2}\right)}{\frac{ka}{2}}\right|$$

where $v_0 = a\sqrt{\frac{C}{M}}$



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Quantisation

Phonons are bosons – when a particular mode is occupied by n phonons, the total energy in the mode is given by;

$$\epsilon = (n + \tfrac{1}{2})\hbar\omega$$

An individual phonon has a particular energy but does not carry momentum…..we are using relative co-ordinates – not absolute coordinates for this "lattice wave". However, the phonon interacts with photons, neutrons, and electrons *as if it had* a "crystal momentum" $\hbar\underline{\mathbf{K}}$

quantisation – individual momentum and energy

$$\vec{p} = \hbar\vec{k}$$

$$E = \hbar\omega(\vec{k})$$

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Phonons…So What!

Phonons are key players in electron-electron and electron-photon interaction

They have energy and (and act as if they have) momentum in satisfying energy and momentum conservation for these processes.

Vital for thermalisation of hot electrons, optical transitions, heat capacity, thermal conductivity, etc., etc.,…..

More later, when we look at the first few of these…..

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Phonon gas

Phonons can be considered to behave as a mutually non-interacting "gas". As they are bosons, the average number of particles, $N(E)$ with energy E is given by the Bose-Einstein distribution

$$N(E)=\frac{1}{\exp\left(\frac{E}{k_b T}\right)-1}$$

where k_b is the Boltzmann constant and T is temperature

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Summary

- introduced phonons: definition and relation to sound
- model for 1D monoatomic system: acoustic branch only
- model for 1D diatomic system: acoustic & optical branch
- described 3D systems – essentially same as diatomic 1D with a little bit of anisotropy
- started to show how quantisation of energy and E-K relationship play a role in defining how electron-electron and electron-hole interactions occur in semiconductors