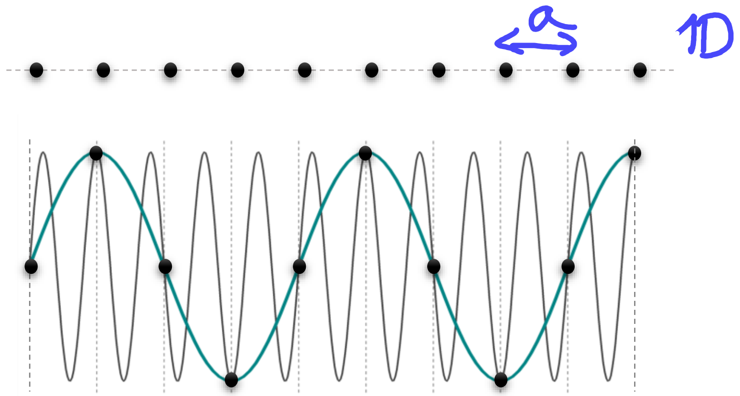
Crystal vibrations - Phonons

Lecture 2

Recap

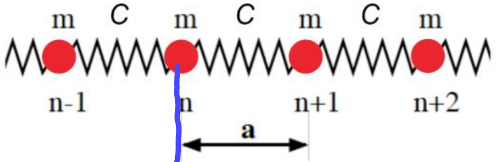
Goal: Describe / understand crystal vibrations (collective motions of atoms)

→ Harmonic Approximation



trick: realize that K and $K+G$ are only equivalent at lattice points

Ex. 1D monoatomic chain

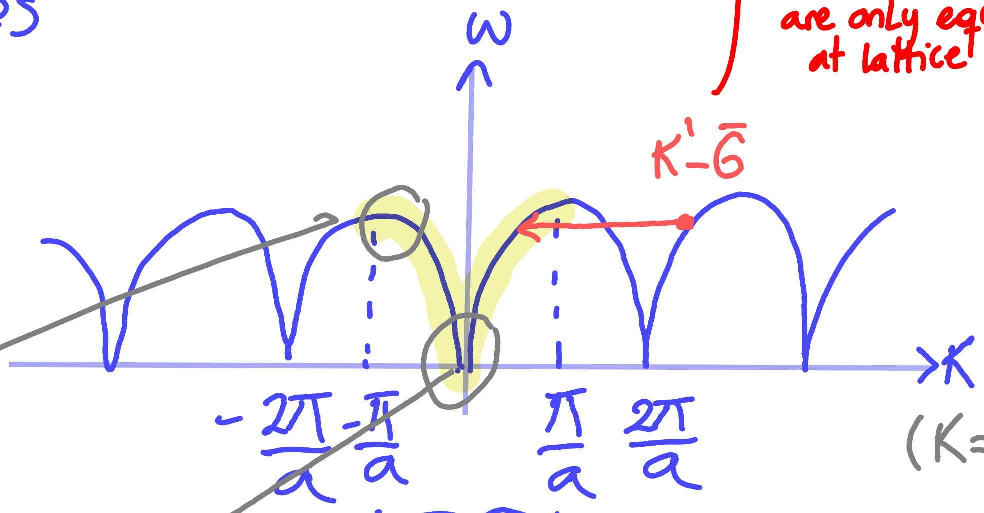


x_0

displacement from eq. position $\delta u = A e^{-i\omega t + iKna}$

Dispersion curves $\omega(K)$

$$\omega = \sqrt{\frac{4C}{m}}\left|\sin\frac{Ka}{2}\right|$$



$\left(K = \frac{2\pi}{\lambda}\right)$

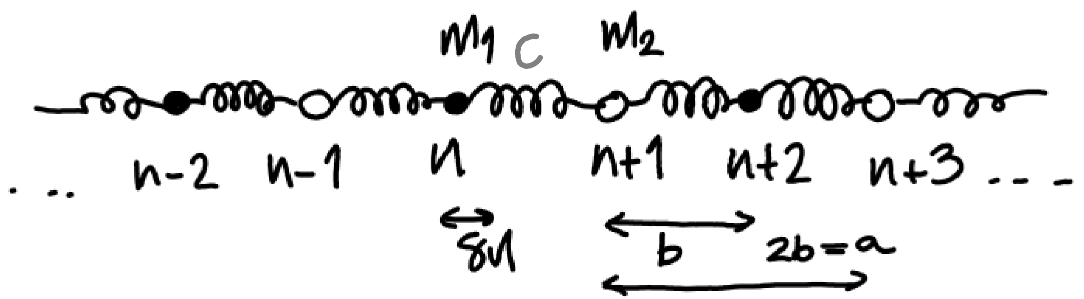
small λ
i.e. $\lambda = 2a$
zone boundary $K = \frac{\pi}{a}$
"standing waves"
$v_g = 0$

Long λ-limit
$\omega \propto K$
Sound velocity $v_p = \frac{\omega}{K} = ct.$

1st Brillouin zone
it contains all information!
(the others are just repetitions)

Recap

Vibrations of 1D diatomic chain



$$m_1 \frac{d^2\delta_n}{dt^2} = c\,(\delta_{n+1} + \delta_{n-1} - 2\delta_n)$$
$$m_2 \frac{d^2\delta_{n+1}}{dt^2} = c\,(\delta_{n+2} + \delta_n - 2\delta_{n+1})$$

Ansatz

in matrix form

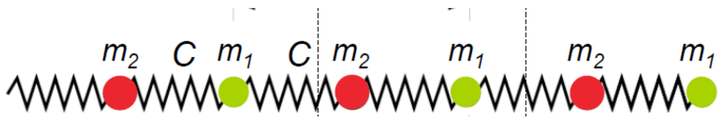
$$\begin{bmatrix} \delta_n \\ \delta_{n+1} \end{bmatrix} = \begin{bmatrix} A_1 e^{iKnb} \\ A_2 e^{iK(n+1)b} \end{bmatrix} e^{-i\omega t}$$

substituting Ansatz in the 2 equations of motion and solving the system of linear homogeneous eqs

Solution →

$$\boxed{\omega^2 = c\left(\frac{1}{m_1}+\frac{1}{m_2}\right) \pm c\sqrt{\left(\frac{1}{m_1}+\frac{1}{m_2}\right)^2 - \frac{4\sin^2 Kb}{m_1 m_2}}}$$

Diatomic chain: dispersion relation

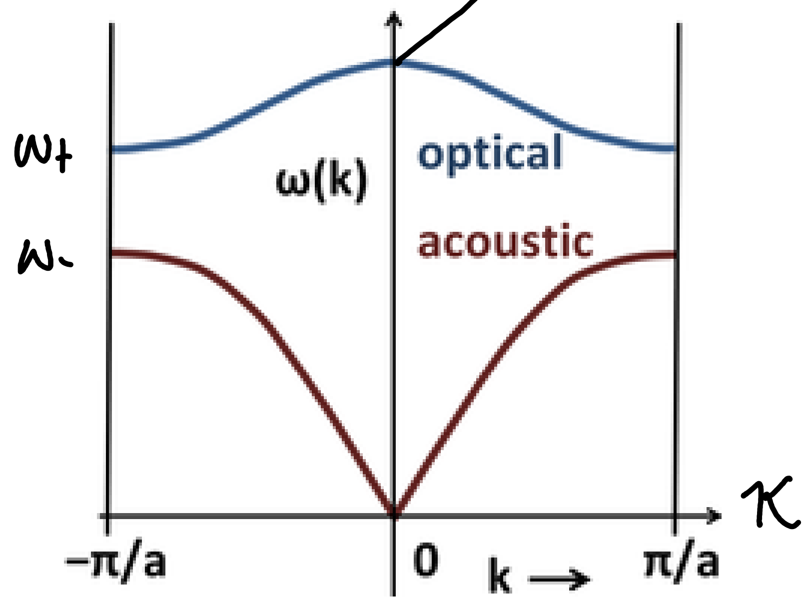


$$\omega^2 = C\left(\frac{1}{m_1}+\frac{1}{m_2}\right) \pm C\sqrt{\left(\frac{1}{m_1}+\frac{1}{m_2}\right)^2 - \frac{4\sin^2 Kb}{m_1 m_2}}$$

$\Longrightarrow$ 2 solutions = 2 dispersion curves (≡ Branches)

ACOUSTIC   OPTICAL

$\omega_{max} = \sqrt{2C\left(\frac{1}{m_1}+\frac{1}{m_2}\right)}$



OPTICAL BRANCH

$K \to 0 \Longrightarrow m_1 A_1 + m_2 A_2 = 0$

→ atoms m_1 and m_2 oscillate in opposite direction

if m_1 and m_2 have opposite charge, these motions can be excited by $\vec{E}$

●→ ←○ ●→ ←○ ●→

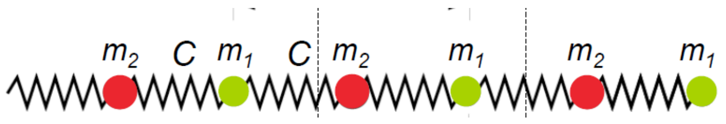
ACOUSTIC BRANCH [as $K \to 0$, $\frac{\omega}{K}$ = sound velocity → ct.]

$K = 0,\ \omega = 0 \Longrightarrow A_1 = A_2$

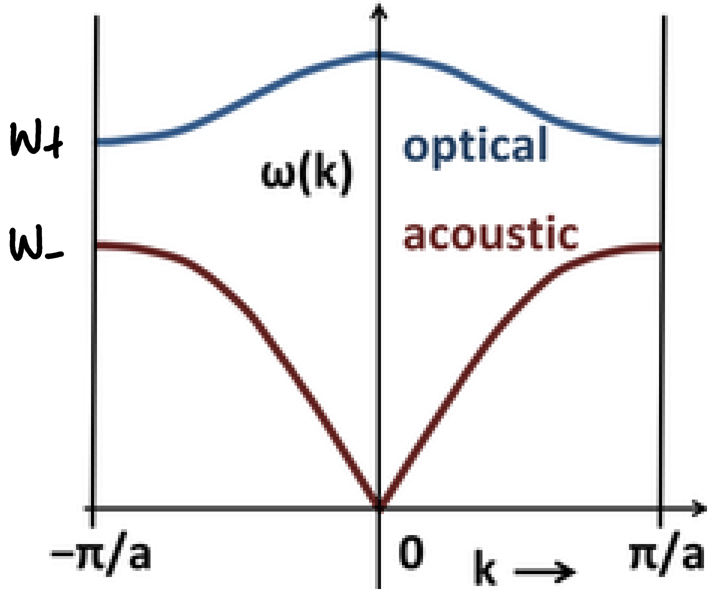
→ atoms m_1 and m_2 oscillate in phase as $K \to 0$

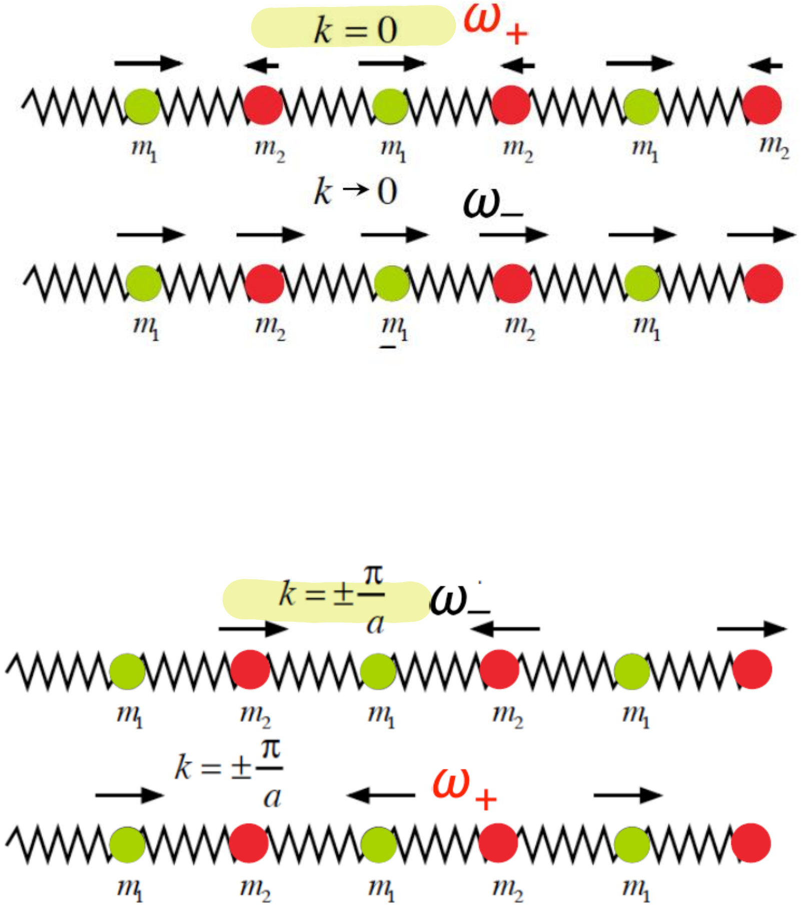
●→ ○→ ●→ ○→ ●→

Diatomic chain: dispersion relation



$$\omega^2 = C\left(\frac{1}{m_1}+\frac{1}{m_2}\right) \pm C\sqrt{\left(\frac{1}{m_1}+\frac{1}{m_2}\right)^2 - \frac{4\,sin^2 Kb}{m_1 m_2}}$$

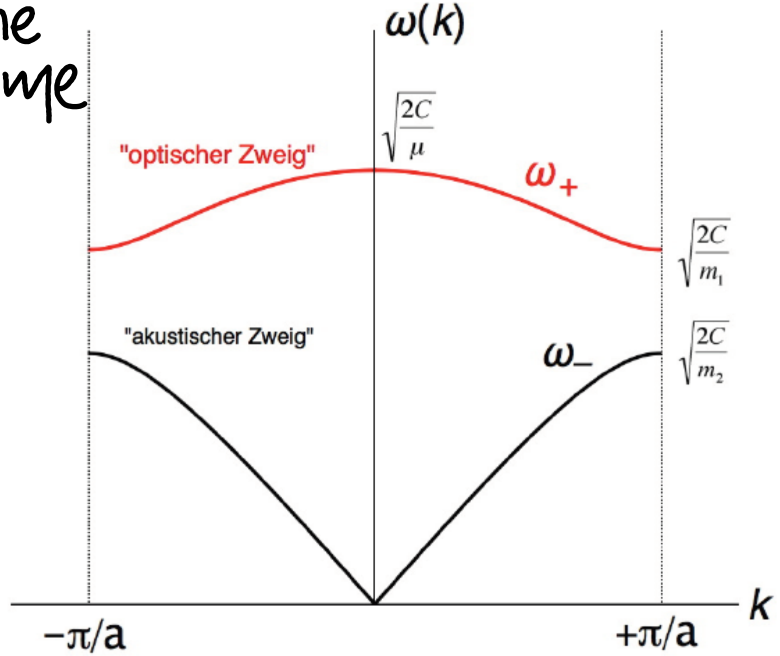


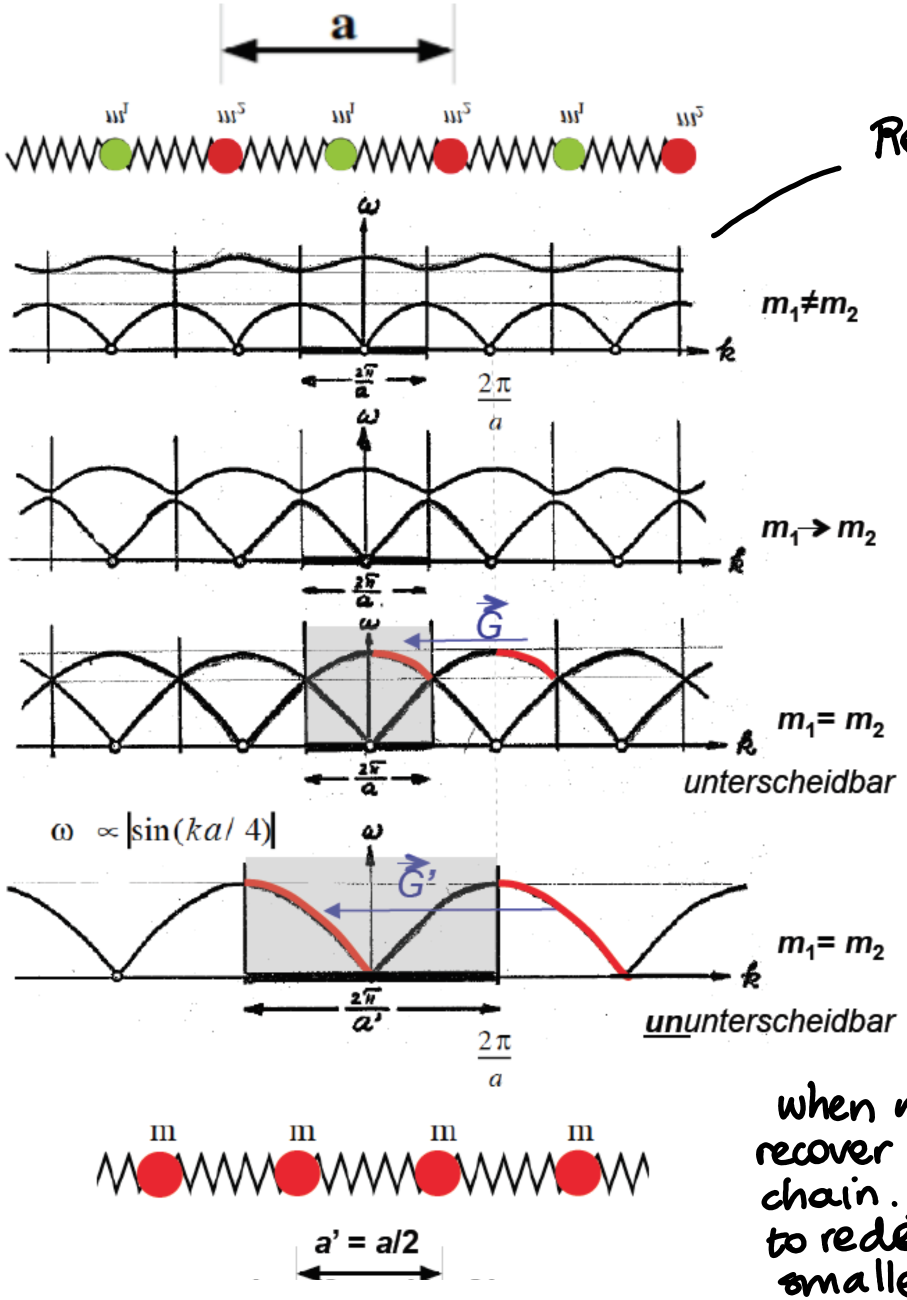


Limit $m_1 \to m_2$:

$$\omega^2 = C\left(\frac{1}{m_1}+\frac{1}{m_2}\right) \pm C\sqrt{\left(\frac{1}{m_1}+\frac{1}{m_2}\right)^2 - \frac{4\sin^2 Kb}{m_1 m_2}}$$

Reduced zone scheme





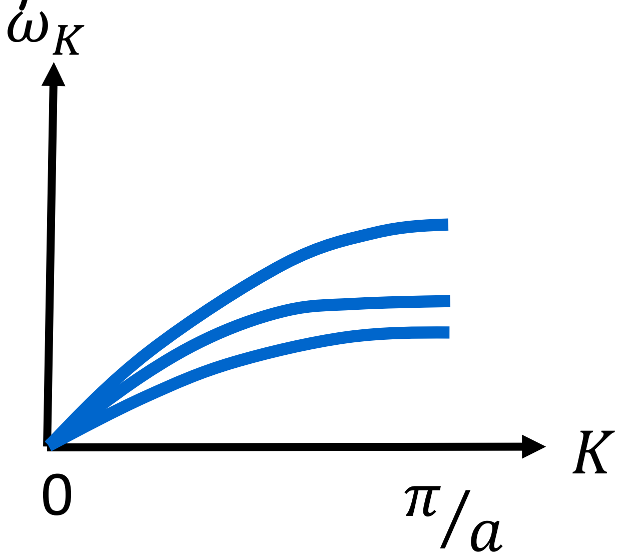
Repeated zone scheme

when $m_1 = m_2$, we recover monoatomic chain. One just need to redefine a new smaller cell.

Vibrations in 3D lattice

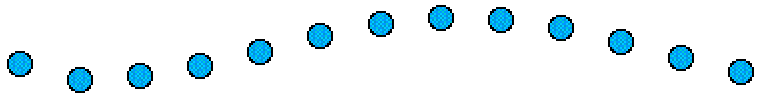
Monoatomic 3D Bravais lattice

(1 atom per cell)



Longitudinal Acoustical Mode:

Transverse Acoustical Mode:



- Equations of motion (like before)
- Ansatz: $\vec{s} = \vec{A}\, e^{i(\vec{K}\cdot\vec{r} - \omega t)}$

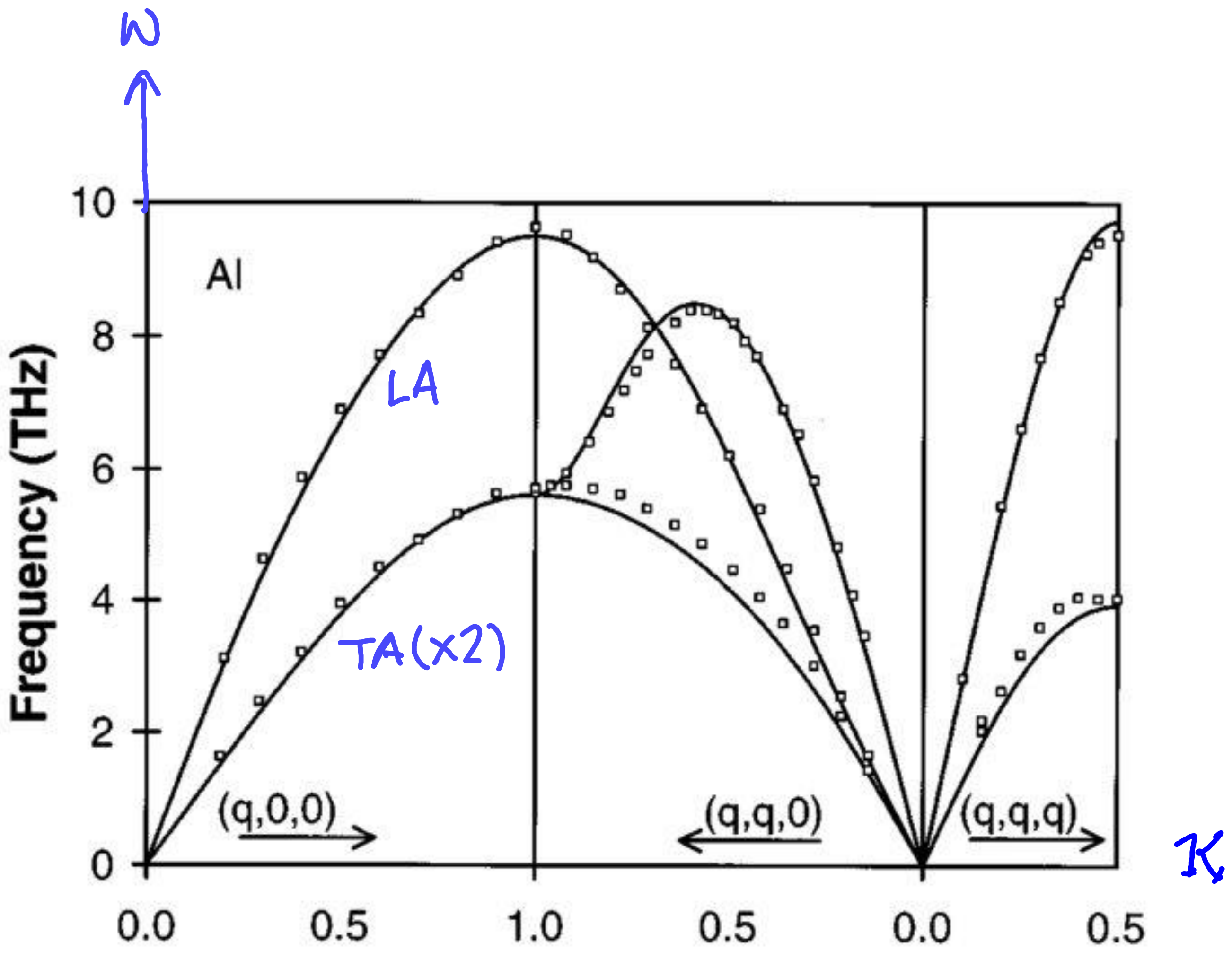
- Amplitude
- direction vibration of atoms → Polarization
  - Longitudinal mode ($\bar{A} \parallel \bar{K}$)
  - Transverse mode ($\bar{A} \perp \bar{K}$) [x2]

- $K = 2\pi/\lambda$
- propagation direction

⇒ 3 dispersion relations

All acoustic: LA, TA_1, TA_2

(remember: monoatomic chain considered)



Notation often
$K \equiv q$

Experimental and theoretical phonon dispersion curves of Al

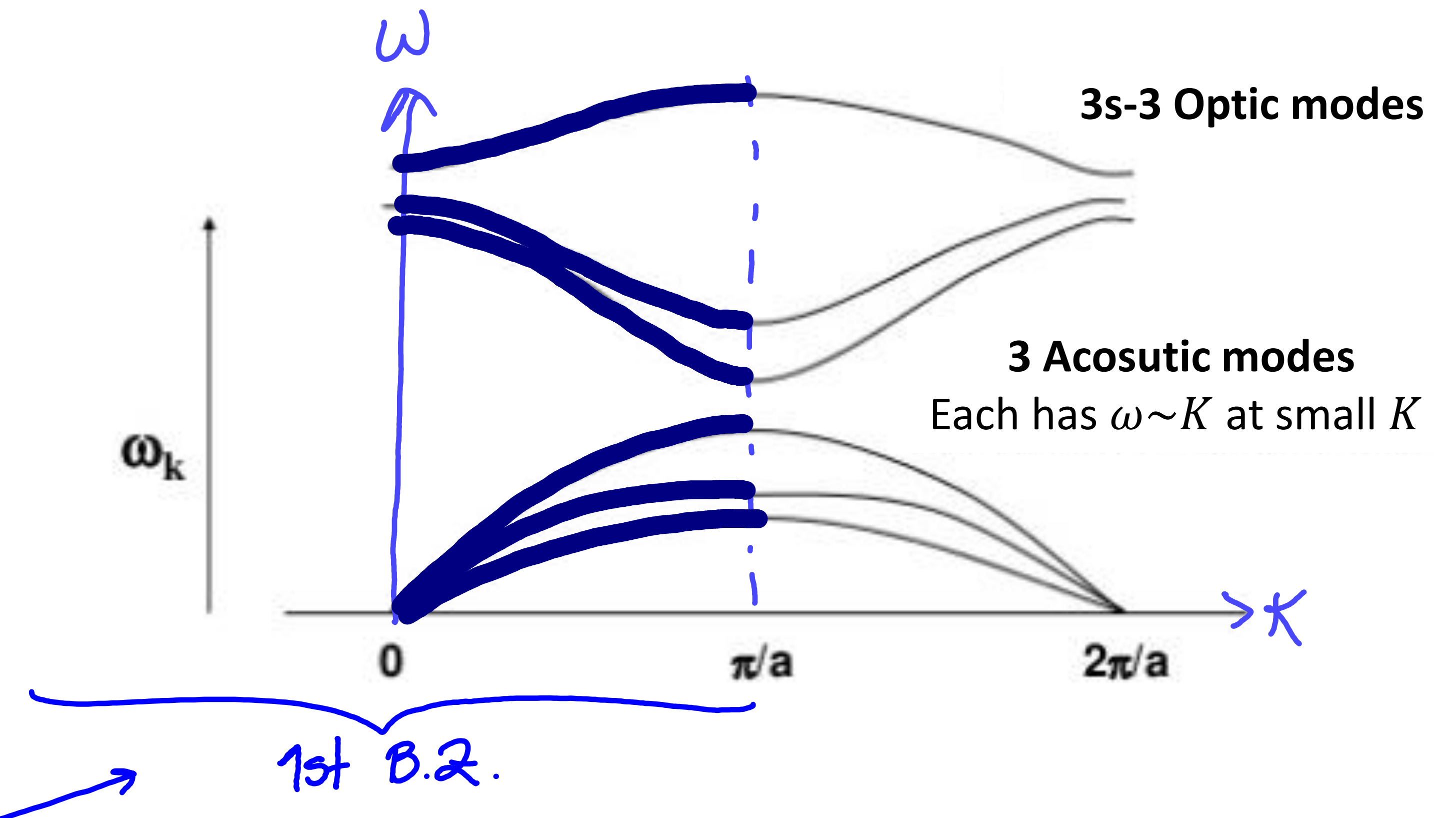
Squares represent experimental data at 300 K

Vibrations in 3D with s atoms per cell

if there are s atoms per primitive cell $\Rightarrow$ 3s dispersion curves

3 ACOUSTICAL BRANCHES

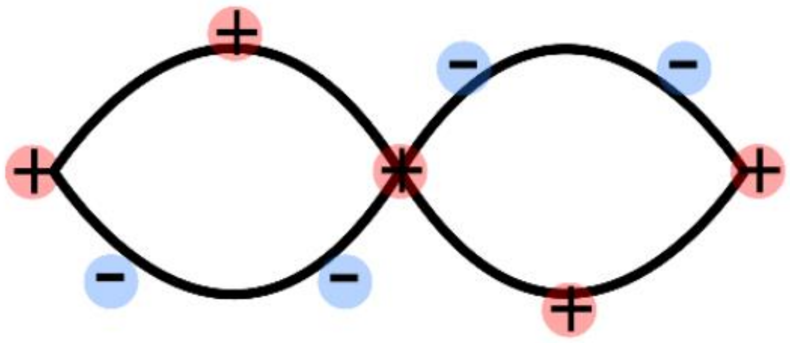
3s – 3 OPTICAL BRANCHES



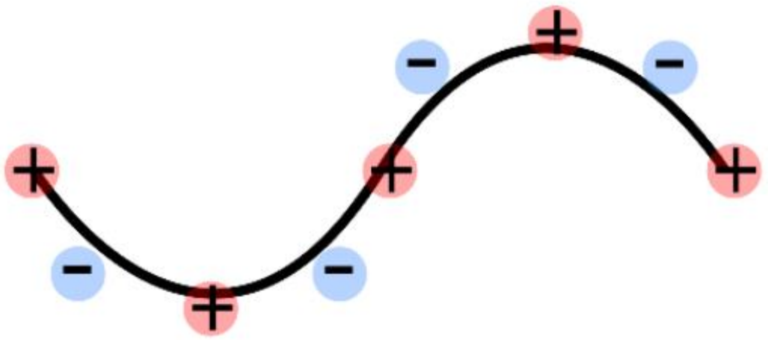
Another way of showing ω(K)

No problem because we know $\omega(K) = \omega(-K)$

Optical Mode



Acoustical Mode



https://www2.warwick.ac.uk/fac/sci/physics/current/postgraduate/regs/mpags/ex5/phonons/

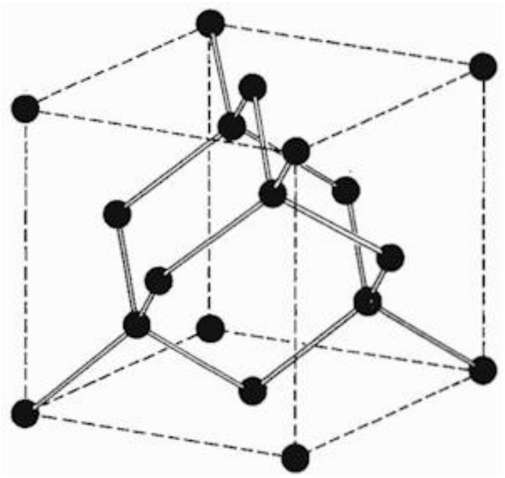
Quiz : Dispersion curves in Diamond

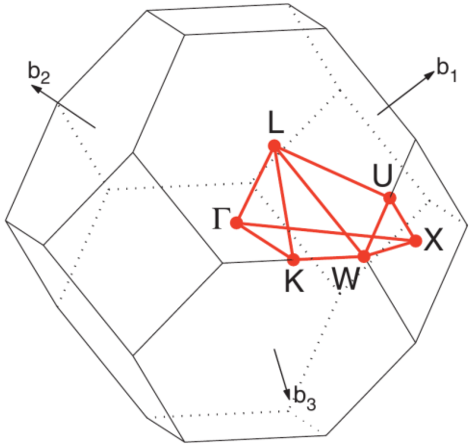
FCC with 2 atoms basis $\Rightarrow$ $3s = 3\times2 = 6$ branches

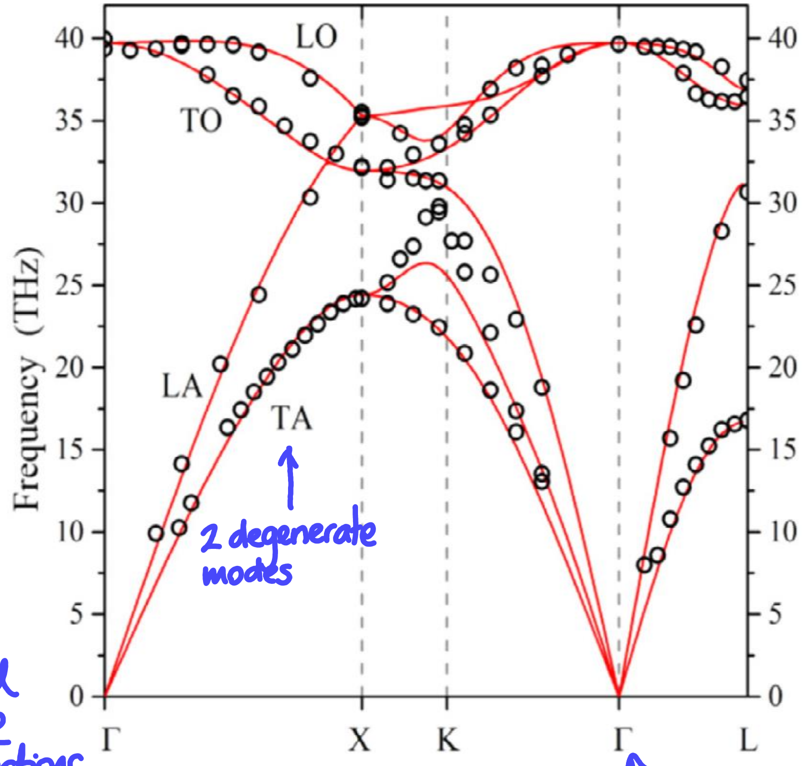
"s

3 acoustic

3 optic







2 degenerate modes

$k=0$

3D info on a 1D diagram is achieved by plotting single line cuts along specific directions of reciprocal lattice

Monteverde *et al.*, *Carboni* 91, 266 (2015)

Quantum modes: Phonons

Quantum correspondence: If a classical harmonic system (i.e. any quadratic Hamiltonian) has a normal oscillation mode at frequency ω, the corresponding quantum system will have eigenstates with energy

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

n = quantum number

PHONON quantum of vibration (in analogy to phonon)

→ its energy is $\hbar\omega$

A phonon is a boson (you can put more than 1 in a k mode)

Phonons can be viewed as particles
(i.e. they can transport energy)

Phonons

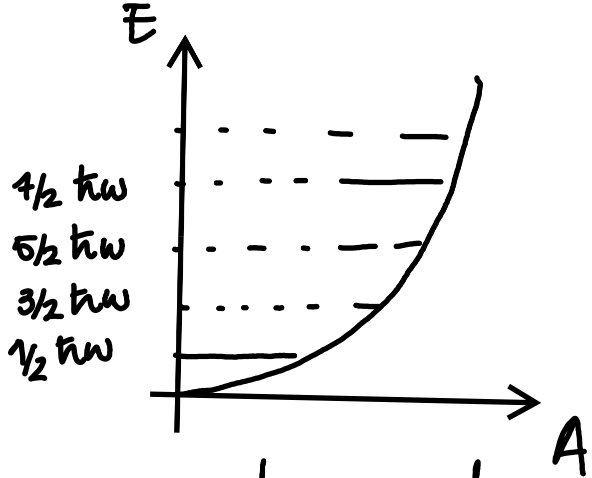
"So, if a normal mode of vibration in a crystal with frequency ω is given by $\bar{\xi} = \bar{A} e^{-i\omega t + i\bar{k}\bar{r}}$,
its energy is given by $E_n = (n + \frac{1}{2})\hbar\omega$, and we say it is occupied by n phonons of energy $\hbar\omega$".

Comparison classical/quantum solutions in 1D

Energy of a normal mode of vibration averaged over time

$$E = \frac{1}{2} m \omega^2 A^2 = \left(n + \frac{1}{2}\right)\hbar\omega$$

Relation Amplitude vibration & phonon occupation of this mode.



In quantum mechanics, only discrete A are allowed.

Phonon momentum

- Phonons can interact with other particles (*i.e.* photons, neutrons, electrons).
- This interaction occurs such as if the photon had a momentum $\hbar\vec{K}$. $\longrightarrow$ pseudomomentum or crystal momentum
- However, a phonon does not carry a real physical momentum.

($\Leftrightarrow$ phonon "coordinates" are relative coordinates)

1 monoatomic chain

$$p_{total} = m\frac{d}{dt}\sum^{N} s_n = -i\omega m A e^{-i\omega t}\sum_{n=1}^{N} e^{iKna} = -i\omega m A e^{-i\omega t}\frac{e^{iKa}}{1-e^{iKa}}\left(1-e^{iKNa}\right)$$

$$s_n = Ae^{i(Kna-\omega t)}$$

$$\sum_{n=1}^{N} S^n = \frac{S^M - S^{N+1}}{1-S}$$

p depends on boundary conditions (note that $Na = L$)

for periodic boundary conditions: $e^{iKna} = e^{iK(n+N)a} = e^{iKna}\underbrace{e^{iKNa}}_{=1}$

$\Rightarrow p_{total} = 0$ and $\hbar\vec{K} \neq p_{total}$

Inelastic scattering by phonons

Remember: Elastic scattering $\vec{K}' = \vec{K} + \vec{G}$

<u>Inelastic scattering</u>: $\vec{K}' = \vec{K} \pm \vec{K} + \vec{G}$

outgoing photon — incident photon — phonon (creation or absorption) — Reciprocal Lattice vector

$\omega(K)$ dispersion curves can be determined by <u>inelastic scattering of neutrons</u>

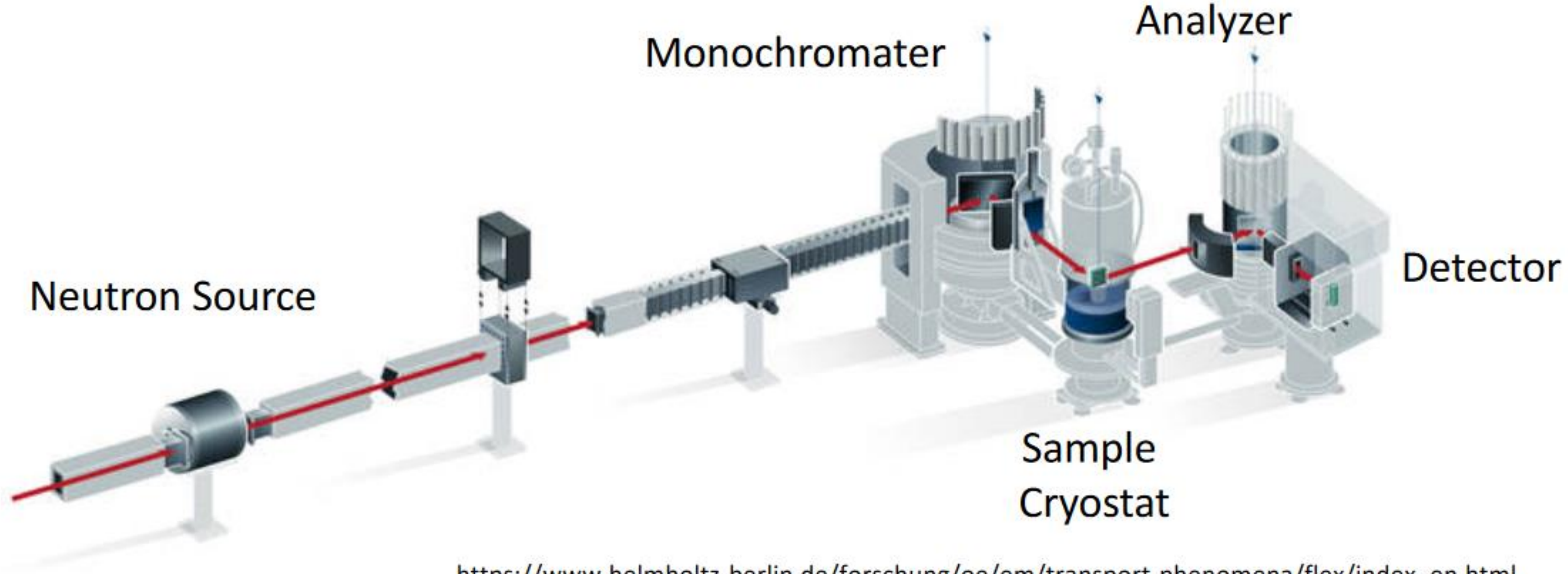
conservation of quasi momentum $\bar{K}' = \bar{K} + \bar{K} + \bar{G}$

phonon

conservation of energy: $\frac{\hbar^2 K^2}{2m} = \frac{\hbar^2 K'^2}{2m} \pm \hbar\omega$

unknown

Triple axis spectrometer



https://www.helmholtz-berlin.de/forschung/oe/em/transport-phenomena/flex/index_en.html

The Nobel Prize in Physics 1994
Bertram N. Brockhouse, Clifford G. Shull

Learning outcomes – Phonons

- **Normal modes are collective oscillations where all particles move at the same frequency.**
- **A normal mode of frequency ω is translated into quantum-mechanical eigenstates $E_n = \hbar\omega\,(n + \frac{1}{2})$.**
- **The quantum unit of a crystal vibration is a *phonon,* which has energy $\hbar\omega$. Phonons can be thought as particles that obey Bose statistics. Thus, if a mode is in the n^{th} eigenstate, we say it is occupied by *n* phonons.**
- **All elastic waves can be described by wavevectors that lie within the first Brillouin zone of the reciprocal space.**
- **If there are s atoms in the primitive cell, the phonon dispersion relation has 3s branches: 3 acoustical phonon branches (i.e. have linear dispersion at small k; sound wave) and 3s-3 optical phonon branches (i.e. have finite frequency at $k = 0$) .**
- **The wavevector selection rule for an inelastic scattering process of a photon or a neutron from wavevector $\vec{k}$ to $\vec{k}'$, when a phonon of wavevector $\vec{K}$ is created, is**

$$\vec{k} = \vec{k}' + \vec{K} + \vec{G}$$

where $\vec{G}$ is a reciprocal lattice vector.