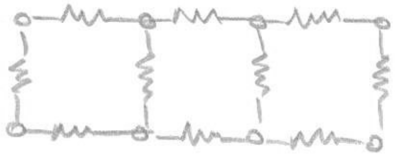
Lattice vibrations



Model of lattice

Phonon

Def: The phonon is the energy quantum of the elastic wave

Compare photon – energy quantum of electromagn. wave

A phonon is described completely by

- ω — $\varepsilon = \hbar\omega$
- $\bar{K}$ — Wave vector, $\lambda = \dfrac{2\pi}{|K|}$ (Propagation along $\bar{K}$)
- polarization direction
  - 3D: 1L, 2T
  - 2D: 1L, 1T
  - 1D: 1L

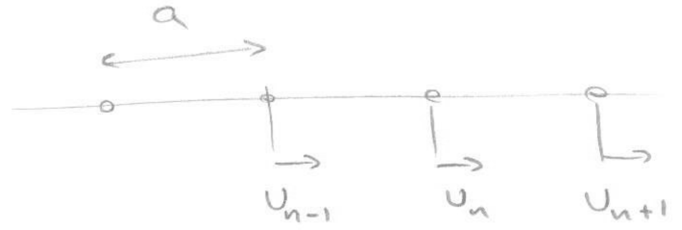
Useful statements

1. There is a highest frequency ω_{max}
2. The number of $\bar{K}$-values is discrete due to boundary cond.
   In practise, it is quasicontinuous, $\sum_K \longrightarrow \int d^3K$ or $\int d\omega$
3. All possible vibration modes can be described with a $\bar{K}$-vector in the 1:st Brillouin zone
4. In a crystal with N atoms there are N vibration modes per polarization direction.

(1) Highest frequency ω_{max}

"$F = C \cdot x$" spring

Model: 1-dim chain, harmonic forces beween nearest neighbors



$L = N \cdot a$

mass M per atom

Eq: $$M \cdot \ddot{u}_n = C \cdot (u_{n+1} - u_n) - C(u_n - u_{n-1}) =$$
$$= C(u_{n+1} - 2u_n + u_{n-1})$$

Ansatz: $$u_n = A \cdot e^{i(K \cdot n \cdot a - \omega t)} \qquad (x = n \cdot a)$$

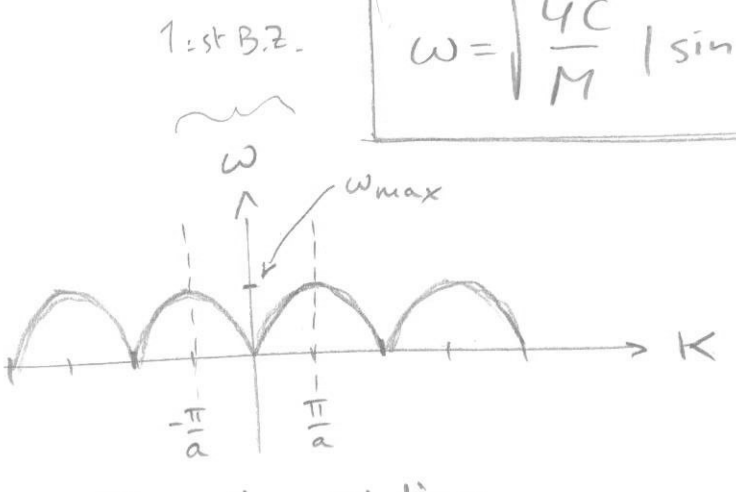
$$\Rightarrow \begin{cases} \ddot{u}_n = -(i\omega)^2 u_n = -\omega^2 u_n \\ u_{n+1} = A e^{i(K(n+1)a - \omega t)} = e^{iKa} u_n \\ u_{n-1} = e^{-iKa} u_n \end{cases}$$

$$-M\omega^2 u_n = C\left(e^{iKa} - 2 + e^{-iKa}\right) u_n$$

$$M\omega^2 = 2C \underbrace{(1 - \cos Ka)}_{2\sin^2 \frac{Ka}{2}}$$

$$\boxed{\omega = \sqrt{\frac{4C}{M}} \left|\sin \frac{Ka}{2}\right|} \qquad \omega_{max} = \sqrt{\frac{4C}{M}}$$

A lattice cannot vibrate with arbitrarily high frequencies



Dispersion relation

② Number of $\bar{K}$-values

Assume periodic boundary conditions

$$U_n(na) = U_n(na + L)$$

$$e^{iKna} = e^{iK(na+L)} \Rightarrow e^{iKL} = 1$$

$$K \cdot L = p \cdot 2\pi \qquad K_x = 0, \pm \frac{2\pi}{L}, \pm \frac{4\pi}{L} \ldots$$

$K_y =$ — " —

$K_z =$ — " —

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③ All vibration modes in 1:st B.Z.

$$U_n = A \cdot e^{i(Kna - \omega t)}$$

Let $K' = K + p \cdot G = K + p \cdot \frac{2\pi}{a}$, p integer

$$\Rightarrow U_n' = \underbrace{e^{iG \cdot na}}_{} U_n = U_n$$

Same state/wave

$$e^{ip \cdot \frac{2\pi}{a} \cdot na} = e^{i \cdot 2\pi \cdot p \cdot n} = 1$$

<u>Example</u>

$$K' = \frac{15}{7} \cdot \frac{\pi}{a} > \frac{2\pi}{a}$$

$$\lambda' = \frac{2\pi}{K'} = \frac{14}{15} a$$

$$K = K' - G = \frac{1}{7} \cdot \frac{\pi}{a}$$

$$\Rightarrow \lambda = \frac{2\pi}{K} = 14a$$

Wavelengths shorter than lattice parameter can be better described with a longer wavelength

(u) N vibration modes per polarization direction

Proof: If N is even $(L = N \cdot a)$:

$$K = 0, \pm\frac{2\pi}{L}, \pm\frac{4\pi}{L}, \dots \pm\frac{N\pi}{a} = \pm\frac{\pi}{a}$$

but $\frac{\pi}{a} - \underbrace{\frac{2\pi}{a}}_{G} = -\frac{\pi}{a}$ same state $\Rightarrow$ keep only $+\frac{n\pi}{L}$

$$\underset{\uparrow 0}{1} + \underset{\uparrow \pm}{2} \cdot \frac{(N-2)}{2} + \underset{\uparrow +\frac{N\pi}{a}}{1} \text{ states} = N - 2 + 2 = \underline{N \text{ states}}$$

If N is odd:

$$K = 0, \pm\frac{2\pi}{L}, \pm\frac{4\pi}{L}, \dots \pm\frac{\overbrace{(N-1)}^{\text{even number}}\pi}{L}, \pm\overbrace{\frac{(N+1)\pi}{L}}^{\text{Larger than } \frac{\pi}{a}}$$

$$1 + 2 \cdot \frac{(N-1)}{2} = \underline{N \text{ states}}$$

Detecting phonons

Elastic scattering $\bar{k}' - \bar{k} = \bar{G}$

modify : $\boxed{\bar{k}' - \bar{k} = \pm \bar{K}_{ph} (+\bar{G})}$ (1)

Energy $\boxed{h\nu' - h\nu = \pm \hbar\omega_{ph}}$ (2)

X-ray : $\lambda \sim 1$ Å $\quad h\nu = \frac{hc}{\lambda} \sim 10$ keV

Phonon : $\hbar\omega \sim 40$ meV

$\}$ x-ray cannot be used

Visible light : $\lambda \sim 500$nm, $\quad h\nu \sim 2$eV $\quad$ maybe possible to resolve 40 meV

BUT : $\quad k = \frac{2\pi}{\lambda} \sim 10^7 \, m^{-1}$

$$|\bar{K}| \lesssim \frac{\pi}{a} \sim 10^{10} \, m^{-1}$$

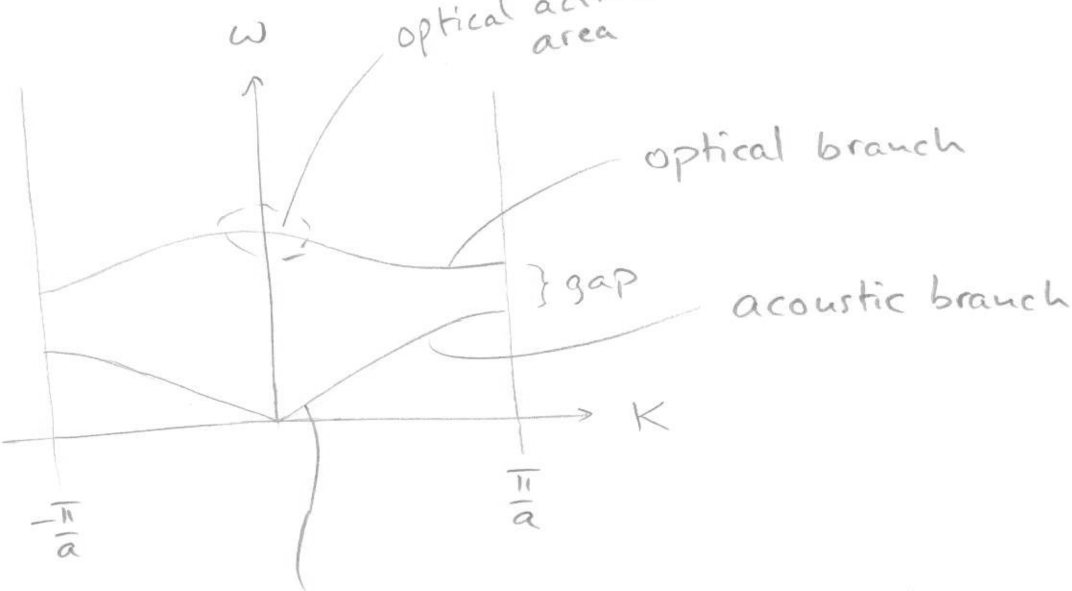
maximum change in k : $\rightleftarrows \quad 2 \cdot k = 2 \cdot 10^7 \, m^{-1}$

much smaller than $10^{10} \, m^{-1}$

$\Longrightarrow \; |\bar{K}|$ cannot be "absorbed"

Neutrons $\quad$ With neutrons both (1) and (2) can be fulfilled over the entire B.Z.

Dispersion relation ω vs k



Sound velocity $v_s = \lim_{K \to 0} \frac{\partial \omega}{\partial K}$

p atoms/ions per cell

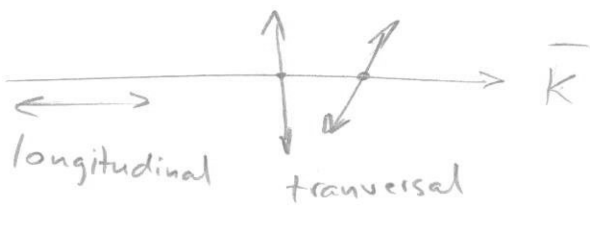
$\Downarrow$

3p acoustic branches $\longrightarrow$ $\omega \to 0$ when $K \to 0$

3(p-1) optical branches

3 $\longrightarrow$ 1 longitudinal, 2 transverse polarizations

(3D crystals)



Wave equation for continuous media

$$\frac{\partial^2 u}{\partial x^2} - \sqrt{\frac{\varrho}{E}} \frac{\partial^2 u}{\partial t^2} = 0$$

E = elasticity modulus

ϱ = density

$$v_s = \sqrt{\frac{E}{\varrho}}$$

Lattice model : $\omega = \sqrt{\frac{4C}{M}} \left| \sin \frac{ka}{2} \right|$

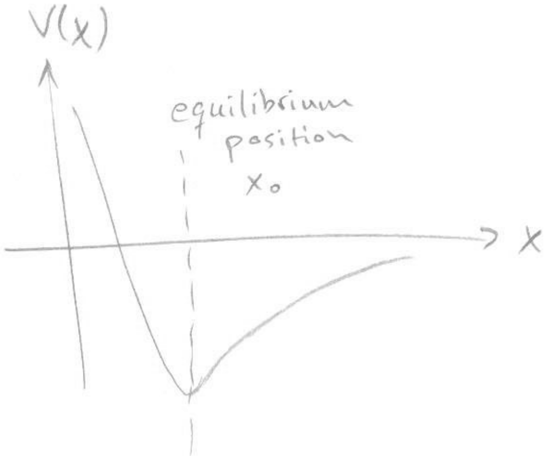
$$v_s = \lim_{k \to 0} \frac{\partial \omega}{\partial k} = \sqrt{\frac{4C}{M}} \cdot \frac{a}{2} = a \cdot \sqrt{\frac{C}{M}}$$

$$M = \varrho \cdot a^3$$

Compare $\sqrt{\frac{E}{\varrho}} = a \cdot \sqrt{\frac{C}{\varrho a^3}} = \sqrt{\frac{C}{\varrho a}}$

$$\Longrightarrow \boxed{C = a \cdot E}$$

Harmonicity



Small displacements

$$V(x) \approx V(x_0) + A\cdot(x-x_0)^2$$

$$F = -\frac{dV}{dx} = -\underbrace{2A}_{C}(x-x_0)$$

spring constant

Hookes law:

$$\boxed{F = -C\cdot(x-x_0)}$$

Harmonic force

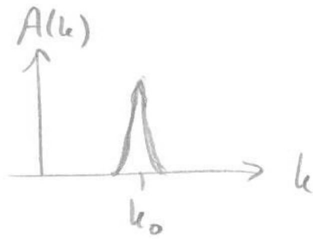
$\Longrightarrow$ harmonic oscillations etc.

Larger amplitudes / displacements

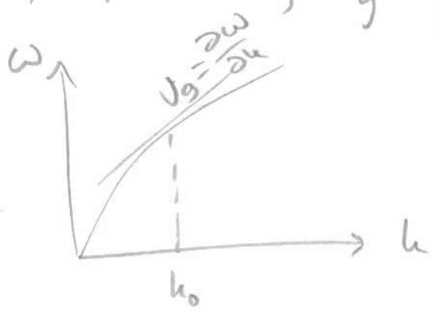
$\Longrightarrow$ anharmonic effects

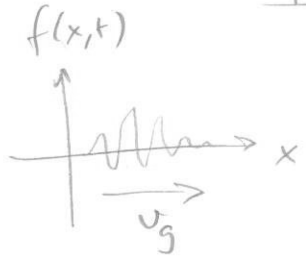
Wave packages

$$f(x,t) = \int_{-\infty}^{\infty} A(k)\, e^{i(kx-\omega t)}\, dk$$



Group velocity $v_g = \frac{\partial \omega}{\partial k}$





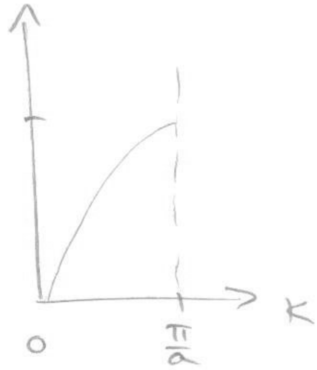
$$3D: \bar{v}_g = \nabla_{\bar{k}}\,\omega(k) = \left(\frac{\partial \omega}{\partial k_x}, \frac{\partial \omega}{\partial k_y}, \frac{\partial \omega}{\partial k_z}\right)$$

Plane waves : Practical set of basis

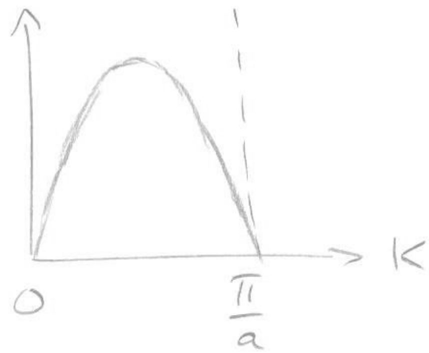
Interaction beyond nearest neighbors

$$\boxed{\omega^2 = \frac{2}{M} \sum_{j>0} C_j \left(1-\cos(Kja)\right)}$$

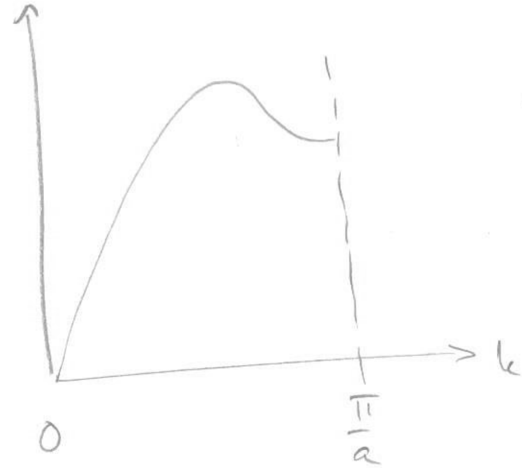
$j=1$ $\qquad \omega^2 = \frac{2}{M} \cdot C_j \cdot \underbrace{2 \cdot \sin\left(\frac{Ka}{2}\right)}_{1-\cos(Ka)}$



$j=2$ $\qquad 1-\cos(2Ka)$

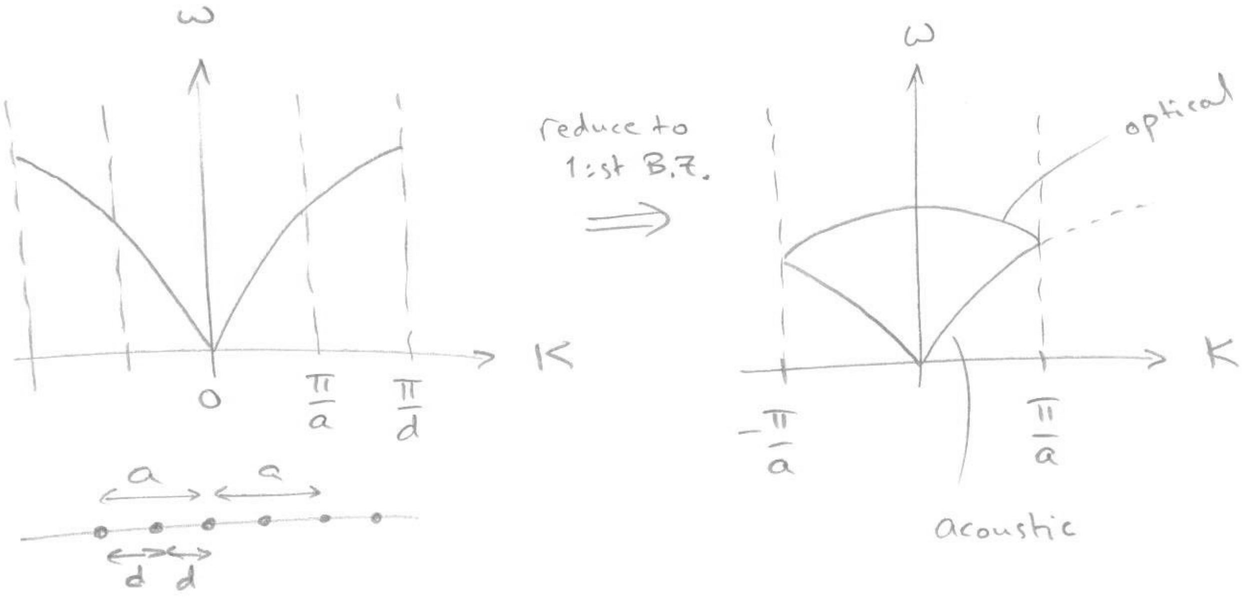


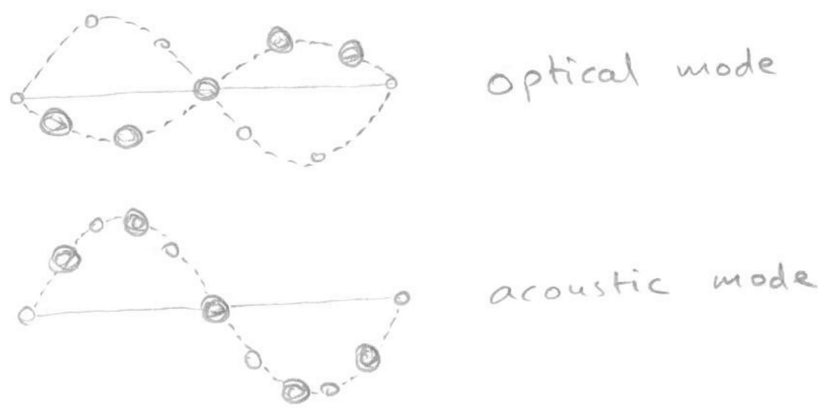
$\boxed{j=1 + j=2}$ $\qquad \omega(K) = \sqrt{\omega^2}$



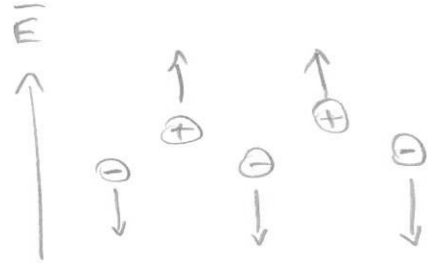
$$\omega^2 = \frac{2C}{M}\left[(1-\cos Ka) + (1-\cos 2Ka)\right]$$

One-dimensional, basis with 2 ions

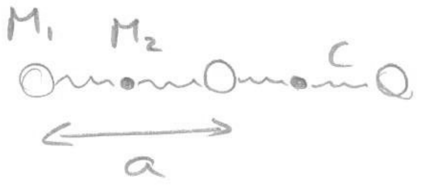




Optical excitation ~ IR



ex. NaCl



M_1: u_s

M_2: v_s

Assume same C

$$\begin{cases} M_1 \cdot \dfrac{d^2 u_s}{dt^2} = C\left(v_s + v_{s-1} - 2u_s\right) \\ M_2 \cdot \dfrac{d^2 v_s}{dt^2} = C\left(u_{s+1} + u_s - 2v_s\right) \end{cases}$$

<u>Ansatz</u>: $\begin{cases} u_s = u \cdot e^{i(Ksa - \omega t)} \\ v_s = v \cdot e^{i(Ksa - \omega t)} \end{cases}$

$$\Longrightarrow \begin{cases} -\omega^2 M_1 u = C \cdot v\left(1 + e^{-iKa}\right) - 2Cu \\ -\omega^2 M_2 v = C \cdot u\left(1 + e^{iKa}\right) - 2Cv \end{cases}$$

or $\begin{cases} (2C - M_1\omega^2)\, u = C \cdot \left(1 + e^{-iKa}\right) v \\ (2C - M_2\omega^2)\, v = C \cdot \left(1 + e^{iKa}\right) u \end{cases}$

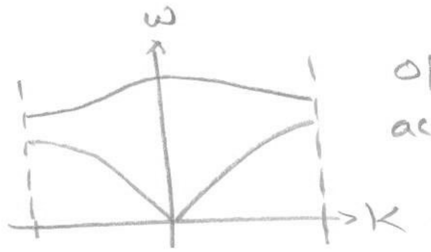
if $u \cdot v \neq 0$

$$\Longrightarrow (2C - M_1\omega^2)(2C - M_2\omega^2) = C^2\left(1 + e^{-iKa}\right)\left(1 + e^{iKa}\right)$$

2nd degree equation for ω^2

$\Rightarrow$ 2 solutions for each ω^2 for each K

with $\omega = +\sqrt{\omega^2}$ $(\omega > 0) \Rightarrow$ 2 solutions $\omega(K)$



optical
acoustic
can also have longitudinal/transversal branches

in 3D $\Rightarrow$ 6 branches (2 ions/cell)