Atomic vibrations in infinite periodic lattices

Dispersion relation - $\omega(k)$ and group velocity - $v_g(k)$ in the 1st BZ of 1D crystal

July 1, 2021

- Period lattices minimize the electric repulsion in a fixed volume
  By assuming linear response to external deformation

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

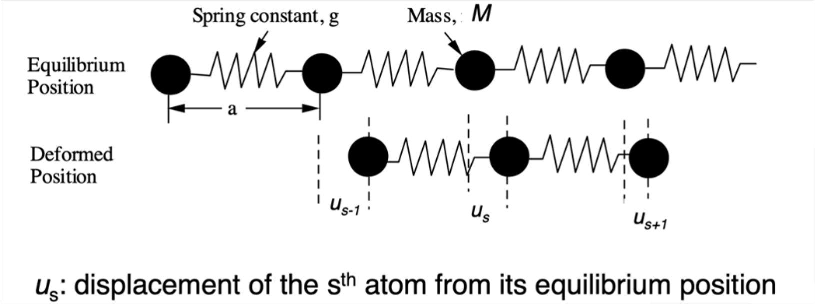

Figure 1: Modelling 1D crystal lattice

Frame Title

- Waves solutions are

$$u_s = u \exp(isKa)$$

- By popping the solutions into the equation one we obtain the dispersion relation

$$\omega = (4C/M)^{1/2} \left| \sin \frac{1}{2} Ka \right|$$

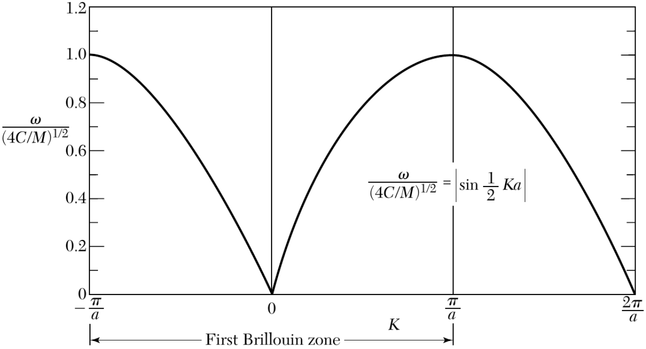

Figure 2: Caption

Elastic waves

- All the properties of the material can be described by the waves in the first Brillouin zone
  k values outside the first Brillouin zone reproduce the same physical properties of those inside

$$\frac{u_s}{u_{s+1}} = e^{ika}$$

- Then if we are at the edge of the Brillouin zone
  $$\frac{u_s}{u_{s+1}} = -1 \quad \Rightarrow \quad \text{standing waves (do not move left or right)}$$
- Waves at the edge of the Brillouin zone satisfy the Bragg's condition

Group velocity

- $$v_g = \frac{d\omega(k)}{dk}$$

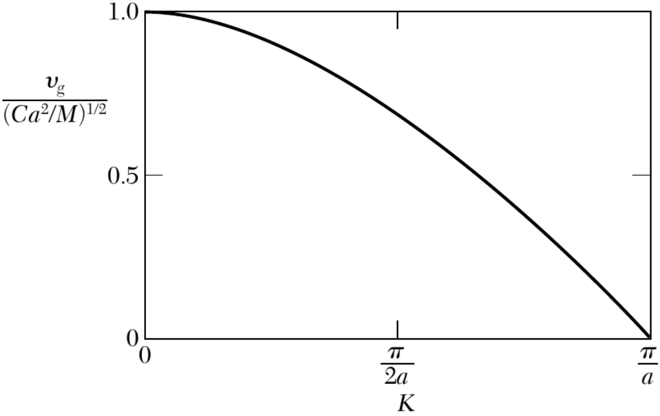

Figure 3: Group velocity of elastic waves in a crystal

Elastic waves

- If the basis is composed of two different atoms we get two dispersion relations (for small ka)

$$\omega^2 \cong 2C\left(\frac{1}{M_1}+\frac{1}{M_2}\right) \qquad \text{(optical branch)}$$
$$\omega^2 \cong \frac{\frac{1}{2}C}{M_1+M_2}K^2a^2 \qquad \text{(acoustical branch)}$$

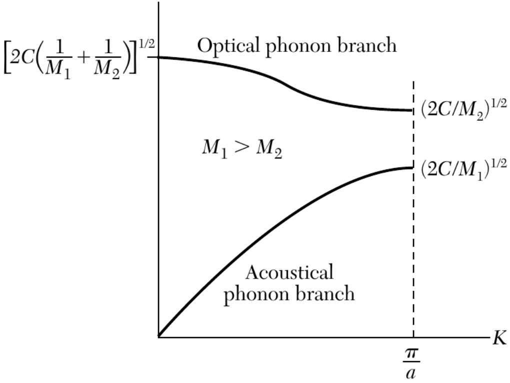

Figure 4: Dispersion relations in biatomic crystals for $ka \ll 1$

Optical and acustical branches

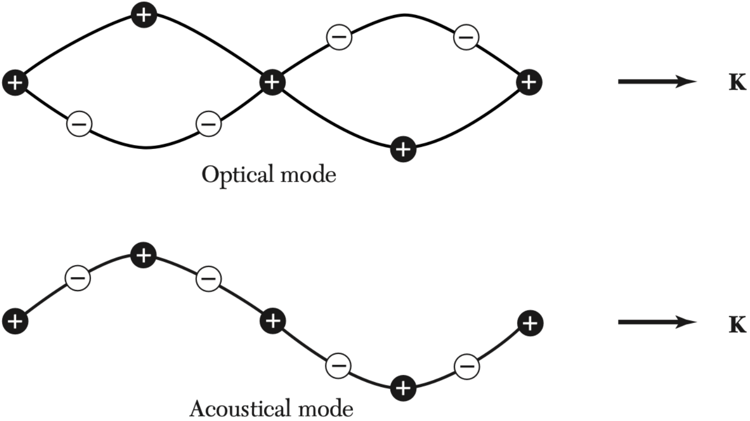

Figure 5: Transverse optical and transverse acoustical waves in a di- atomic linear lattice, illustrated by the particle displacements for the two modes at the same wavelength