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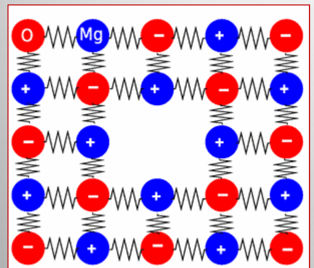
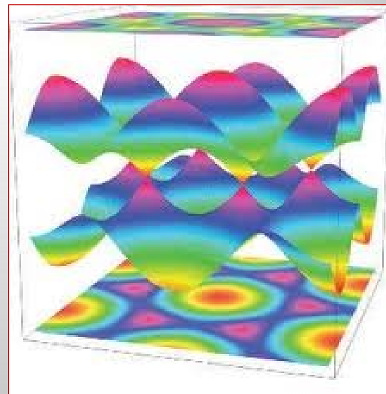
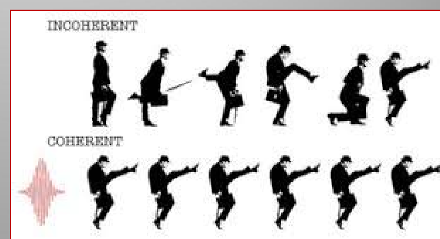




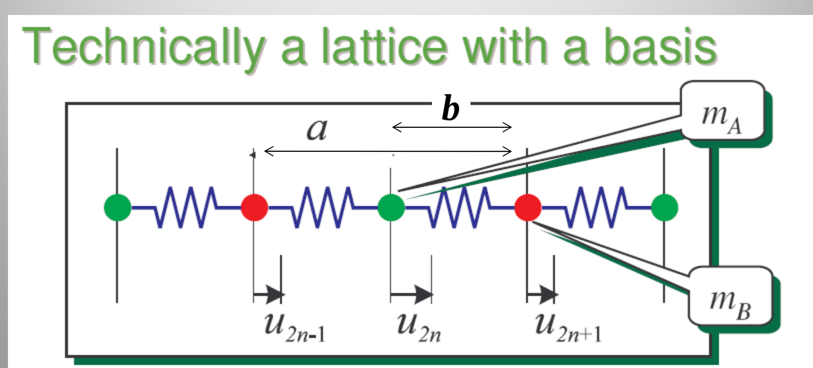


PHYS432

Materials Physics

Diatomic Lattice

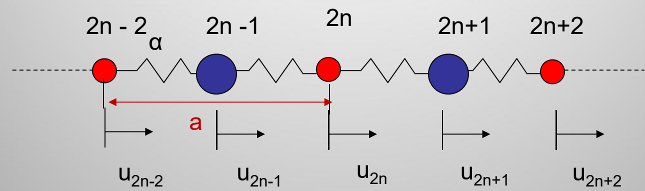
- Now try two different masses connected by same strength "spring" bonds



Dispersion relation: $\omega^2 = \alpha\left(\frac{1}{m_A}+\frac{1}{m_B}\right) \pm \alpha\sqrt{\left(\frac{1}{m_A}+\frac{1}{m_B}\right)^2 - \frac{4\sin^2(ka/2)}{m_A m_B}}$

Vibrational Spectrum for structures with 2 atoms/primitive basis

Linear diatomic chain:



Equation of motion for atoms on even positions: $\ddot{u}_{2n} = \frac{\alpha}{m_A}\left(u_{2n+1} + u_{2n-1} - 2u_{2n}\right)$

Equation of motion for atoms on odd positions: $\ddot{u}_{2n+1} = \frac{\alpha}{m_B}\left(u_{2n+2} + u_{2n} - 2u_{2n+1}\right)$

Solution with: $u_{2n} = A_1\, e^{i(2knb - \omega t)}$ and $u_{2n+1} = A_2\, e^{i((2n+1)kb - \omega t)}$

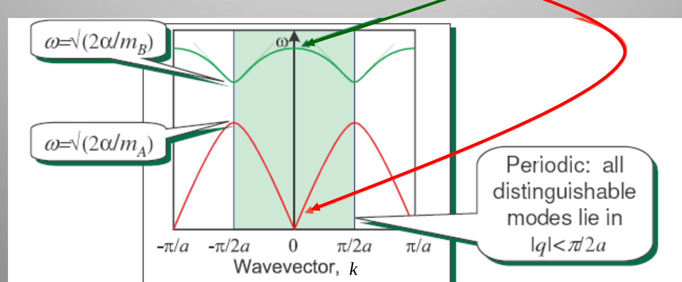
➢ For small k: $\omega^2 \approx \alpha\left(\frac{1}{m_A} + \frac{1}{m_B}\right)\left\{1 \pm \left[1 - \frac{2k^2b^2 m_A m_B}{(m_A + m_B)^2}\right]\right\}$

Optical branch (or mode) [higher frequency]:

$$\omega \approx \sqrt{2\alpha\left(\frac{1}{m_A} + \frac{1}{m_B}\right)}$$

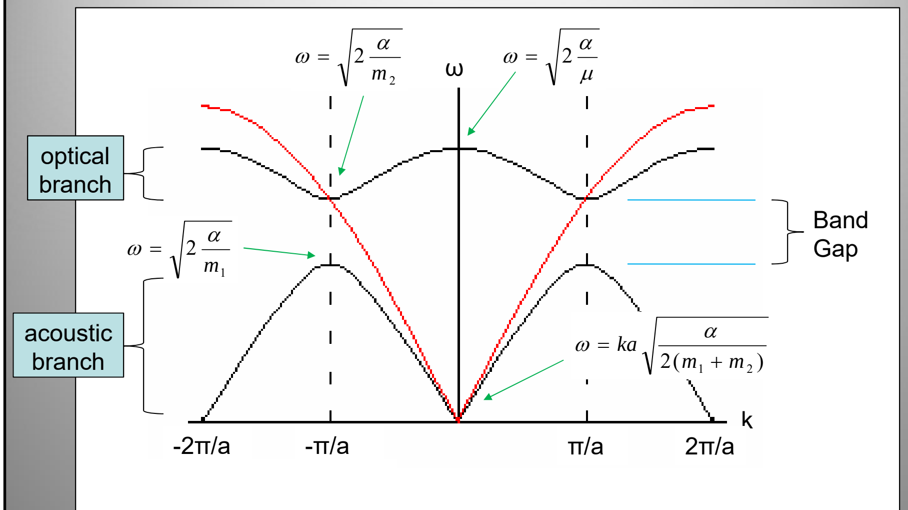
Acoustic branch (or mode) [lower frequency]:

$$\omega \approx kb\sqrt{\frac{2\alpha}{m_A + m_B}} = ka\sqrt{\frac{\alpha}{2(m_A + m_B)}}$$



Dispersion plot

Diatomic Lattice

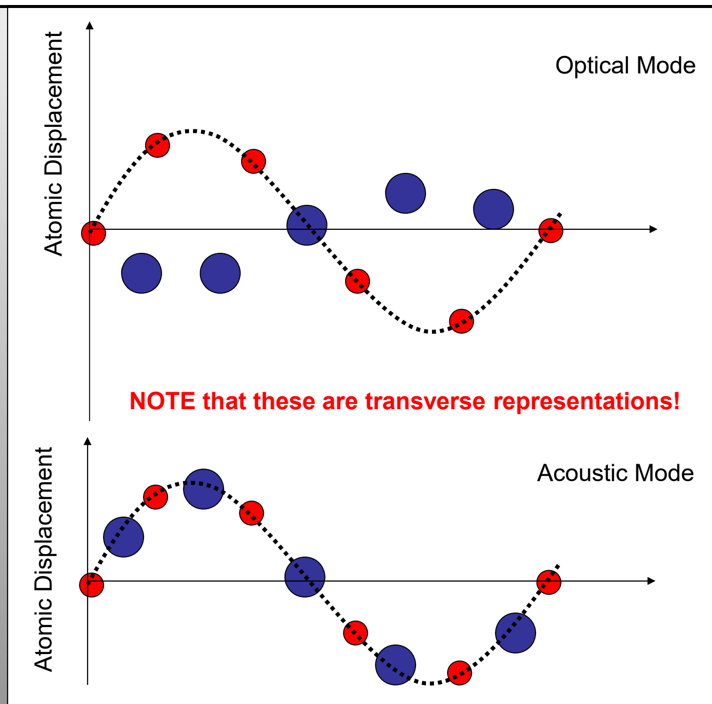


$$\left.\frac{A_2}{A_1}\right|_{k=0} = -\frac{m_1}{m_2}$$

Stokes' models

Animations

$$\left.\frac{A_2}{A_1}\right|_{k\to 0} = 1$$



Diatomic Lattice

Acoustic modes:

- Correspond to sound-waves in the long- λ limit.
- $\omega \to 0$ as k → *0*

Optical modes:

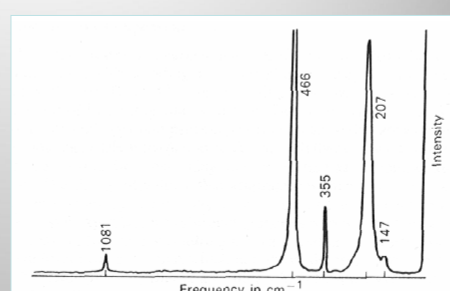
- In the long-λ limit, optical modes interact strongly with electromagnetic radiation in polar crystals.
- Strong optical absorption is observed (photons annihilated, phonons created; often in IR part of spectrum).
- w → finite value as k → *0*
- Optical modes arise from folding back the dispersion curve as the lattice periodicity is doubled (halved in k-*space).*

Zone boundary:

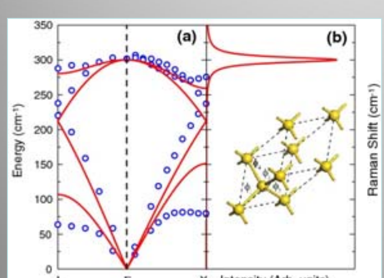
- All modes are standing waves at zone boundary, $\partial\omega / \partial k = 0$: a necessary consequence of the lattice periodicity.
- In a diatomic chain, the frequency-gap between the acoustic and optical branches depends on the mass difference. In the limit of identical masses the gap → zero.

e.g., exciting optical modes

- Raman scattering:
- near-IR, vis, near-UV



Scattered light has peaks at $h\nu = h\nu_o \pm \hbar\omega_{phonon}$



Raman response of c-Ge