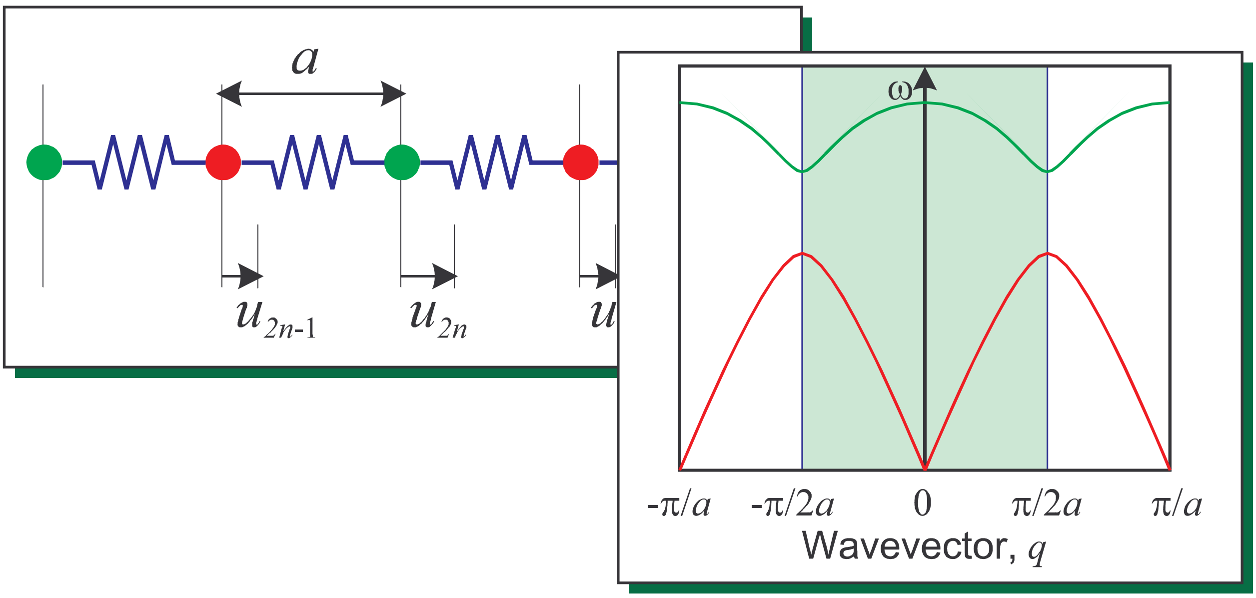
Lecture 12: Lattice vibrations

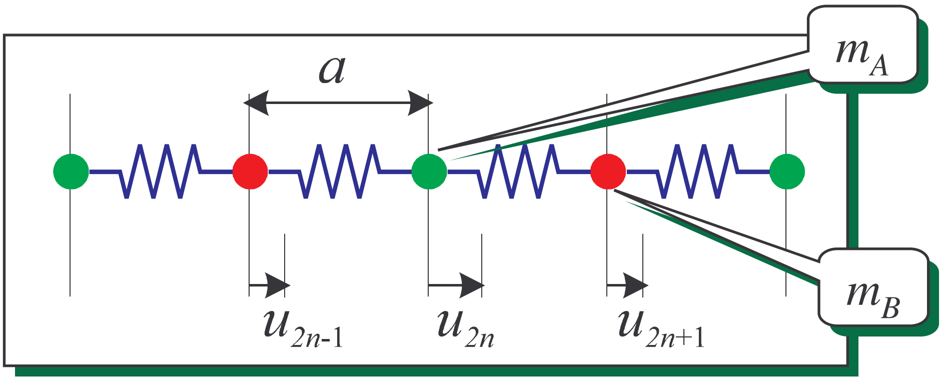
Quantised Lattice vibrations: Diatomic systems in 1-D and in Phonons in 3-D

- **Aims:**
  - Model systems (continued):
    - Lattice with a basis:
      - Phonons in a diatomic chain
      - origin of optical and acoustic modes
  - Phonons as quantised vibrations
  - Real, 3-D crystals:
    - Examples of phonon dispersion:
      - Rare gas solids
      - Alkali halides



Diatomic lattice

- Technically a lattice with a basis



  - proceeding as before. Equations of motion are:

$$m_A \ddot{u}_{2n} = \alpha\left(u_{2n+1} + u_{2n-1} - 2u_{2n}\right)$$

$$m_B \ddot{u}_{2n+1} = \alpha\left(u_{2n+2} + u_{2n} - 2u_{2n+1}\right)$$

Trial solutions:

$$u_{2n} = U_1 \exp\{i(2nqa - \omega t)\}$$

$$u_{2n+1} = U_2 \exp\{i((2n+1)qa - \omega t)\}$$

substituting gives

$$\left(m_A\, \omega^2 - 2\alpha\right)U_1 + (2\alpha \cos qa)U_2 = 0$$

$$(2\alpha \cos qa)U_1 + \left(m_B\, \omega^2 - 2\alpha\right)U_2 = 0$$

homogeneous equations require determinant to be zero giving a quadratic equation for ω^2.

$$\omega^2 = \frac{\alpha}{m_A m_B}[(m_A + m_B) \pm$$

Two solutions for each q

$$\left\{(m_A + m_B)^2 - 4m_A m_B \sin^2 qa\right\}^{1/2}]$$

Acoustic and Optic modes

- **Solutions**
  - $q \to 0$:
    - Optic mode (higher frequency)

$$\omega = \sqrt{\frac{\alpha 2(m_A + m_B)}{m_A m_B}} = \sqrt{\frac{2\alpha}{\mu}}$$

Effective mass μ

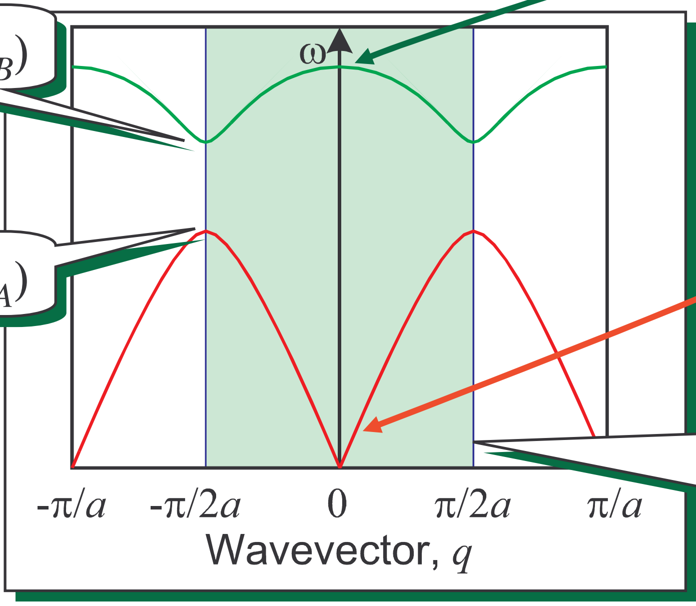
    - Acoustic mode (lower frequency)

$$\omega^2 \approx \frac{\alpha}{m_A m_B}\left[(m_A + m_B) - (m_A + m_B)\left\{1 - 4\frac{m_A m_B}{(m_A + m_B)^2}(qa)^2\right\}^{1/2}\right]$$

$$\omega \approx \sqrt{\frac{2\alpha a^2}{m_A + m_B}}\,q$$

$\omega = \sqrt{(2\alpha/m_B)}$

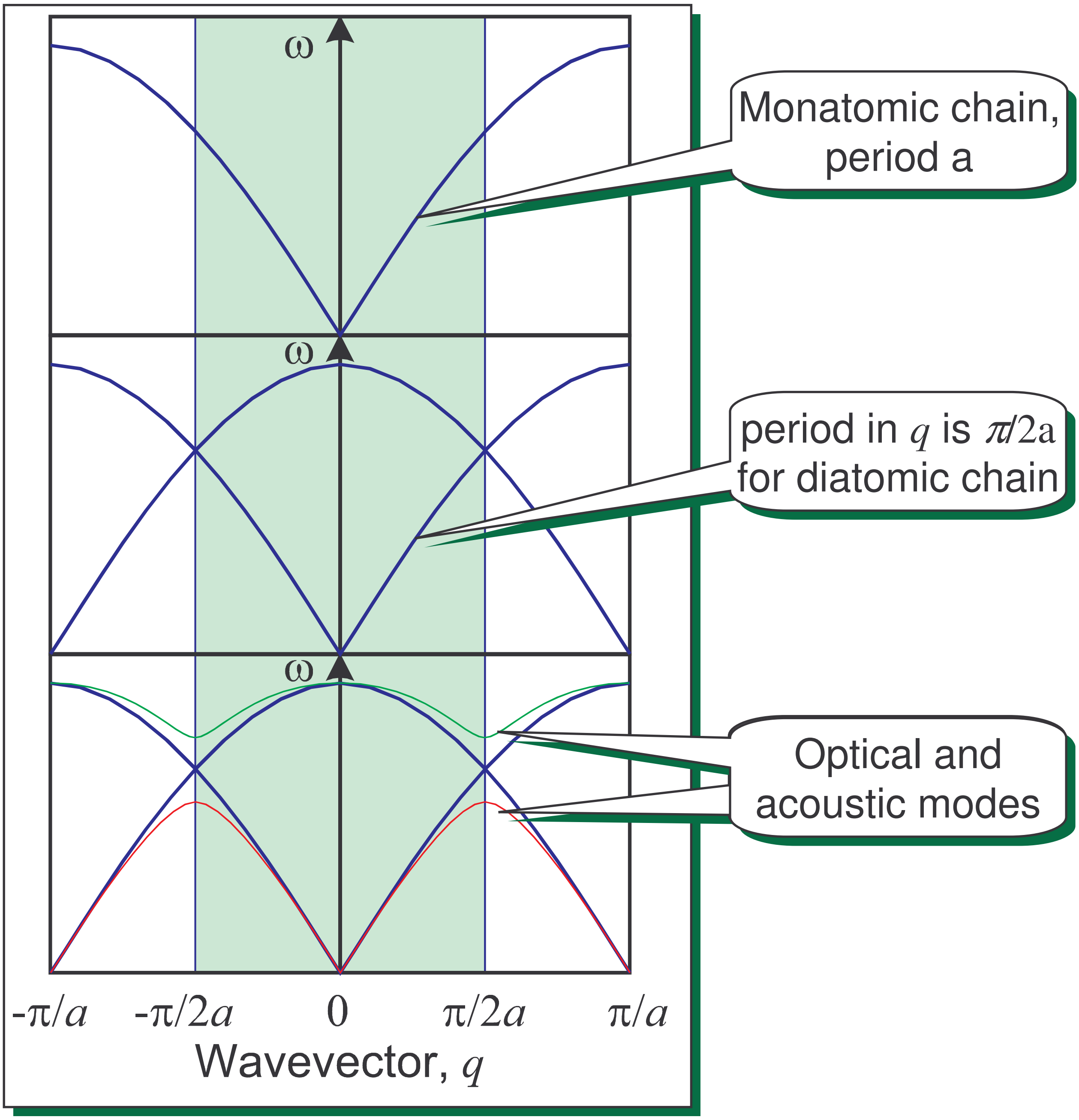
$\omega = \sqrt{(2\alpha/m_A)}$



Periodic: all distinguishable modes lie in $|q| < \pi/2a$

Origin of optic and acoustic branches

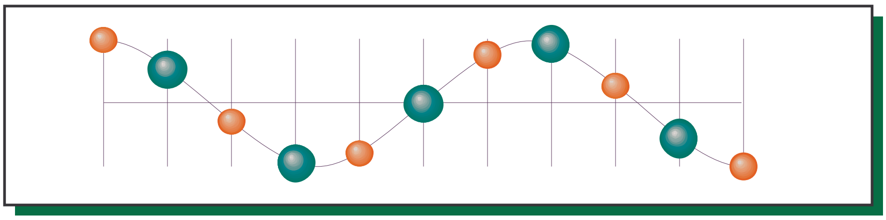
- **Effect of periodicity**
  - The modes of the diatomic chain can be seen to arise from those of a monatomic chain. Diagrammatically:



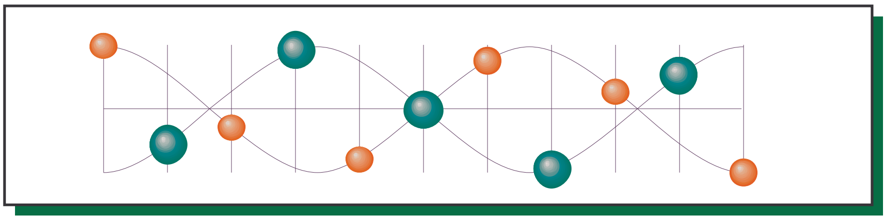
Displacement patterns

- Displacements shown as transverse to ease visualisation.

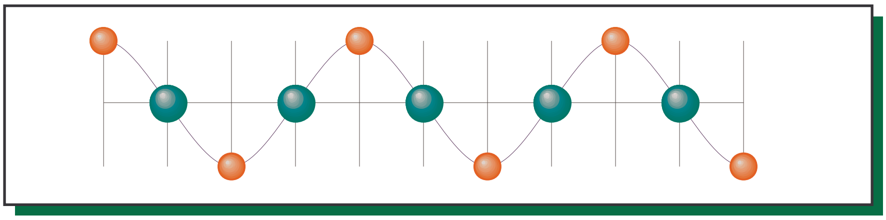
- **Acoustic modes:** Neighbouring atoms in phase



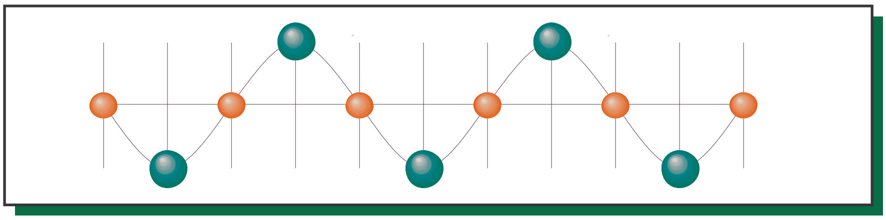
- **Optical modes:** Neighbouring atoms out of phase



- **Zone-boundary modes**
  - $q=\pi/2a;\ \lambda=2\pi/q=4a$ (standing waves)
  - Higher energy mode – only light atoms move



  - Lower energy mode – only heavier atoms move

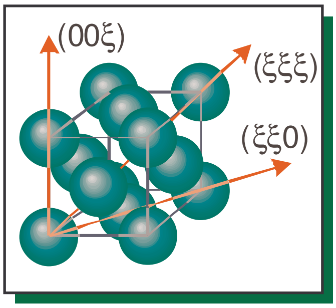


Diatomic chain: summary

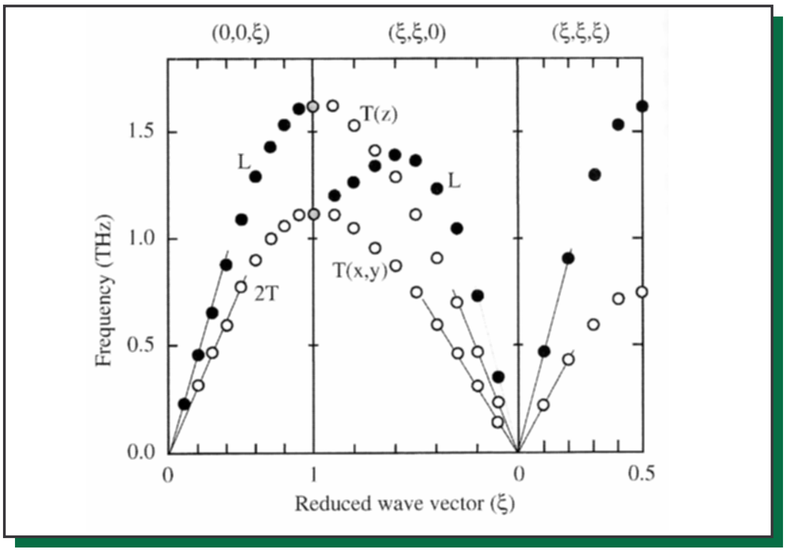
- **Acoustic modes:**
  - correspond to sound-waves in the long-wavelength limit. Hence the name.
  - $\omega \to 0$ as $q \to 0$
- **Optical modes:**
  - In the long-wavelength limit, optical modes interact strongly with electromagnetic radiation in polar crystals. Hence the name.
  - Strong optical absorption is observed (Photons annihilated, phonons created).
  - $\omega \to$finite value as $q \to 0$
  - Optical modes arise from folding back the dispersion curve as the lattice periodicity is doubled (halved in q-space).
- **Zone boundary:**
  - All modes are standing waves at the zone boundary, $\partial\omega/\partial q = 0$: 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 tends to zero.

Phonons in 3-D crystals: Monatomic lattice

- Example: Neon, an f.c.c. solid:
  - Inelastic neutron scattering results in different crystallographic directions



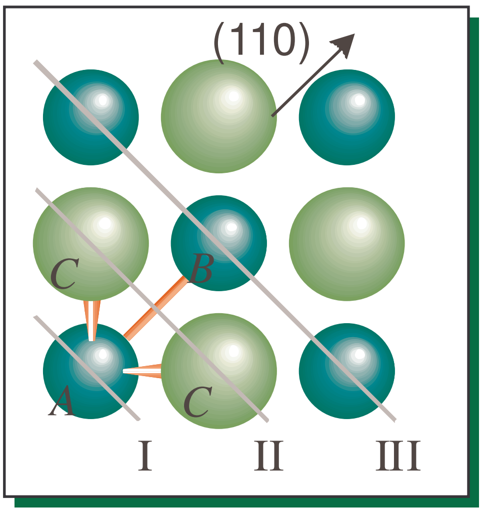
Phys. Rev. *B* **11**, 1681, (1975)



  - Many features are explained by our 1-D model:
  - Dispersion is sinusoidal (n.n. interactions)
  - All modes are acoustic (monatomic system)

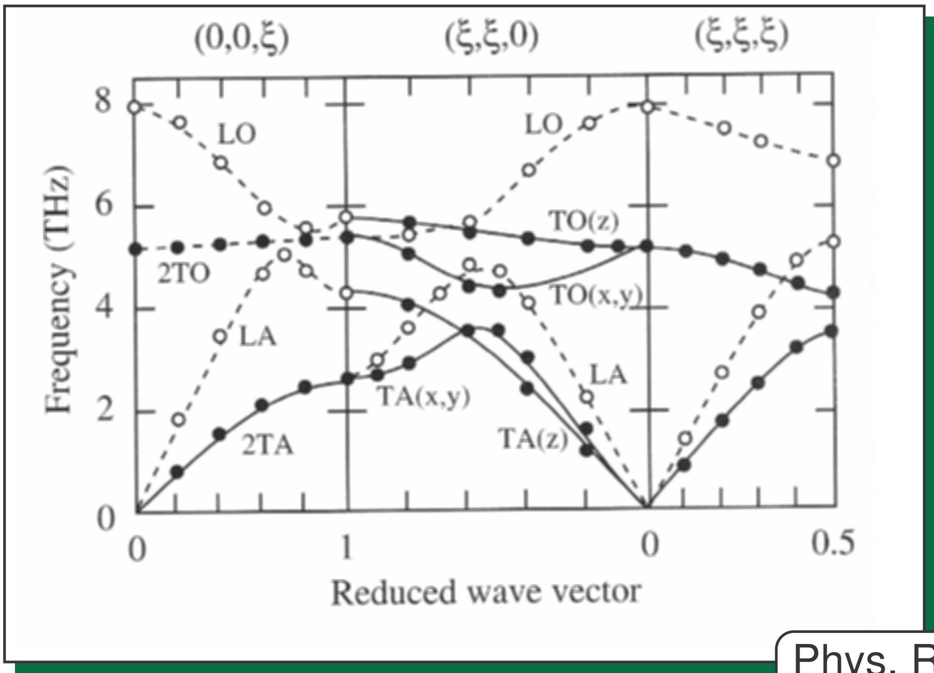
Neon: a monatomic, f.c.c. solid

- Notes: (continued)
  - There are two distinct types of mode:
    - Longitudinal (L), with displacements parallel to the propagation direction,
      - These generally have higher energy
    - Transverse (T), with displacements perpendicular to the propagation direction
      - These generally have lower energy
      - They are often degenerate in high symmetry directions (not along (ξξ0))
  - Minor point (demonstrating that real systems are subtle and interesting, but also complicated):
    - L mode along (ξξ0) has 2 Fourier components, suggesting next-n.n. interactions (see Q 8, sheet 2). In fact there are only n.n. interactions
    - The effect is due to the fcc structure. Nearest-neighbour interactions from atom, A (in plane I) join to atom C (in plane II) and to atom B (in plane III) thus linking nearest- and next-nearest-planes.



Phonons in 3-D crystals: Diatomic lattice

- Example: NaCl, has sodium chloride structure!
  - Two interpenetrating f.c.c. lattices



Phys. Rev. **178** 1496, (1969)

- Main points:
  - The 1-D model gives several insights, as before. There are:
    - Optical and acoustic modes (labels O and A);
    - Longitudinal and transverse modes (L and T).
  - Dispersion along (ξξξ) is simplest and most like our 1-D model
    - (ξξξ) planes contain, alternately, Na atoms and Cl atoms (other directions have Na and Cl mixed)

NaCl phonons

- Notes, continued…
  - Note the energy scale. The highest energy optical modes are ~8 THz (i.e. approximately 30 meV). Higher phonon energies than in Neon. The strong, polar bonds in the alkali halides are stronger and stiffer than the weak, van-der-Waals bonding in Neon.
  - Minor point:
    - Modes with same symmetry cannot cross, hence the avoided crossing between acoustic and optical modes in (00ξ) and (ξξ0) directions.
    - Ignore the detail for present purposes