

Crystal Structure

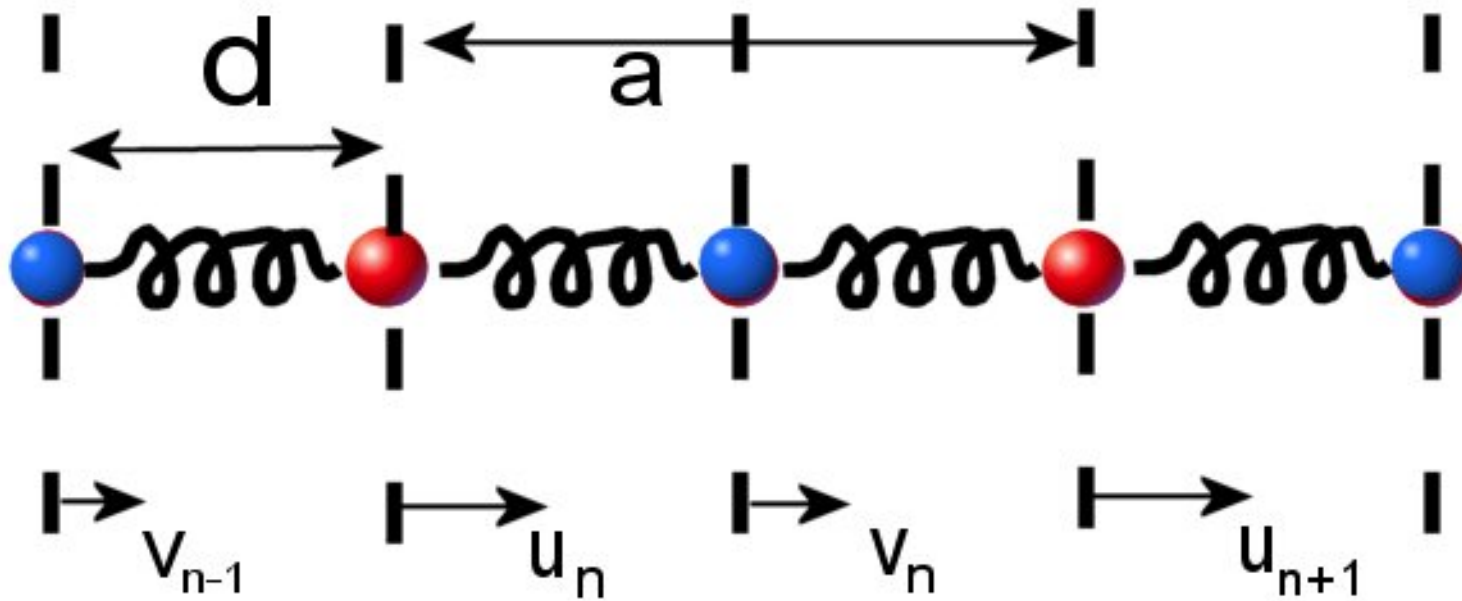
LATTICE VIBRATIONS

Lecture 9

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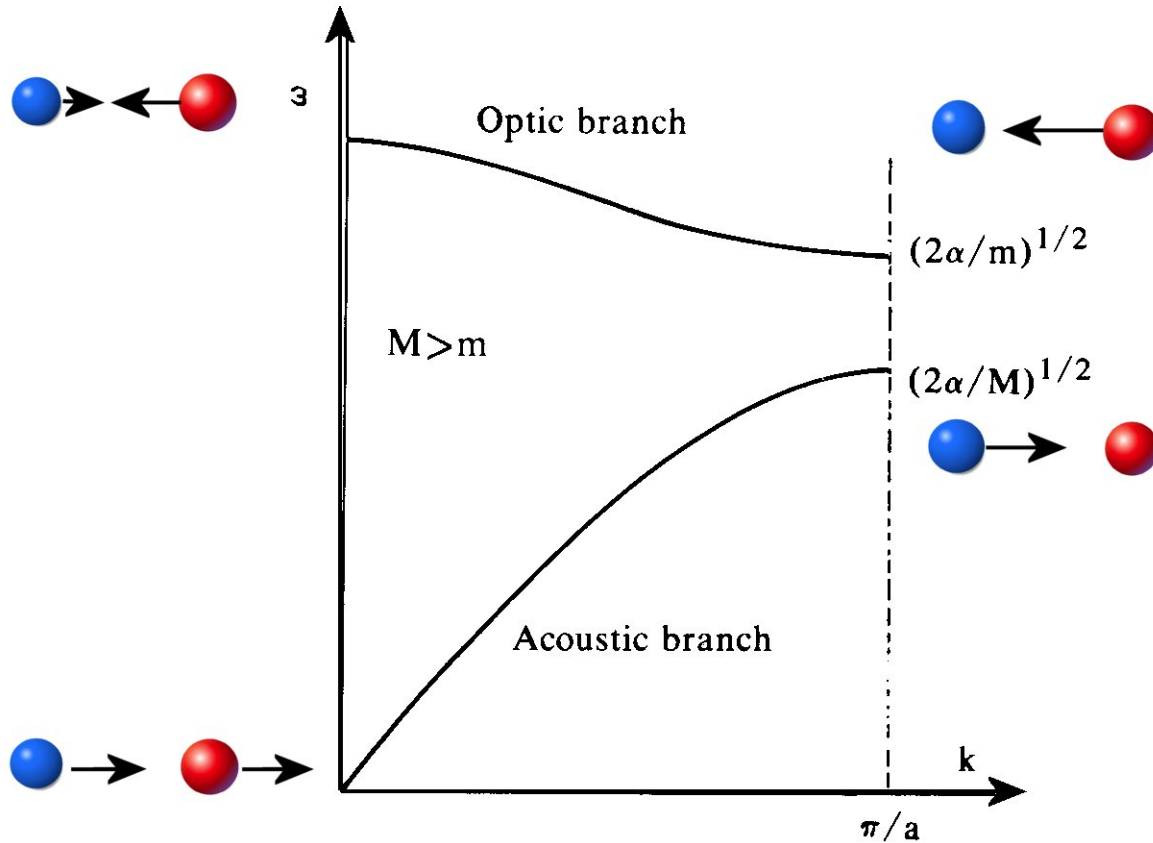
Lattice Vibrations

4.1.3 More than one atom per cell (contd)



Two solutions: if atomic spacing $d = a/2$

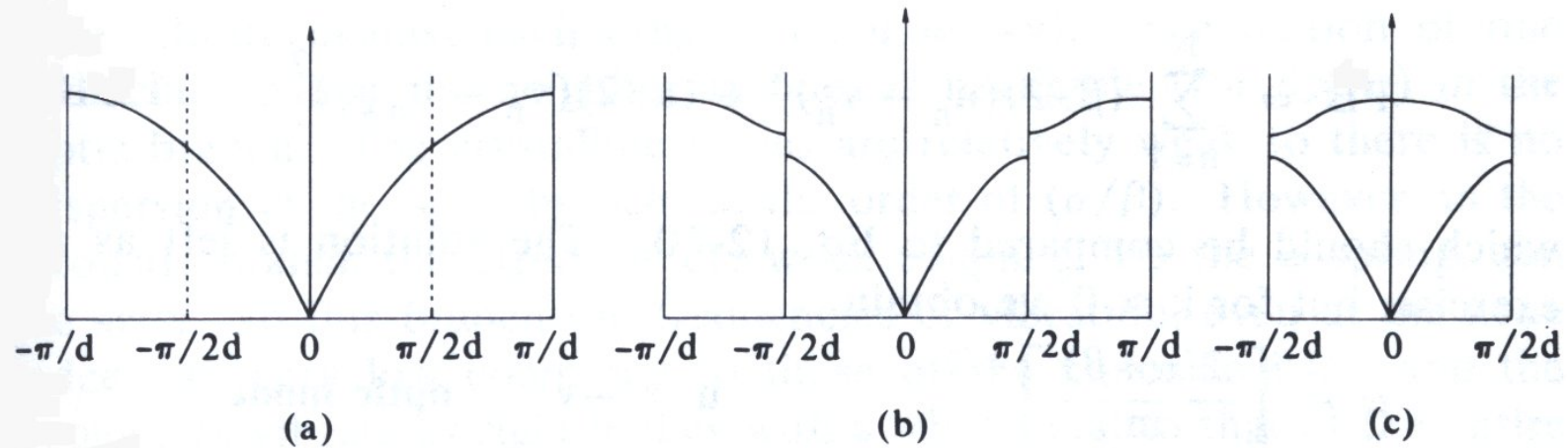
$$\omega^2 = \alpha \left(\frac{1}{m} + \frac{1}{M} \right) \pm \alpha \sqrt{\left(\frac{1}{m} + \frac{1}{M} \right)^2 - \frac{4 \sin^2(ka/2)}{mM}}$$



Notes on diatomic linear chain:

- **Acoustic branch has $\omega = 0$ at $k = 0$.**
- **Optic branch has $\omega \neq 0$ at $k = 0$.**
- **At $k = 0$**
 - **on acoustic branch, atoms move in phase**
 - **on optic branch, atoms move in antiphase, keeping centre of mass of cell static.**
 - **if atoms have different charges, optic mode gives oscillating electric dipole moment to unit cell**
 - **dipole moment couples to electromagnetic field - hence optic mode**
- **At $k = \pi/a$ only one atomic species moves in each mode.**

4.1.4 Degenerate case of diatomic chain



Diagrams showing the folding back of a Brillouin zone. (a) ω vs. k in the first Brillouin zone k between $\pm\pi/d$. (b) The primitive unit cell has become twice as large so the Brillouin zone is twice as small. (c) The same as (b) but the pieces of the ω vs. k curve are translated into the first Brillouin zone.

If the masses become equal, the diatomic chain is identical with the monatomic chain except that the unit cell is larger than it need be. Larger unit cell in real space \rightarrow smaller unit cell in reciprocal space ($-\pi/a < k < \pi/a$) Same *physics* from monatomic cell, one branch of spectrum, or diatomic cell, two branches.

4.1.5 Three dimensions

- **Atoms can move in three directions (for chain, parallel + 2 transverse).**
- **Transverse force constants weaker, so transverse frequencies usually less than longitudinal**
- **Similarly, transverse wave speeds less than longitudinal**
- **3-D monatomic crystal: 3 acoustic branches (L + 2T)**
- **Transverse branches degenerate along some symmetry directions.**

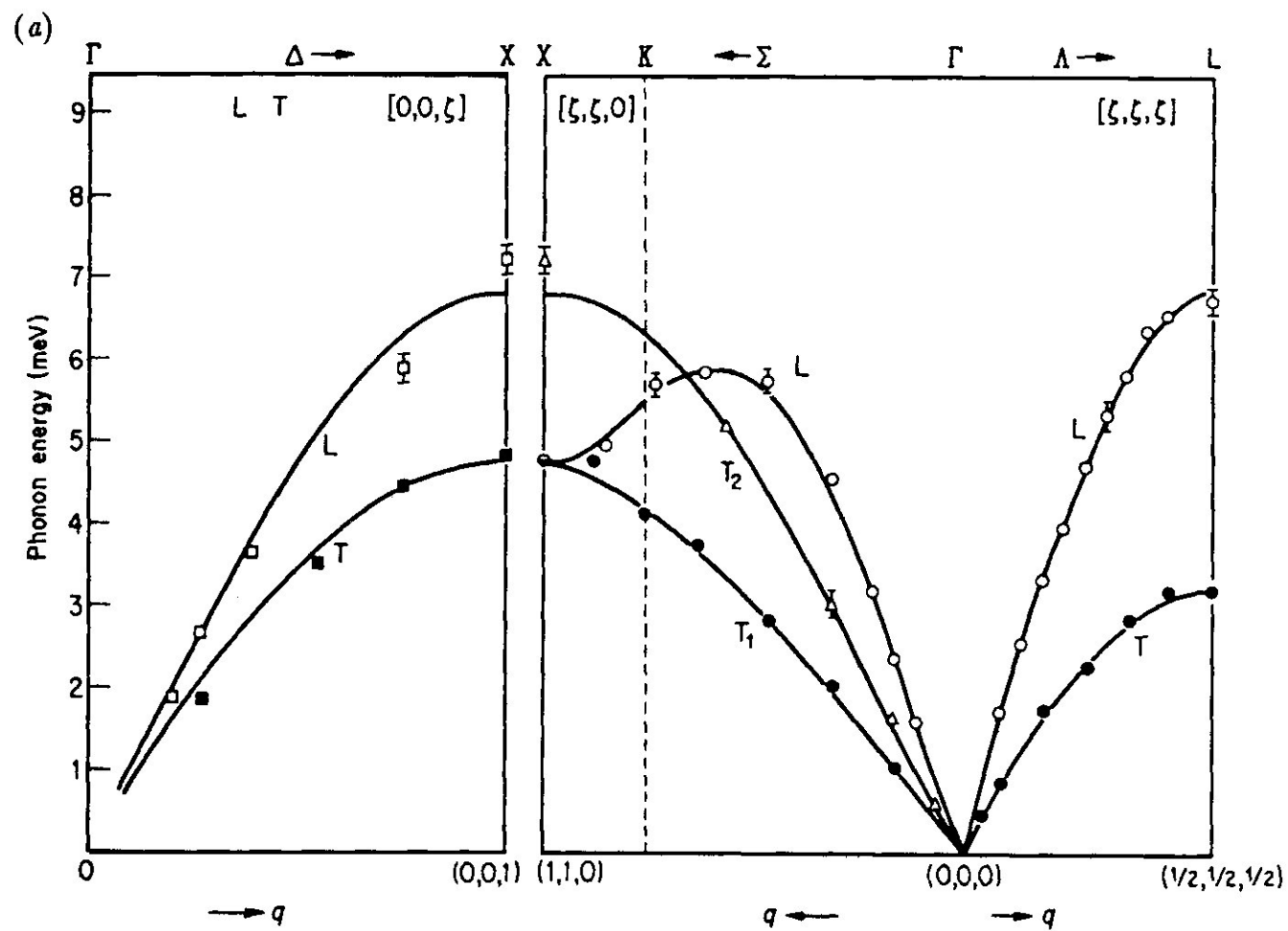
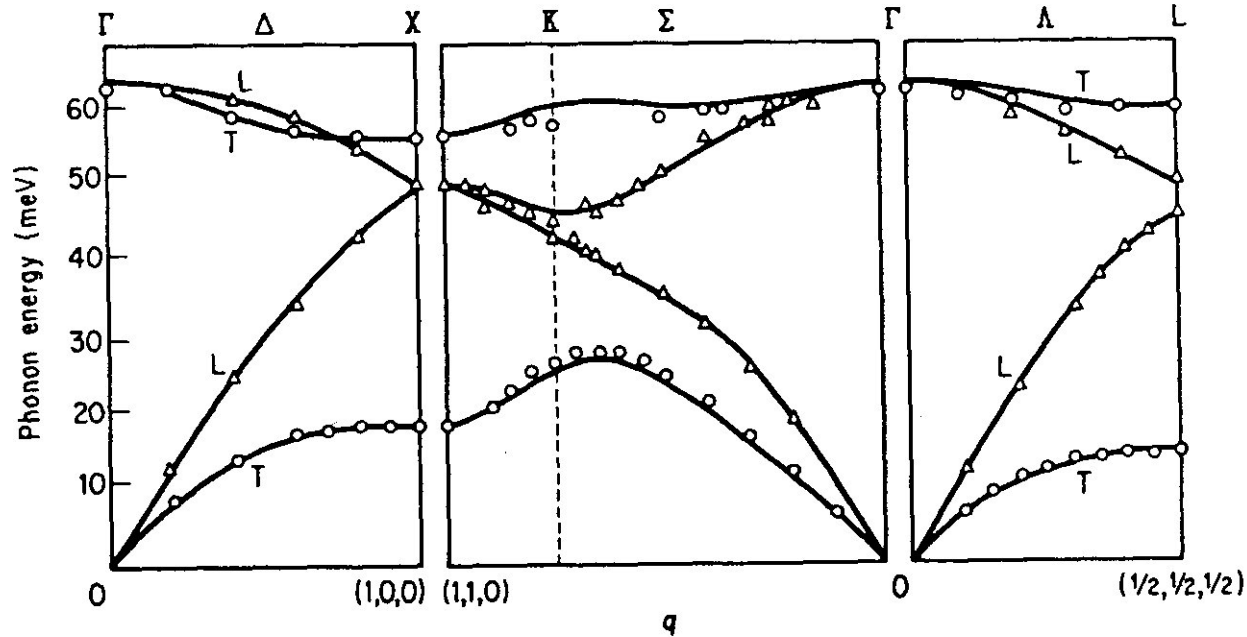


Figure (a) Measured phonon dispersion in Ne (after Leake *et al* (1969); reproduced from Elliott and Gibson (1982)).

3-D diatomic crystal: 3 acoustic branches (L + 2T) and 3 optical.

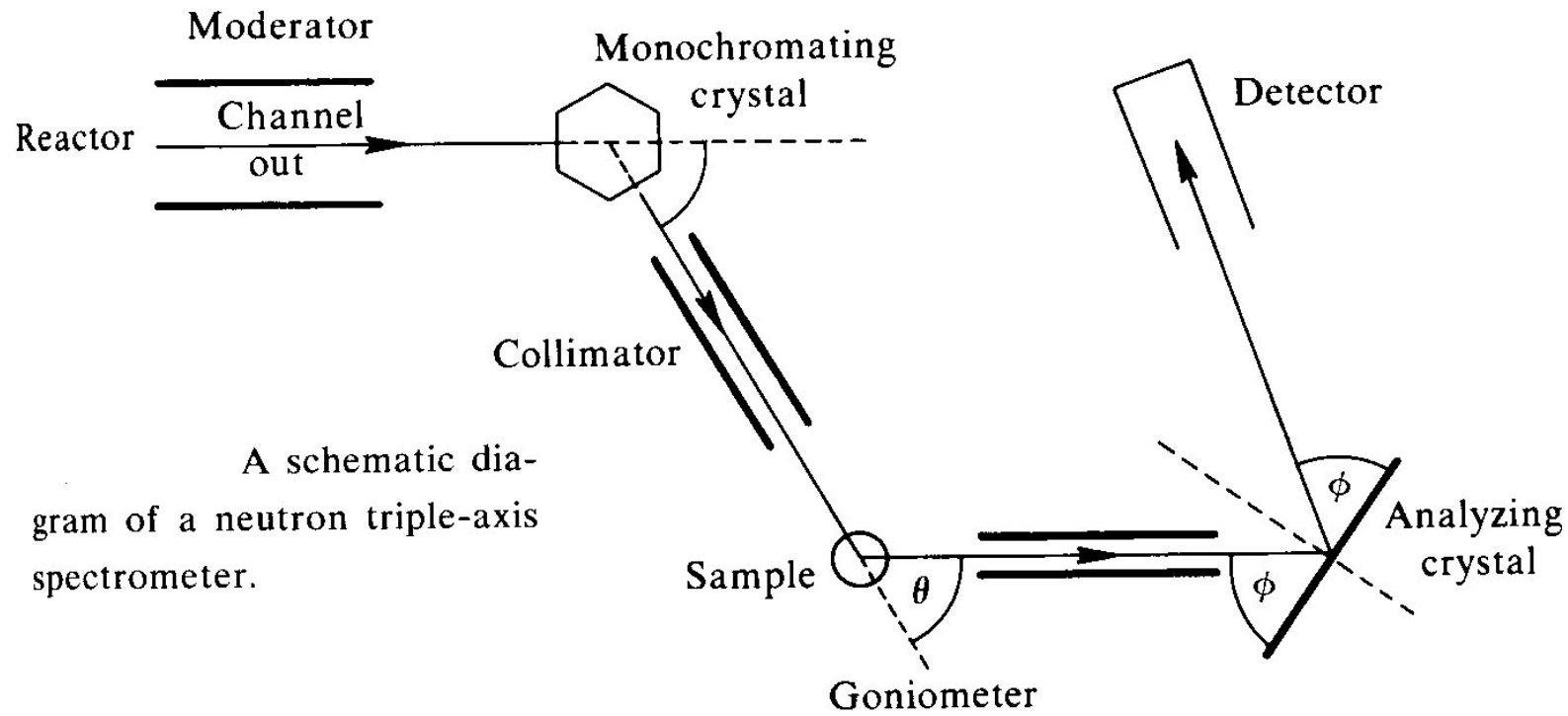


Measured phonon dispersion in Si (after Dolling (1963))

In general: N atoms in the unit cell \rightarrow 3 acoustic branches and $3(N - 1)$ optical branches.

4.1.6 Measuring Phonon Spectra

- **Phonon energy** $E = \hbar\omega \approx 10^{-34}10^{13} = 10^{-21} \text{ J} \approx 0.01 \text{ eV}$
- **Comparable with neutron energies**
- **Inelastic neutron scattering: measure Δk and ΔE .**



- Know input k and E
- Scatter output beam from analyser crystal of known structure.
- From Bragg angles out of analyser, know wavelength of original scattered beam
- hence scattered energy, hence Δk

4.2 Normal Modes

In formal terms, the energy of the crystal is a function of the displacements of all the atoms from their equilibrium positions:

$$U(\{u_n\}) = U_0 + \frac{1}{2} \sum_{n,n'} u_n u_{n'} \left(\frac{\partial^2 U}{\partial u_n \partial u_{n'}} \right)_0 + \frac{1}{3!} \sum_{n,n',n''} u_n u_{n'} u_{n''} \left(\frac{\partial^3 U}{\partial u_n \partial u_{n'} \partial u_{n''}} \right) + \dots$$

Note that the linear term is zero – this is the definition of the equilibrium structure. In the *harmonic approximation*

$$U(\{u_n\}) = U_0 + \frac{1}{2} \sum_{n,n'} D_{nn'} u_n u_{n'}$$

add the kinetic energy

$$\sum_n \frac{p_n^2}{2m_n},$$

and then change variables, forming linear combinations of the form

$$u(k) = \sum_n A_n u_n e^{ikr_n}.$$

These are the *normal modes*, in terms of which the Hamiltonian is diagonal.

We find we can rewrite the Hamiltonian of the system in the form

$$\mathcal{H} = \sum_k \left(n_k + \frac{1}{2} \right) \hbar \omega_k.$$

In the harmonic approximation, the lattice vibrations are the same as a collection of harmonic oscillators, with frequencies ω_k . These normal modes do not interact: put energy into one mode k by altering n_k and it will stay in that mode. The normal modes are called *phonons*. The allowed values of k will be determined by the boundary conditions at the edges of the material.

4.3 Phonon Density of States

4.3.1 One Dimension - $g(k)$

Take crystal of length L , and impose *periodic boundary conditions*, so that for a wave

$$\exp(ikx) = \exp(ik(x + L)),$$

so

$$\exp(ikL) = 1,$$

or

$$k = n \frac{2\pi}{L},$$

where n is an integer. The allowed states are uniformly distributed in reciprocal space (k-space) with spacing $2\pi/L$. The density of states is the inverse of the spacing,

$$g(k) = \frac{L}{2\pi}.$$

The number of allowed states with wavevectors between k and $k + dk$ is $g(k) dk$.