

Lecture 6 Static Lattice Failure and Phonons

Simon: Chapter 9 (p77-86); Kittel: Chapter 4 (p90-95)

We now move on to consider a more complete description of crystals as being composed of *vibrating atoms*. By implication much of the previous discussion has treated crystals as immobile atoms at fixed lattice points. This so called “static lattice” model may only be valid at zero temperature, and even then there is zero point energy. At all finite temperature the atoms (or more correctly the ion cores) in the lattice must have some thermal energy which will manifest as motion about an equilibrium position. (Note that quantum mechanics also has some bearing on this through the uncertainty principle expressed as $\Delta x \Delta p \geq \hbar$ which requires strongly localised atoms to have a non-zero momentum).

There are a number of properties of crystals which cannot be described by the static lattice model. These include:

- Transmission of sound
- Superconductivity
- Inelastic scattering of light from crystal surfaces
- Heat capacity of solids at constant volume
- Thermal expansion
- Melting

(More details in Ashcroft and Mermin Chapter 21 – see background reading folder on duo)

We now consider a crystal in which the atoms vibrate elastically about a mean position. The description is simplified at the outset by limiting the description to having only one atom in the primitive unit cell. This will be extended to a two-atom basis later.

The vibrations of atoms in crystals will be quantised. The quanta of vibration are called phonons. (From Greek phono means sound/voice).

The phonon is one of a family of excitations in solids. Each can be set up by a corresponding exciting field which supplies the energy necessary for the excitation to be created.







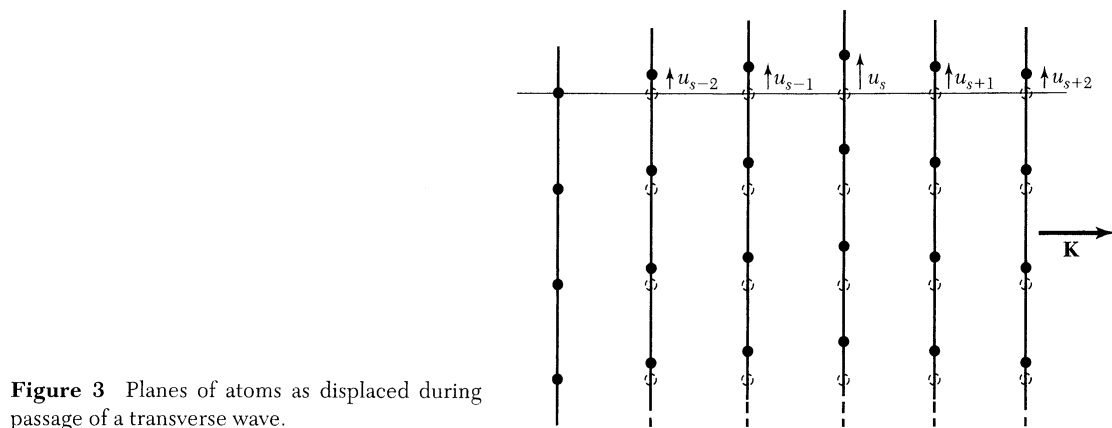
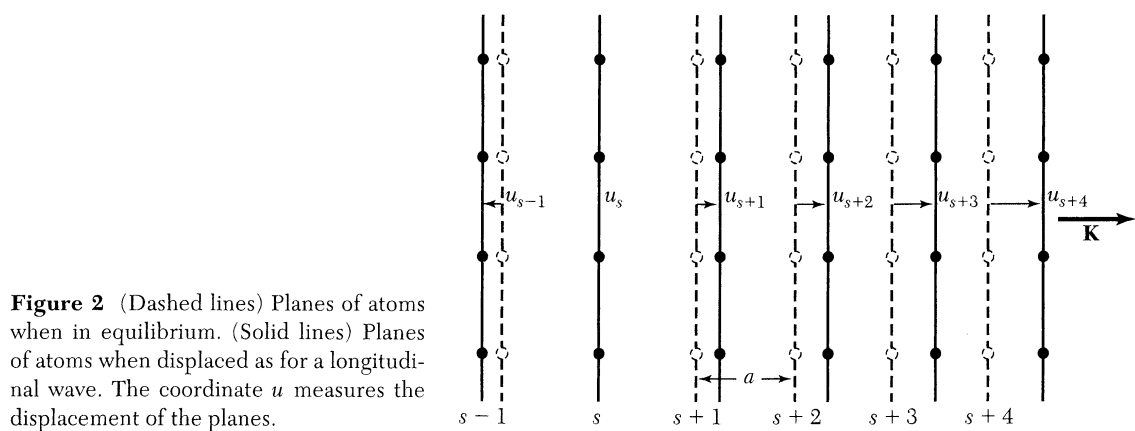
	Name	Field
	Electron	
	Photon	Electromagnetic wave
	Phonon	Elastic wave
	Plasmon	Collective electron wave
	Magnon	Magnetization wave
—	Polaron	Electron + elastic deformation
—	Exciton	Polarization wave

Figure 1 Important elementary excitations in solids.

Based on our previous description of waves and wavevectors we want to describe the resulting vibrational wave in terms of a wavevector. We also want to be able to relate the wavevector to the elastic constants of the crystal.

Consider a cubic crystal. The directions of high symmetry provide the simplest picture for developing a description of vibrational waves. These are the $[100]$ $[110]$ and $[111]$ directions which correspond to the cube edge, the cube face diagonal and the cube body diagonal.

When a wave propagates in one of these directions a full plane of atoms moves in phase with displacements either parallel or perpendicular to the direction of propagation.



The displacement of the plane of atoms is described by a single coordinate u_s for plane s . The problem is now reduced to *one dimension*.

In the case where the displacement is parallel to the direction of propagation, this is described as a **longitudinal** wave or polarisation.

Waves with displacements perpendicular to the direction of propagation are called **transverse** waves or polarisations.

(There is one longitudinal wave and two transverse waves for each wavevector.)

We assume that the elastic response of the crystal is a linear function of the force (this is the crystalline equivalent of Hooke's Law). These are described as elastic waves

From vibrations and waves we know that the energy of an oscillating system (simple harmonic motion) is given by:

$$E = \frac{1}{2} k A^2$$

where k is the spring constant given by: $\omega = \sqrt{\frac{k}{m}}$ and A is the maximum amplitude of vibration. (Young and Freedman section 13.3)

The elastic energy is a quadratic function of the displacement from the mean position.

In considering the forces acting on a plane s with a displacement from equilibrium given by u_s it is usual to consider only the nearest neighbour interactions $s \pm 1$.

The total force on the plane from Hooke's Law is then:

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

C is the force constant between nearest neighbour planes (this will be different for longitudinal and transverse waves). C is also the force constant for individual atoms in the plane.

The equation of motion for an atom in the plane s is then:

$$M \frac{d^2 u_s}{dt^2} = C(u_{s+1} + u_{s-1} - 2u_s)$$

where M is the mass of the atom.

From our knowledge (!) of Hooke's law we expect solutions to be of simple harmonic motion. These are described by a time dependent function of the form: $\exp(-i\omega t)$. This means

$$\frac{d^2 u_s}{dt^2} = -\omega^2 u_s$$

and we then have:

$$-M\omega^2 u_s = C(u_{s+1} + u_{s-1} - 2u_s)$$

This equation describes the motion of adjacent planes of atoms u_s , u_{s+1} and u_{s-1} .

The solution of this equation will be a wave equation. The general form will be:

$$u_{s\pm 1} = u \exp i(s \pm 1)ka = u \exp(isKa) \exp(\pm iKa)$$

where a is the spacing between adjacent planes, K is the wavevector and u is the maximum amplitude. Note that the separation of planes will be different in different directions and so the value of a will depend on the direction of propagation of any wave.

Substituting the solution into the equation gives:

$$-\omega^2 M u \exp(isKa) = Cu\{ \exp[i(s+1)Ka] + \exp[i(s-1)Ka] - 2 \exp[isKa] \}$$

This can be reduced to:

$$\omega^2 M = -C[\exp(iKa) + \exp(-iKa) - 2]$$

Using the identity that $2 \cos Ka = \exp(iKa) + \exp(-iKa)$ we then have:

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

Using trigonometric identities we can write the relation above as:

$$\omega^2 = \left(\frac{2C}{M}\right) (1 - \cos Ka) = \left(\frac{2C}{M}\right) \sin^2 \frac{1}{2} Ka \quad ; \text{ and } \omega = \left(\frac{4C}{M}\right)^{\frac{1}{2}} \left| \sin \frac{1}{2} Ka \right|$$

This is the **dispersion relation** describing the frequency dependence of propagation. In simple terms: waves of certain frequency (or wavevector k) travel faster than others.

Dispersion is a key concept in understanding the behaviour of phonons (and other aspects of condensed matter physics).

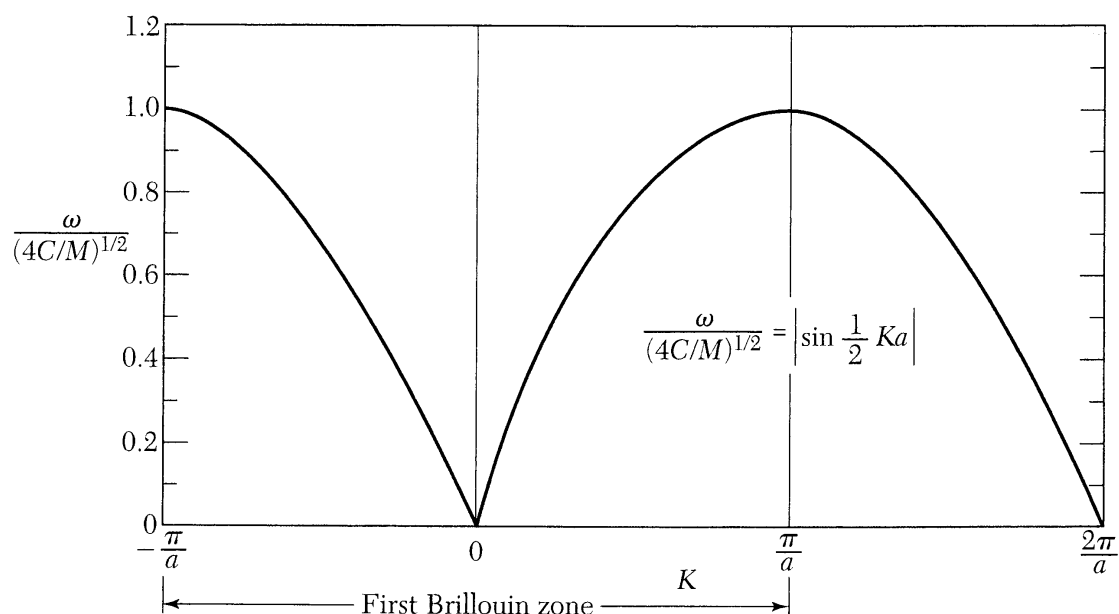


Figure 4 Plot of ω versus K . The region of $K \ll 1/a$ or $\lambda \gg a$ corresponds to the continuum approximation; here ω is directly proportional to K .

Graph shows dispersion behaviour. Remember the boundary of the first Brillouin zone lies at $K = \pm \pi / a$. (The unit cell in reciprocal or frequency space)

Group Velocity

If we consider the propagation of a displacement wave in a crystal as a wave packet (phonon) then the concept of group velocity will describe the velocity of the displacement through the crystal. We remind ourselves that *group velocity* is defined by:

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

or expressing it in vector notation

$$\mathbf{v}_g = \nabla_{\mathbf{K}} \omega(\mathbf{K})$$

Mathematically this is the gradient of the frequency with respect to \mathbf{K} , physically this is the velocity of energy propagation in the medium (the energy of the elastic wave).

Applying this to the dispersion relation above gives a group velocity of

$$v_g = \left(\frac{Ca^2}{M} \right)^{\frac{1}{2}} \cos \frac{1}{2} Ka$$

This is zero at the edge of the first Brillouin zone where $K = \pi / a$, this corresponds to a standing wave and we have zero net velocity (see diagram next page).

Conceptually the group velocity of a wave packet represents the velocity of a phonon.

Long wavelength limit

This regime is important in considering the propagation of sound through materials. These are very long wavelength waves covering many unit cells. They therefore have a very small wavevector close to $K \sim 0$. The long wavelength limit can be defined by having $Ka \ll 1$.

When $Ka \ll 1$ we expand $\cos(Ka) \approx 1 - \frac{1}{2}(Ka)^2$ so the dispersion relation then becomes:

$$\omega^2 = (C/M)K^2 a^2$$

$$\omega = \sqrt{\frac{C}{M}} Ka$$

This shows that the frequency ω is directly proportional to the wavevector K in the long wavelength limit. (i.e. the graph is a straight line at very small K values). This is equivalent to stating the velocity of sound is independent of frequency in this regime. In this situation $v = \omega/K$ as for elastic waves in a continuum.

The long wavelength limit is a common approximation and applies to all waves where the wavelength is significantly larger than the lattice constant a .

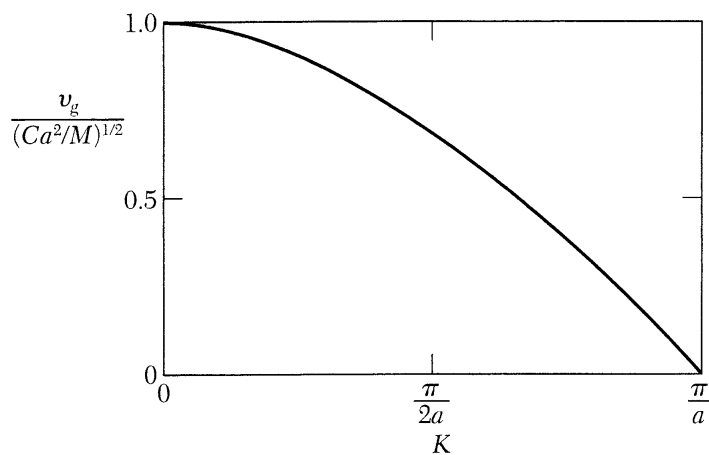


Figure 6 Group velocity v_g versus K , for model of Fig. 4. At the zone boundary $K = \pi/a$ the group velocity is zero.

Figure illustrates the group velocity as a function of wavevector k across the first Brillouin zone.