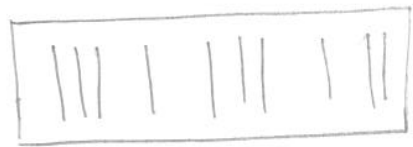


### 4.0 Elastic waves in a solid.

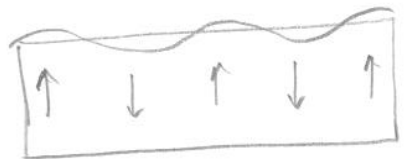
Before we put in the atoms / crystal, let's review the vibrational properties of a solid:



→ ← → ← → ←  
 comp. exp

mechanical excitation  
 → waves.

= longitudinal wave.



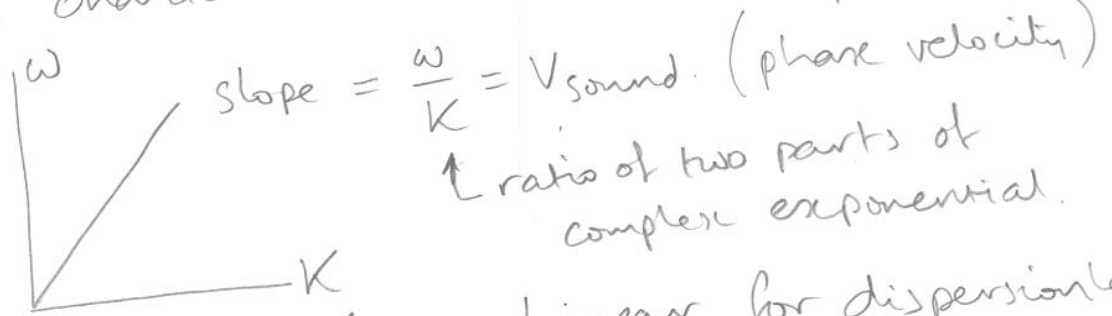
→ propagation } transverse  
 ↑↓ displacement } wave

Both waves propagate at "speed of sound".  
 (not the same)  
 $i(kx - \omega t)$

$u = u_0 e^{i(kx - \omega t)}$   
 $\vec{u} = \vec{u}_0 e^{i(\vec{k} \cdot \vec{r} - \omega t)}$  full 3D form.

$\vec{k}$  = direction of propagation  $|\vec{k}| = 2\pi/\lambda$   
 $\vec{k} \parallel \vec{u}$  longitudinal  $\vec{k} \perp \vec{u}$  transverse

Basic characteristic of linear medium:  
 $v = f\lambda$



Dispersion relation. Linear for dispersionless solid. Group velocity of wave:

$v_g = \frac{d\omega}{dk} = v_p$  for dispersionless case

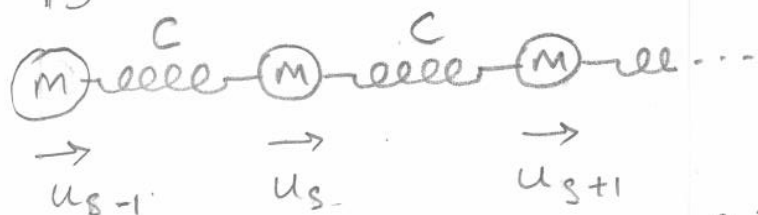
Crystals are different because of discrete sampling of  $\vec{u}$  at lattice positions → dispersion  
 $\lambda \sim$  atomic spacing  $\leftrightarrow k \sim$  Zone boundary.

### 4.1 Vibrations

Big subject which will lead to strong predictions about the thermal properties of solids. We will also see in the counting of modes how the reciprocal space notation is valuable.

We will start with simple models and build up towards the more general case. We will not study formal elasticity theory, although this is strictly necessary. We start with the:

"1D monatomic chain" ← good for single directions 3D.



This could represent masses suitably constrained or lattice planes in a crystal.

Force on mass  $M_s$  is (to the right)

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

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

Solution is a wave. We use the complex notation

$$u_s = u_{s0} e^{-i\omega t}, \text{ but we drop the "0"}$$

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

This is now an algebraic difference equation, for which we assume a wave-like spatial dependence:

$$u_s = u e^{ik(sa)}$$

Some wave vector  $\uparrow$  integer  $s \times$  lattice spacing = distance along chain

$$-M\omega^2 e^{iksa} = C e^{iksa} \left( e^{ika} + e^{-ika} - 2 \right)$$

$s+1 \qquad s-1$

Using  $\cos x = \frac{1}{2}(e^{ix} + e^{-ix})$  identity:

$$-M\omega^2 = 2C(\cos Ka - 1)$$

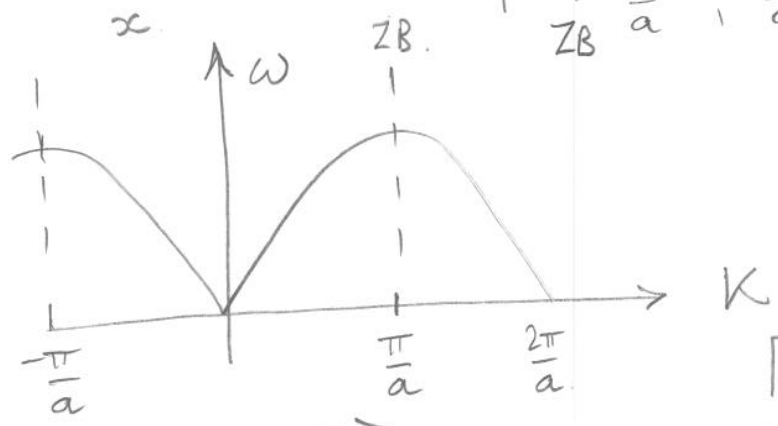
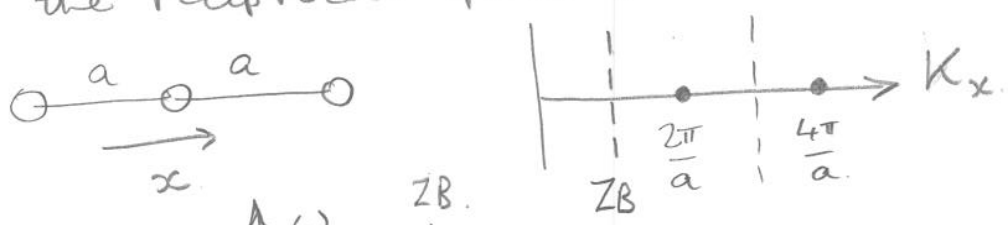
$$\omega^2 = 2 \frac{C}{M} (1 - \cos Ka) = \frac{4C}{M} \sin^2 \frac{1}{2} Ka$$

28.01.10

This is called a dispersion relation. It tells us how the frequency of the wave changes with its wavevector. Every  $K$  is a solution.

### 4.2 First Brillouin Zone.

The wave vector  $K$  (units =  $m^{-1}$ ) naturally maps into the reciprocal space of the 1D crystal:



not repeating.

First Brillouin Zone = unique set of solutions  
 $K$ -points outside FBZ are redundant and represent the same wave:

$$K \rightarrow K + \frac{2\pi}{a}$$

$$e^{iKsa} \rightarrow e^{i(K + \frac{2\pi}{a})sa} = e^{iKsa} e^{2\pi i s}$$

integer

Discrete atoms on a high-frequency wave:



can't distinguish the two waves.

### First Brillouin Zone

What range of  $K$  is physically significant for elastic waves? Only those in the first Brillouin zone. From (4) the ratio of the displacements of two successive planes is given by

$$\frac{u_{s+1}}{u_s} = \frac{u \exp[i(s+1)Ka]}{u \exp(isKa)} = \exp(iKa) . \quad (10)$$

The range  $-\pi$  to  $+\pi$  for the phase  $Ka$  covers all independent values of the exponential.

The range of independent values of  $K$  is specified by

$$-\pi < Ka \leq \pi , \quad \text{or} \quad -\frac{\pi}{a} < K \leq \frac{\pi}{a} .$$

This range is the first Brillouin zone of the linear lattice, as defined in Chapter 2. The extreme values are  $K_{\max} = \pm\pi/a$ . Values of  $K$  outside of the first Brillouin zone (Fig. 5) merely reproduce lattice motions described by values within the limits  $\pm\pi/a$ .

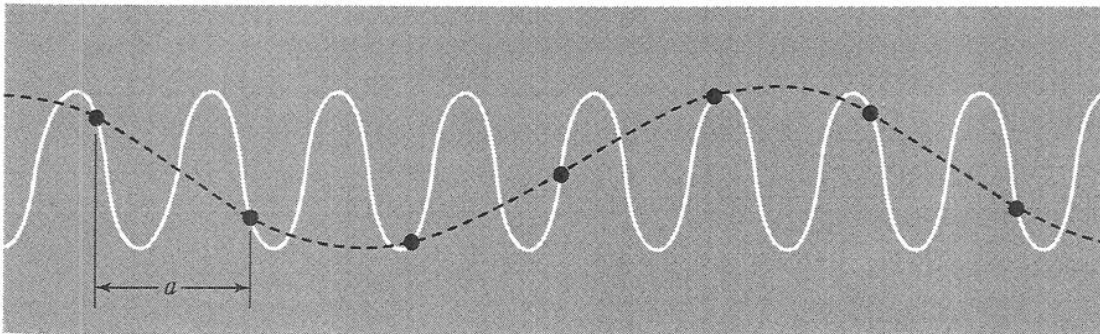
We may treat a value of  $K$  outside these limits by subtracting the integral multiple of  $2\pi/a$  that will give a wavevector inside these limits. Suppose  $K$  lies outside the first zone, but a related wavevector  $K'$  defined  $K' = K - 2\pi n/a$  lies within the first zone, where  $n$  is an integer. Then the displacement ratio (10) becomes

$$u_{s+1}/u_s = \exp(iKa) \equiv \exp(i2\pi n) \exp[i(Ka - 2\pi n)] \equiv \exp(iK'a) , \quad (11)$$

because  $\exp(i2\pi n) = 1$ . Thus the displacement can always be described by a wavevector within the first zone. We note that  $2\pi n/a$  is a reciprocal lattice vector because  $2\pi/a$  is a reciprocal lattice vector. Thus by subtraction of an appropriate reciprocal lattice vector from  $K$ , we always obtain an equivalent wavevector in the first zone.

At the boundaries  $K_{\max} = \pm\pi/a$  of the Brillouin zone the solution  $u_s = u \exp(isKa)$  does not represent a traveling wave, but a standing wave. At the zone boundaries  $sK_{\max}a = \pm s\pi$ , whence

$$u_s = u \exp(\pm is\pi) = u (-1)^s . \quad (12)$$



**Figure 5** The wave represented by the solid curve conveys no information not given by the dashed curve. Only wavelengths longer than  $2a$  are needed to represent the motion.

The  $\pm K$  points are distinguishable, but only because of the time dependence:

$$u_s(t) = u_{s0} e^{iKsa - i\omega t} = u_{s0} e^{i(Ksa - \omega t)}$$

The phase velocity is  $\omega/K$  which can be positive or negative.

However at the Zone Boundary,  $K = \pm \frac{\pi}{a}$  we lose the sense of direction

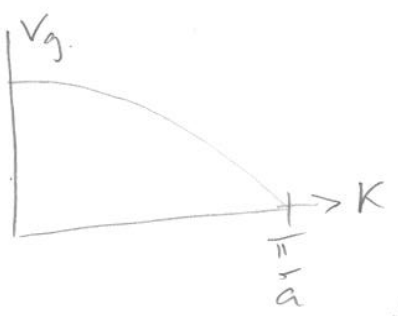
$$u_s(t) = u_{s0} e^{i(\pm \pi s - \omega t)} = u_{s0} (-1)^s e^{-i\omega t}$$

This represents a standing wave with alternate atoms oscillating with opposite phase. No longer a travelling wave.

### 4.3 Group Velocity.

The more important measure of the velocity represents the motion of wave packets:

$$v_g = \frac{d\omega}{dk} = \frac{d}{dk} \left( 2 \left( \frac{c}{m} \right)^{1/2} \sin \frac{Ka}{2} \right) = a \left( \frac{c}{m} \right)^{1/2} \cos \frac{Ka}{2}$$



Group velocity falls smoothly to zero at the zone boundary (where it is a standing wave)

Long wavelength limit:  $K \ll \frac{\pi}{a}$

$$v_g \approx a \left( \frac{c}{m} \right)^{1/2} = \text{constant}$$

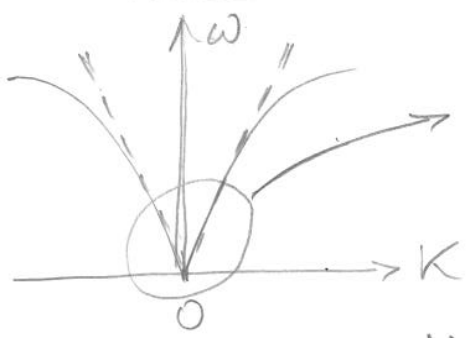
This can also be seen as the linear region of the dispersion relation. Same value as phase velocity  $\omega/K$  here:

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

Phase velocity  $v_p = \frac{\omega}{K} = a \left( \frac{C}{M} \right)^{1/2} = v_g = \text{Group vel.}$

This is the velocity of long-wavelength elastic waves in the solid, commonly called the speed of sound,  $v_s = v_p = v_g$ .

2.02.09 I



Linear region is said to be "dispersionless", meaning frequency ∝ wave-vector.

Dispersionless medium has  $v_g = v_p$  ✓  
 Dispersion effects kick in near zone boundary.  
 Can consider this as interference with the Bragg-diffracted wave moving in the opposite direction, slowing down the wave packets until they make a standing wave at the Z.B.

27.01.08 II

i) Easy to generalise to 3D:

Dispersion relation  $\omega(k) \rightarrow \omega(\vec{k})$   
 Group velocity  $\vec{v}_g = \vec{\nabla}_k \omega(\vec{k})$

Isotropic (eg cubic) medium has  $v_g$  the same in all directions in the long-wavelength limit.  
 → two polarization L & T; 3 modes 1xL 2xT altogether.

30.01.06 I

ii) Typical numbers:

$$\left. \begin{aligned} M &= Z m_p \sim 50 \times 10^{-27} \text{ kg.} \\ a &= 0.3 \text{ nm} \\ v_s &= 10^4 \text{ m/s} \end{aligned} \right\}$$

$$\begin{aligned} C &= M \left( \frac{v_s}{a} \right)^2 \\ &= 5 \times 10^{-26} \times (3 \times 10^{13})^2 \\ &= 45 \text{ N/m} \end{aligned}$$

typical macroscopic value.

(35)

$$-\omega^2 M_1 u = C(v + v e^{-ika} - 2u)$$

$$-\omega^2 M_2 v = C(u e^{ika} + u - 2v)$$

These coupled (bi)linear equations form a matrix

$$\begin{pmatrix} 2C - \omega^2 M_1 & -C(1 + e^{-ika}) \\ -C(e^{ika} + 1) & 2C - \omega^2 M_2 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = 0$$

This is an eigenvalue problem that has no solution unless the determinant of the matrix is zero; then it has many solutions with fixed ratios of the amplitudes  $u$  and  $v$ :

We solve for  $\omega$ , so keep separate powers of  $\omega^2$ :

$$\omega^4 M_1 M_2 - \omega^2 (2CM_1 + 2CM_2) + 4C^2 - C^2 \underbrace{(1 + e^{-ika})(e^{ika} + 1)}_{2 + 2\cos Ka} = 0 \quad \left[ \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \right]$$

$$\omega^4 M_1 M_2 - \omega^2 2C(M_1 + M_2) + 2C^2(1 - \cos Ka) = 0$$

$$\omega^2 = \frac{2C(M_1 + M_2) \pm \sqrt{4C^2(M_1 + M_2)^2 - 8C^2 M_1 M_2 (1 - \cos Ka)}}{2M_1 M_2}$$

There are two frequencies for each  $K$  wavevector. Two "branches" of the dispersion relation.

Before we plot the result, let's examine the limiting cases:

i) Small  $K$ :  $K \ll \frac{\pi}{a}$   $1 - \cos Ka \approx \frac{1}{2} K^2 a^2$

$$\omega^4 M_1 M_2 - \omega^2 2C(M_1 + M_2) + C^2 K^2 a^2 = 0$$

Limiting roots of quadratic when " $C$ " is small

$$\frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \rightarrow \frac{-b}{a} \text{ or } \frac{-b + b(1 - 4ac/2b^2)}{2a} = \frac{-c}{b}$$

(-ve) (+ve)

So the two small-K solutions are:

$$\omega_1^2 = \frac{2C(M_1+M_2)}{M_1M_2} = 2C \left( \frac{1}{M_1} + \frac{1}{M_2} \right) \leftarrow \text{reduced mass}$$

this branch has no dispersion (K-dependence)

$$\omega_2^2 = \frac{c^2 K^2 a^2}{2C(M_1+M_2)} = \frac{c}{2(M_1+M_2)} K^2 a^2$$

this branch is just like our previous soln with the <sup>phase</sup>group velocity containing both masses added together

$$V_p = V_g = a \left( \frac{c}{m} \right)^{1/2} \rightarrow a \left( \frac{c}{2(M_1+M_2)} \right)^{1/2} \text{ cf } a \left( \frac{c}{M} \right)^{1/2}$$

29.01.2007

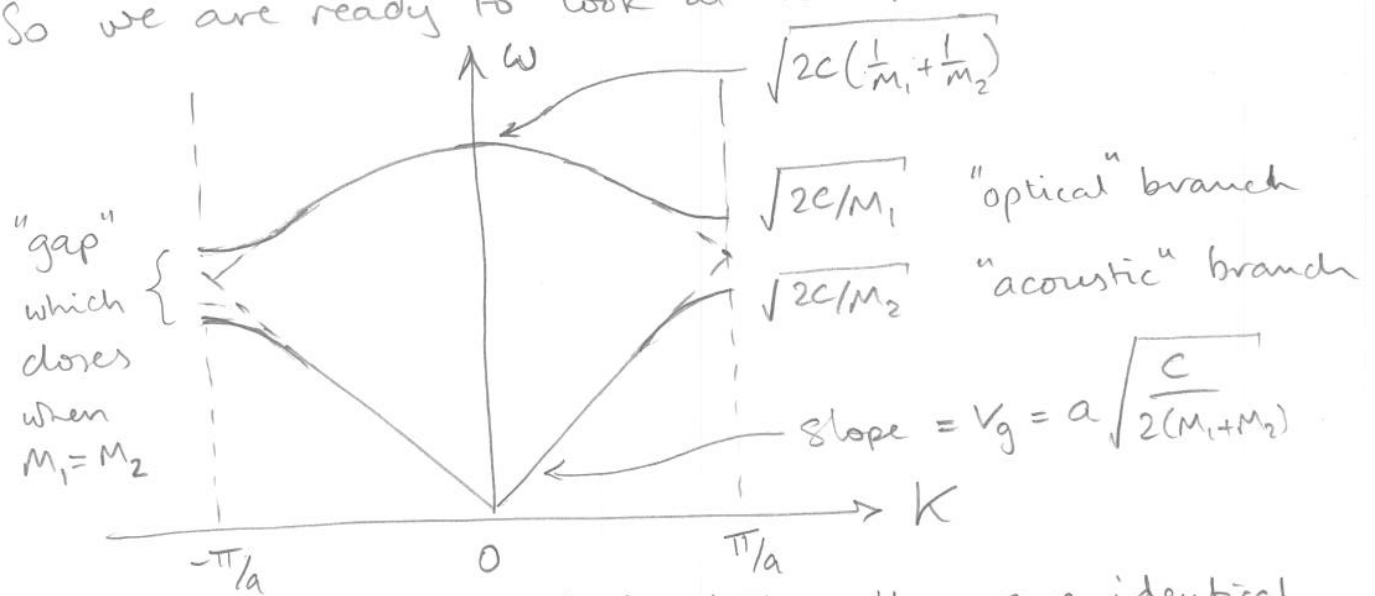
ii) Zone boundary is also easy:  $K = \frac{\pi}{a} \cos Ka = -1$

$$\omega^4 M_1 M_2 - \omega^2 2C(M_1+M_2) + 4C^2 = 0$$

$$b^2 - 4ac = 4C^2(M_1+M_2)^2 - 16C^2 M_1 M_2 = 4C^2(M_1 - M_2)^2$$

$$\text{So } \omega^2 = \frac{2C(M_1+M_2) \pm 2C(M_1-M_2)}{2M_1M_2} = \frac{2C}{M_1} \text{ or } \frac{2C}{M_2}$$

So we are ready to look at the full curve:



As before no states outside  $\pm\pi/a$ : they are identical to those within (for discrete atoms)

- 30.01.06 II
- 29.01.08
- 2.02.09 I
- 1.02.10



4.5 Nature of branches.

This breakup of the dispersion relation into optical and acoustic branches is a fundamental paradigm of solid state physics.

That is why we study it so closely.

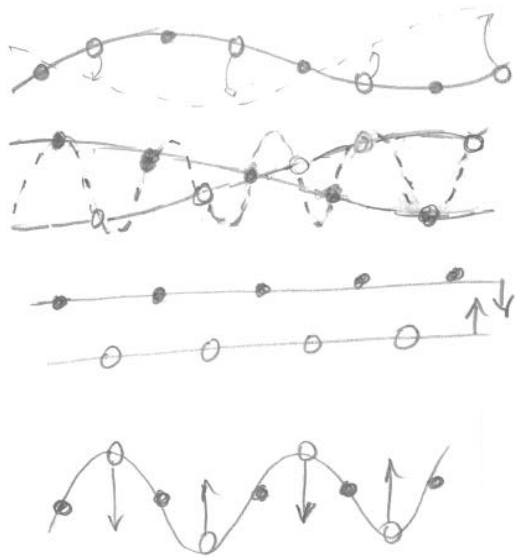
i) nature of modes, obtained from eigenvalues of matrix equation:

optical mode:  $u \neq v$  have opposite sign.

acoustic mode: " " " same sign

ratio of  $u/v$  varies across  $K$ -range.

Picture of transverse modes [we studied longd.]

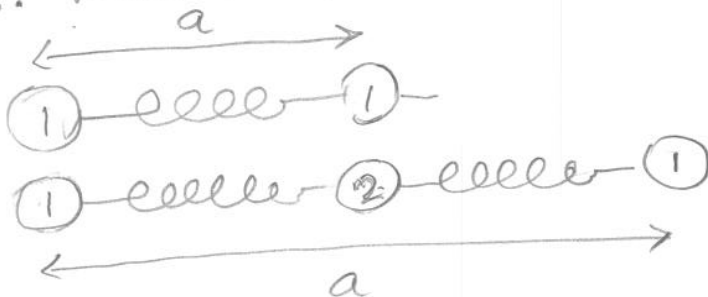


acoustic (low frequency) }  $|K| < \frac{\pi}{a}$   
 optical (high frequency) }  
 Zone centre ( $K=0$ )  $\omega = \sqrt{\frac{2c}{m^*}}$   
 of optical mode. red. mass

Zone Boundary  $K = \frac{\pi}{a}$   $M_1$  or  $M_2$   
 only one ion moving.

ii) How does 2-branch dispersion relation "morph" into a single branch when  $M_1 = M_2$ ? [ob exam].

Ans: needs redefinition of  $a$ :



monatomic  
 diatomic basis

Call the second case  $a' = 2a$ :  $\frac{\pi}{a'} = \frac{1}{2} \frac{\pi}{a}$

**Answer EVERY question from section A and TWO questions from section B.**

The numbers in square brackets in the right-hand margin indicate the provisional allocation of maximum marks per sub-section of a question.

Mass of the electron	$m_e$	=	$9.11 \times 10^{-31}$	kg
Charge on the electron	$e$	=	$-1.602 \times 10^{-19}$	C
Boltzmann's constant	$k_B$	=	$1.38 \times 10^{-23}$	J K <sup>-1</sup>
Planck's constant/ $2\pi$	$\hbar$	=	$1.05 \times 10^{-34}$	J s

**SECTION A**

**[Part marks]**

1. Explain how a real metal can be deformed by stresses that are considerably smaller than its theoretical elastic limit. [2]

Stating your assumptions, estimate the room-temperature concentration of vacancies in a sample of copper, which melts at  $1358K$ , if the energy difference between a copper atom deep inside the bulk and one attached to the surface is  $1.21eV$ . [5]

2. Sketch the dispersion relation for longitudinal phonons on a linear monatomic chain. In a separate diagram, sketch the dispersion relation for a diatomic chain made up of alternating atoms with two different masses. Be careful to label your axes so that the two relations can be compared. [3]

EXplain carefully how the diatomic dispersion relation converts into the monatomic result as the masses of its two atoms are made to be the same? [4]

3. According to the tight-binding method, the energy of an electron in a crystal is usually given by a form,

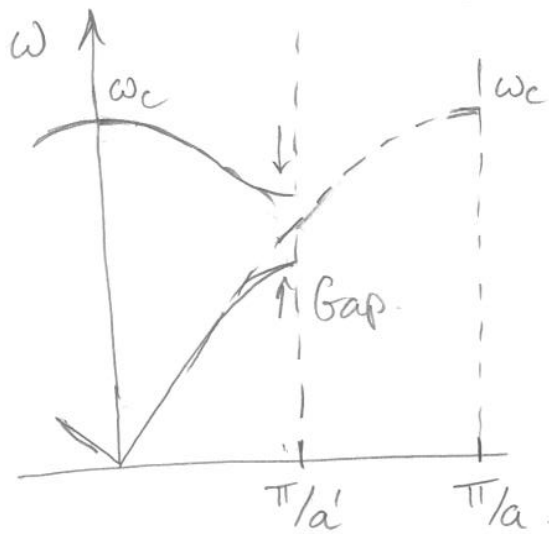
$$U = -\alpha - \gamma \sum_m \exp(-i\mathbf{k} \cdot \rho_m).$$

What is the meaning of the symbols  $\alpha$  and  $\gamma$  in this expression? [3]

Give an expression for the energy of an electron in a simple cubic lattice with lattice parameter  $a$  as a general function of the  $\mathbf{k}$ -vector according to this model. [4]

4. Explain with the aid of a diagram how the  $\mathbf{k}$ -states of a free electron metal should change under the application of an electric field and show how this explains why the electrical conductivity is proportional to the relaxation time,  $\tau$ . [3]

If the effects of impurity scattering and phonon scattering on the electrical conductivity



a) Unfold optical branch into doubled Brillouin Zone.

b) Close "gap" by letting  $M_1 = M_2$

c) Check frequencies:

$$\omega_c = \sqrt{2c \left( \frac{1}{m_1} + \frac{1}{m_2} \right)} \text{ diatomic}$$

$$\rightarrow \sqrt{4c/M} \text{ monatomic ans.}$$

iii) General Case (degrees of freedom).

3D has 3 acoustic branches always

2 × transverse } 3 modes (ie 3 freq's for every  $\vec{k}$ )  
 1 × longitudinal.

2-atom basis has double this number (6 in 3D)

p-atom basis has p × the number:

3(p-1) optical modes. (mixed polarization)  
 3 acoustic modes.

### 4.6 Quantization of Vibrations

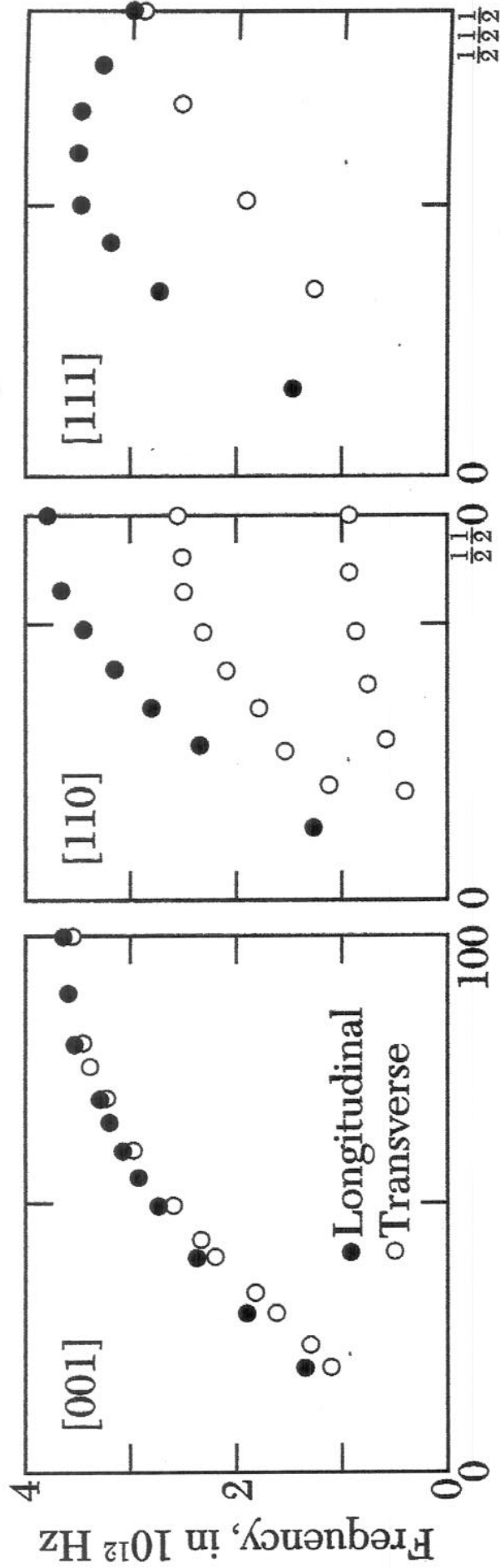
A mechanical oscillator has discrete energies of excitation. The quantum number of the excitation is  $n$ , with energy:

$$E = \left( n + \frac{1}{2} \right) \hbar \omega \quad = \text{"harmonic oscillator"}$$

$\omega$  is the frequency of the vibration. Vibrations are bosons, so  $n$  can have any integer value.

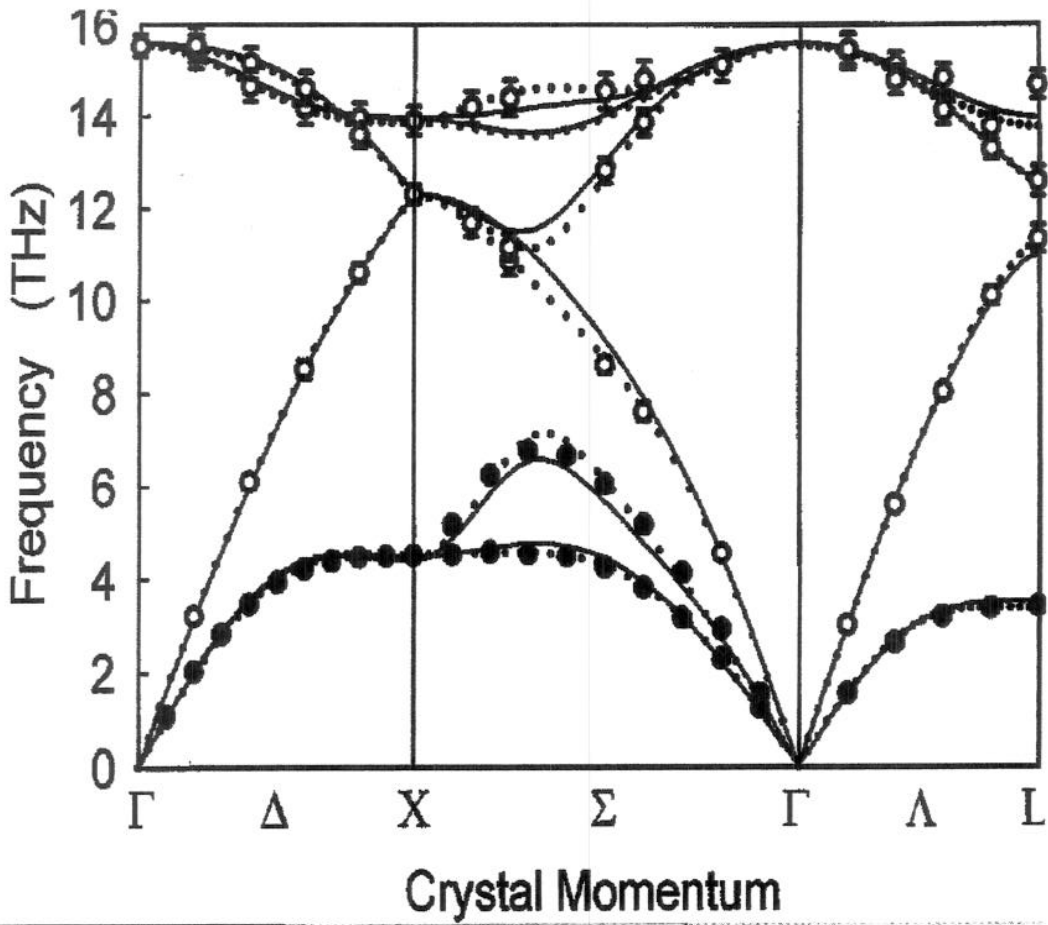
Quanta of mech. excitation are called phonons by analogy with light oscillators  $\rightarrow$  photons.

The  $\frac{1}{2} \hbar \omega$  is zero-point energy due to the Heisenberg uncertainty principle.

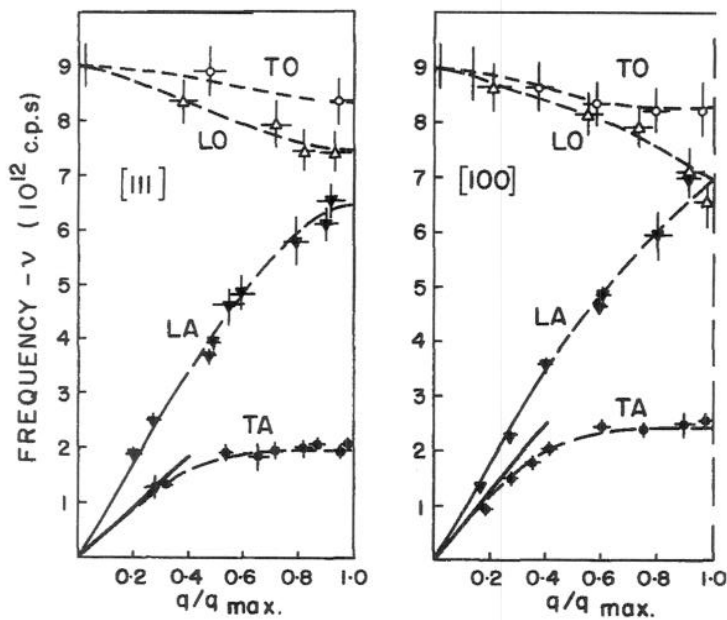


Wavevector, in units  $2\pi/a$

**Figure 11** The dispersion curves of sodium for phonons propagating in the [001], [110], and [111] directions at 90 K, as determined by inelastic scattering of neutrons, by Woods, Brockhouse, and Bowers.



Silicon. Holt et al PRL



Germanium. Brockhouse et al.

Each  $K$ -value of the excitations of a crystal corresponds to a different mode.

- like an independent oscillator.
- every  $K$  is orthogonal to every other  $K$  (later)

Energy  $E_K = (n + \frac{1}{2}) \hbar \omega(K)$

Since we think of a phonon as a kind of particle inside the crystal, we can consider it to carry momentum:

$\vec{P}_K = \hbar \vec{K}$

This is not a genuine physical momentum but a crystal momentum that can be gained or lost by interaction with an external probe, such as a photon or neutron.

Neutron scattering is the best way of measuring phonon dispersion relations.

Neutron energy  $\frac{1}{2}mv^2$  is gained or lost upon interaction with a crystal:  $\frac{1}{2}mv^2 = \frac{\hbar^2}{2m} k^2$

- inelastic scattering, not conserving energy
- $\vec{k}' = \vec{k} + \vec{G} \pm \vec{K}$  conservation of "momentum".  
 " " " energy.  
 $E' = E \pm \hbar \omega(K)$

- neutron spectrometer measures  $(\vec{k}', E')$

So can reconstruct both  $\vec{K}$  and  $\omega(\vec{K})$

plot as experimental dispersion curve [pic]

Brockhouse Nobel prize (1994)

Profs: McMorrow, Finney, McEwen, Acapli