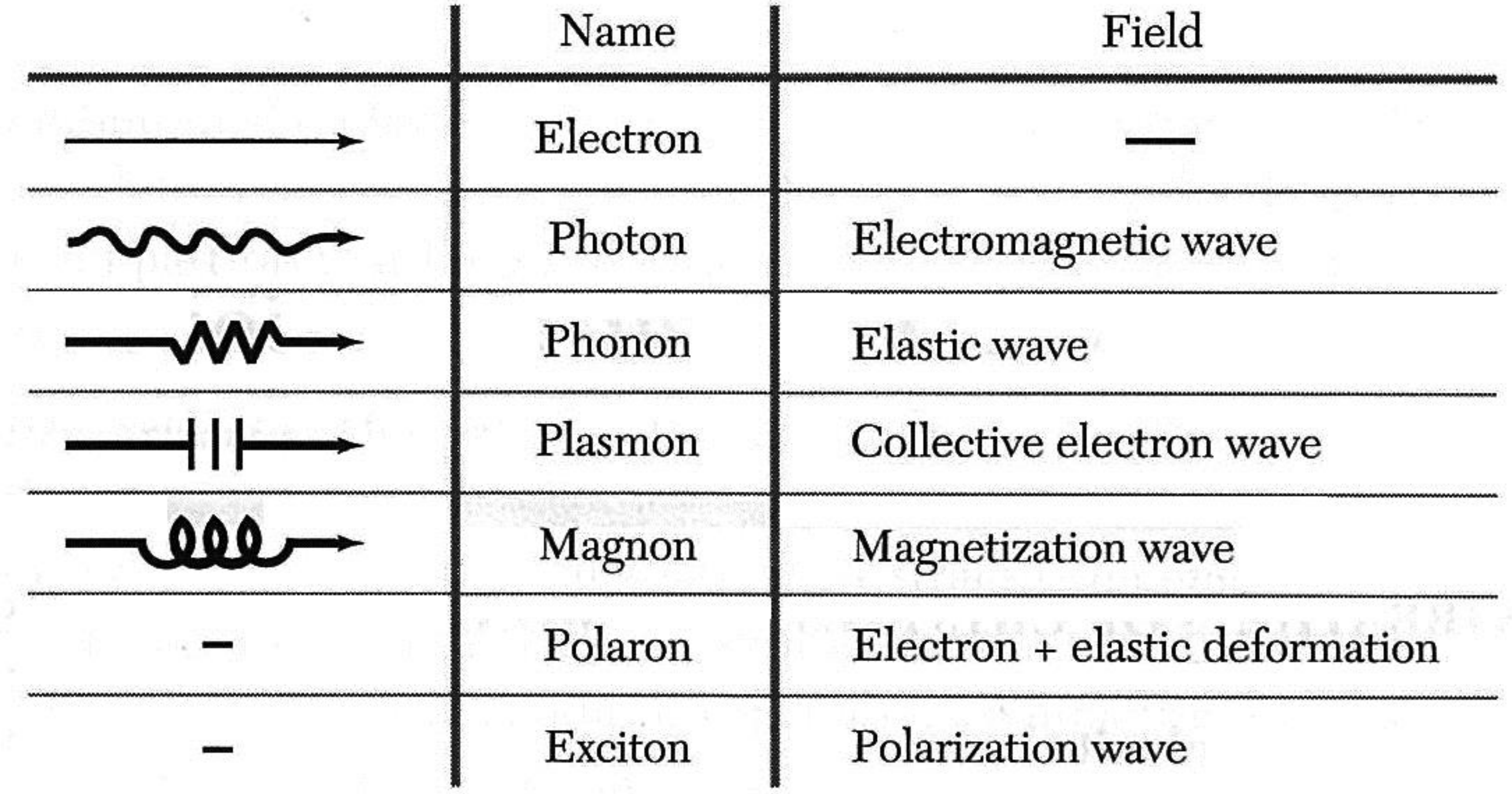
Chap 4: Phonons I
Crystal Vibrations

Major Elementary Excitation in Solids

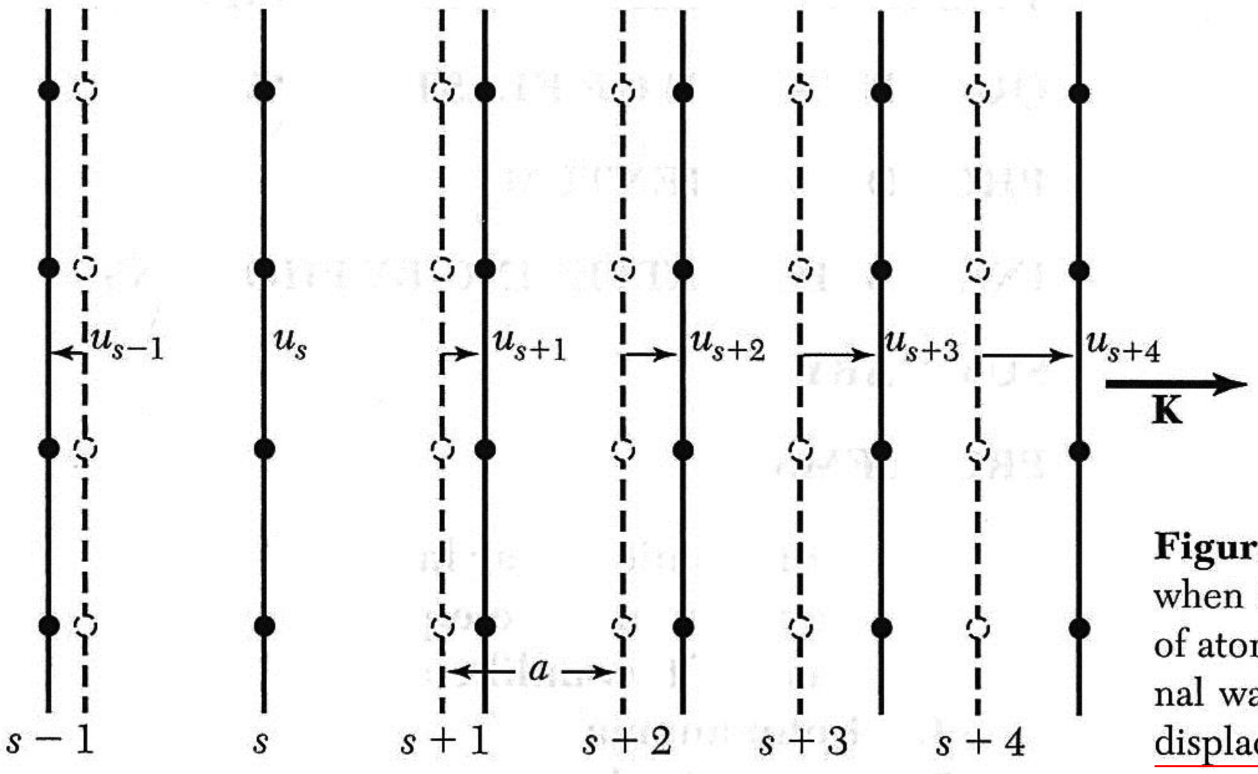


	Name	Field
→	Electron	—
	Photon	Electromagnetic wave
	Phonon	Elastic wave
	Plasmon	Collective electron wave
	Magnon	Magnetization wave
–	Polaron	Electron + elastic deformation
–	Exciton	Polarization wave

Figure 1 Important elementary excitations in solids.

Displacement of Planes of Atoms in a Longitudinal Wave

U_s is defined as the displacement for the plane ***s*** from its equilibrium position



$U_s \,//\, \vec{K}$

Longitudinal wave

Figure 2 (Dashed lines) Planes of atoms when in equilibrium. (Solid lines) Planes of atoms when displaced as for a longitudinal wave. The coordinate u measures the displacement of the planes.

Displacement of Planes of Atoms in a Transverse Wave

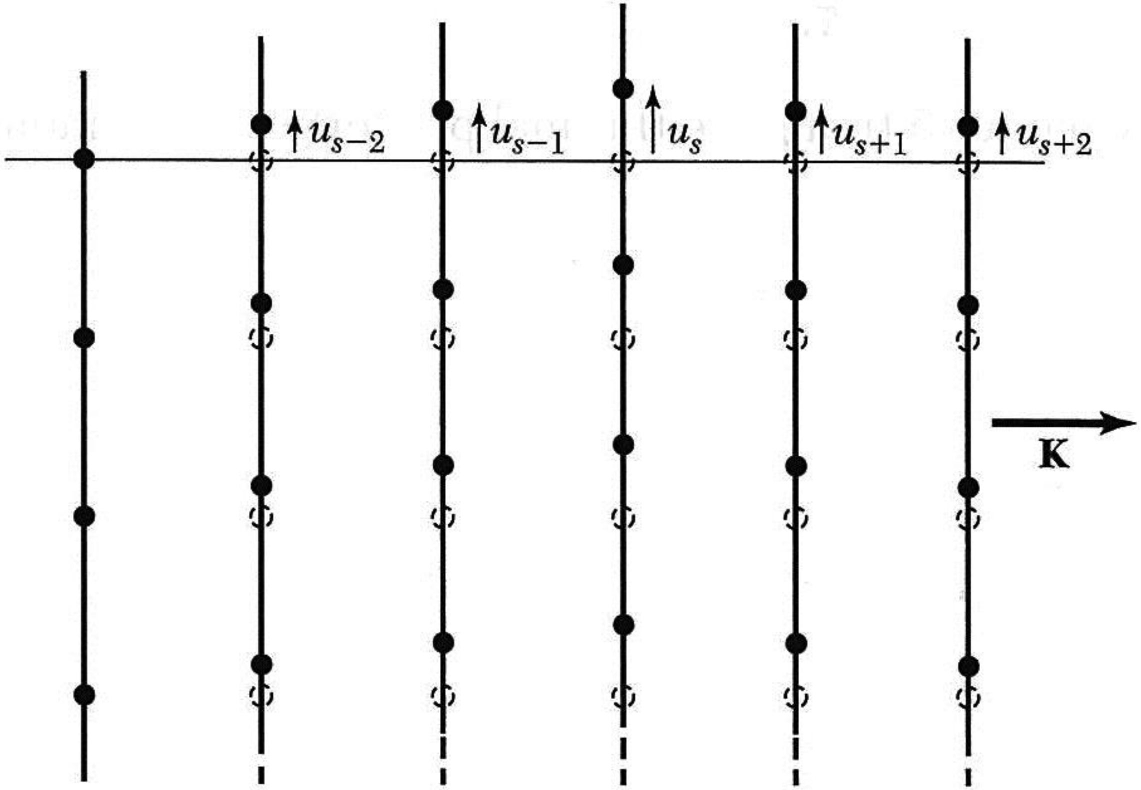


Figure 3 Planes of atoms as displaced during passage of a transverse wave.

$U_s \perp$ K

Transverse Wave

Hooke's Law

- We assume the elastic response of the crystal is a linear function of the forces.
- The elastic energy is a quadratic function of the relative displacement of any two points in the crystal.
- Hooke's Law : The force exerted on the plane *s* as caused by the displacement of the plane *s+p* is directly proportional to the difference of the displacement $u_{s+p} - u_s$. For nearest neighbor interaction, $p = \pm 1$
- The total force on plane *s* from planes *s+1*, and *s-1* is

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

The equation of motion of the plane *s* is

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

With time dependence, $u = u \exp(-i\omega t)$

$$-M\omega^2 u_s = C(u_{s+1} + u_{s-1} - 2u_s) \tag{3}$$

By traveling wave solution in the form of $u_s = u \exp(isKa)$

$$u_{s\pm1} = u \exp(isKa)\exp(\pm iKa) \quad , \tag{4}$$

$$\begin{aligned} &-\omega^2 M u \exp(isKa) \\ &= Cu\{\exp[i(s+1)Ka] + \exp[i(s-1)Ka] - 2\exp(isKa)\} \ . \qquad (5) \end{aligned}$$

$$\omega^2 M = -C[\exp(iKa) + \exp(-iKa) - 2] \ . \qquad (6)$$

$$\omega^2 = (2C/M)(1 - \cos Ka) \ . \qquad (7)$$

At the first Brillouin zone boundary, *K = π/a, and -π/a ,*

$$d\omega^2/dK = (2Ca/M) \sin Ka = 0 \qquad (8)$$

$$\omega^2 = (4C/M)\sin^2 \tfrac{1}{2}Ka \ ; \qquad \boxed{\omega = (4C/M)^{1/2}\left|\sin \tfrac{1}{2}Ka\right|} \ . \qquad (9)$$

ω vs κ Dispersion for Monoatomic Lattice

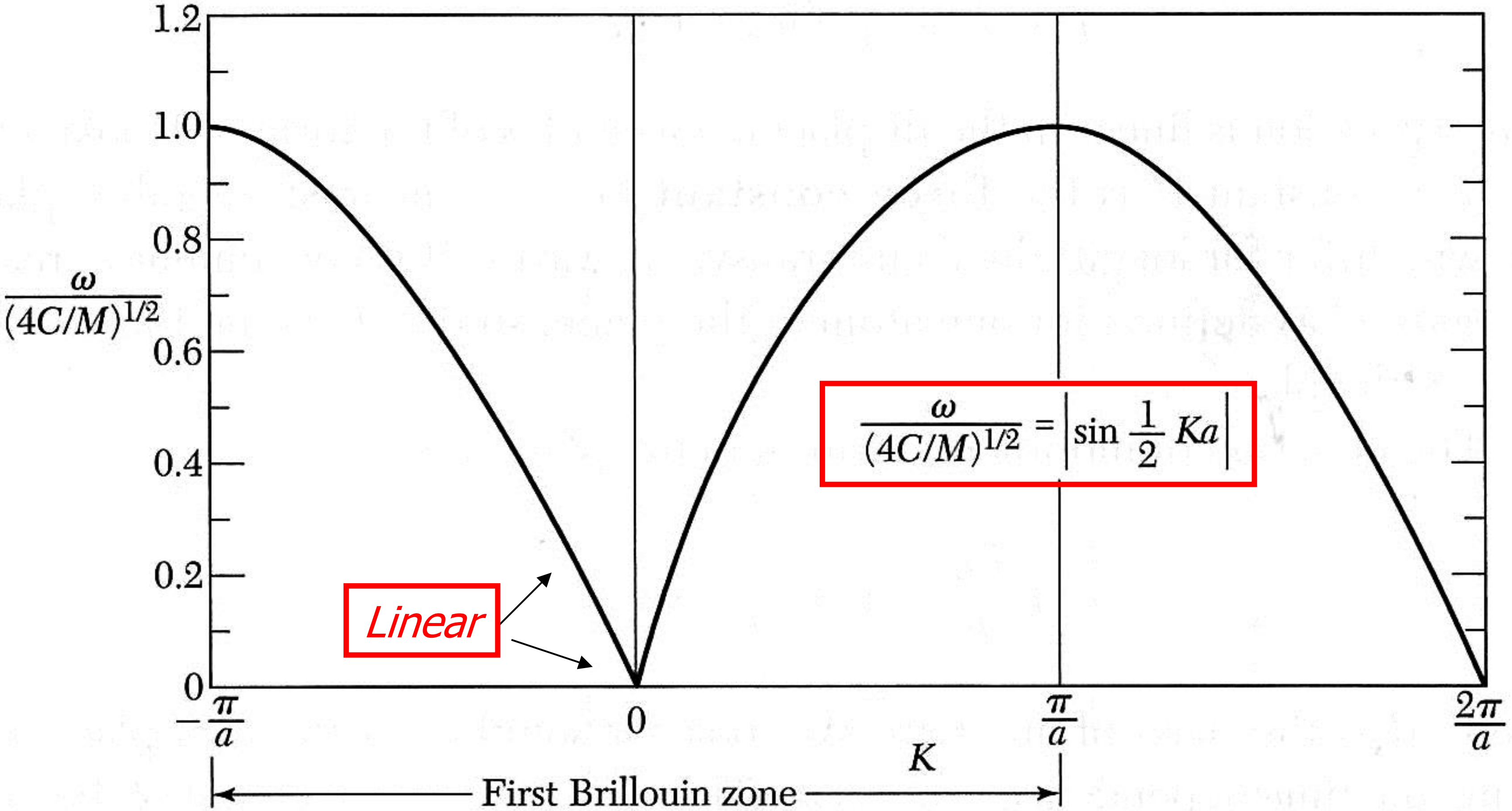


Figure 4 Plot of ω versus K. The region of $K \ll 1/a$ or $\lambda \gg a$ corresponds to the continuum approximation; here ω is directly proportional to K.

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

$-\pi < Ka < \pi$

$-\pi/a < K < \pi/a$

The meaningful range of ***K*** is only inside the first Brillouin Zone of the linear lattice.

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

$K' = K - 2n\pi/a = K - nG$

We can always subtract a reciprocal lattice vector ***G*** from ***K*** to become ***K'***, to be inside the first Brillouin zone.

At the zone boundary, $K_{max} = \pi/a$, *and* $-\pi/a$

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

This is **a standing wave**, $U_s = u$ *or* $-u$, depending on ***s*** is an even, or odd integer.

Group Velocity

The trasmission velocity of a wave packet is the group velocity

$$v_g = d\omega/dK \ ,$$

or

$$\mathbf{v}_g = \mathrm{grad}_{\mathbf{K}}\, \omega(\mathbf{K}) \ , \tag{13}$$

From Eq. 9,

$$\boxed{v_g = (Ca^2/M)^{1/2} \cos \tfrac{1}{2} Ka \ .} \tag{14}$$

At zone boundary, $K = \pi/a$, $\upsilon_{\mathbf{g}} = 0$ for standing wave

At the zone center, $Ka << 1$, the continuum approximation

$$\omega^2 = (C/M)K^2a^2 \ . \tag{15}$$

$\boldsymbol{v_g} = (C/M)^{1/2}\, a$ $V_g \sim$ is nearly a constant

The Traveling Wave Description of the Atomic Displacement

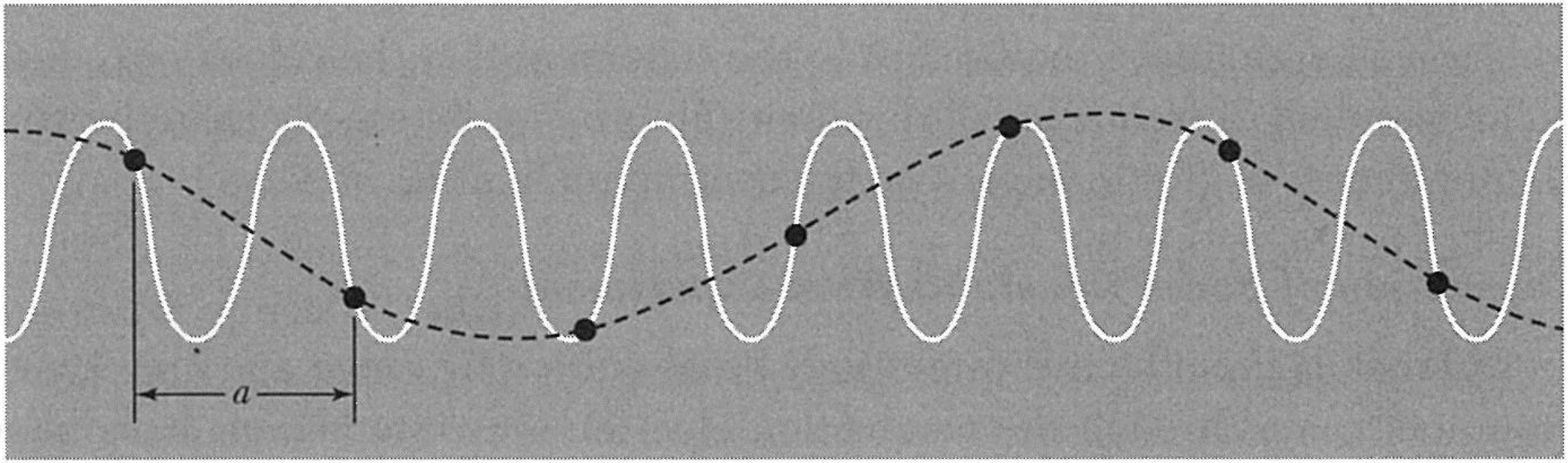


Figure 5 The wave represented by the solid curve conveys no information not given by the dashed curve. Only wavelengths longer than 2*a* are needed to represent the motion.

$\lambda > 2a$

$K < \pi/a$

Group Velocity Vg vs k of Mono Atomic Lattice

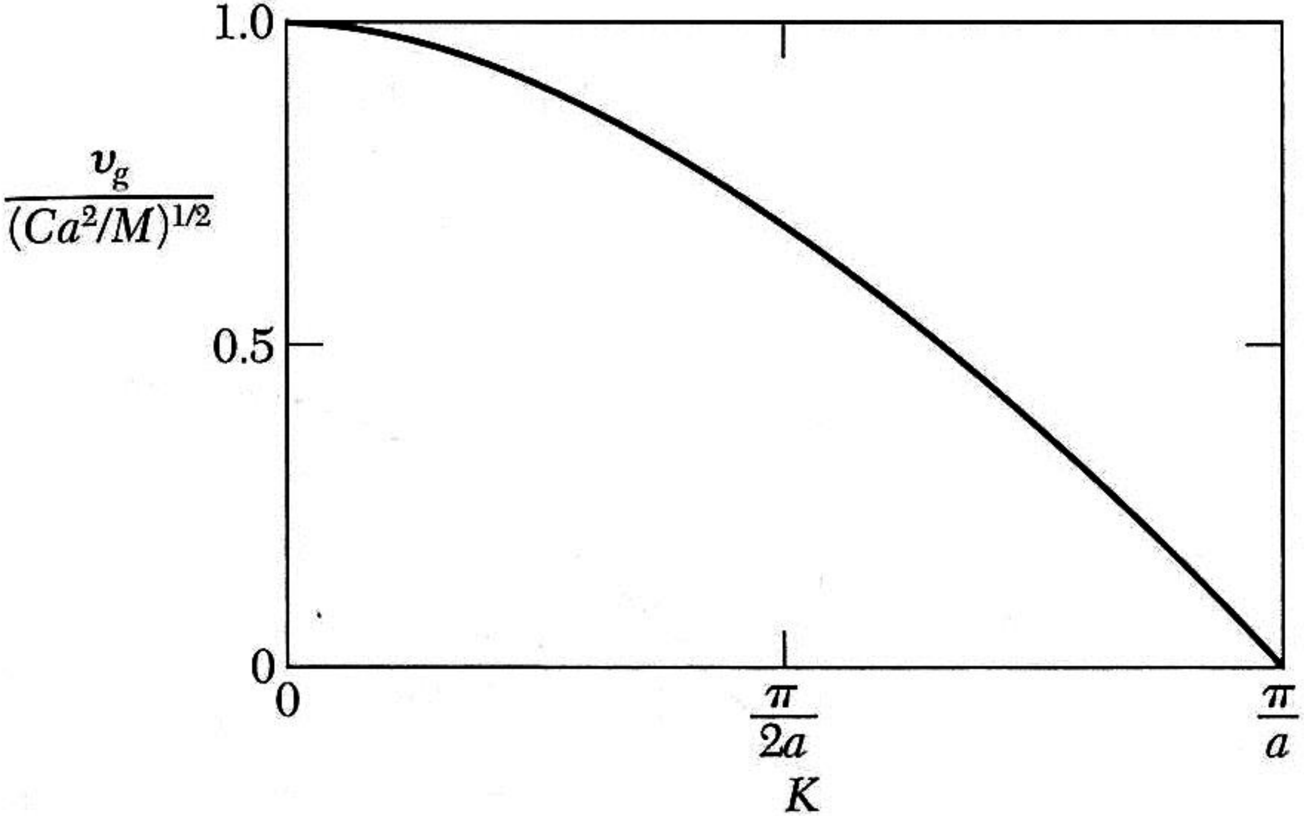


Figure 6 Group velocity v_g versus K, for model of Fig. 4. At the zone boundary $K = \pi/a$ the group velocity is zero.

Derivation of Force Constant from Experiment

For longer range force, we include ***p*** nearest planes of contributions to ω

$$\omega^2 = (2/M)\sum_{p>0} C_p(1-\cos pKa) \ . \tag{16a}$$

We times *M cos rKa* term on both sides, and integrate over *K*

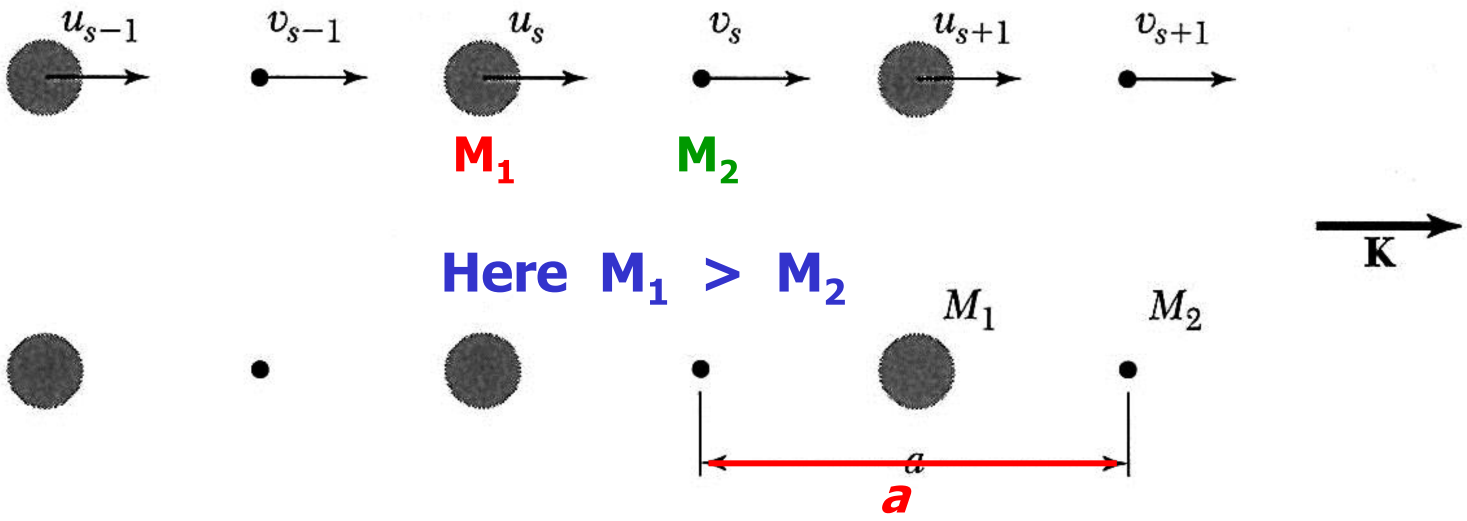
$$\begin{aligned} M\int_{-\pi/a}^{\pi/a} dK\, \omega_K^2 \cos rKa &= 2\sum_{p>0} C_p \int_{-\pi/a}^{\pi/a} dK\,(1-\cos pKa)\cos rKa \\ &= -2\pi C_r/a \ . \end{aligned} \tag{16b}$$

Note the integral vanishes, except for $p = r$

$$C_p = -\frac{Ma}{2\pi}\int_{-\pi/a}^{\pi/a} dK\, \omega_K^2 \cos pKa \tag{17}$$

From experimentally measured ω_K, we will derive $\boldsymbol{C_p}$

Displacement of a Diatomic Linear Crystal Structure



Here M_1 > M_2

Figure 9 A diatomic crystal structure with masses M_1, M_2 connected by force constant C between adjacent planes. The displacements of atoms M_1 are denoted by u_{s-1}, u_s, u_{s+1}, . . . , and of atoms M_2 by v_{s-1}, v_s, v_{s+1}. The repeat distance is a in the direction of the wavevector K. The atoms are shown in their undisplaced positions.

Considering only nearest neighbor interaction, force constants are identical between all pairs of near-neighbor planes

Equation of Motion for a Diatomic Linear Crystal

$$M_1 \frac{d^2 u_s}{dt^2} = C(v_s + v_{s-1} - 2u_s) \ ; \qquad (18)$$
$$M_2 \frac{d^2 v_s}{dt^2} = C(u_{s+1} + u_s - 2v_s) \ .$$

Traveling wave solution

$$\left\{ \begin{aligned} u_s &= u \exp(isKa) \exp(-i\omega t) \ ; \\ v_2 &= v \exp(isKa) \exp(-i\omega t) \ . \end{aligned} \right. \qquad (19)$$

a as the distance between nearest identical planes, not nearest neighbor planes.

$$-\omega^2 M_1 u = Cv[1 + \exp(-iKa)] - 2Cu \ ; \qquad (20)$$
$$-\omega^2 M_2 v = Cu[\exp(iKa) + 1] - 2Cv \ .$$

ω vs K for a Diatomic Linear Crystal

Solution exists only if the determinant of the coefficients vanishes

$$\begin{vmatrix} 2C - M_1\omega^2 & -C[1+\exp(iKa)] \\ -C[1+\exp(iKa)] & 2C - M_2\omega^2 \end{vmatrix} = 0 \ , \qquad (21)$$

$$M_1M_2\omega^4 - 2C(M_1+M_2)\omega^2 + 2C^2(1-\cos Ka) = 0 \ . \qquad (22)$$

At *Ka << 1,* the zone center

$$\omega^2 \cong 2C\left(\frac{1}{M_1}+\frac{1}{M_2}\right) \qquad \text{(optical branch)} \ ; \qquad (23)$$

Nearly a constant with *K*

$$\omega^2 \cong \frac{\frac{1}{2}C}{M_1+M_2}K^2a^2 \qquad \text{(acoustical branch)} \ . \qquad (24)$$

Nearly linear with *K*

At *Ka =* π, $-\pi$, the zone boundary

$$\omega^2 = 2C/M_1 \ ; \qquad \omega^2 = 2C/M_2 \ . \qquad (25)$$

Optical and Acoustic Branches of the Dispersion for a Diatomic Linear Lattice

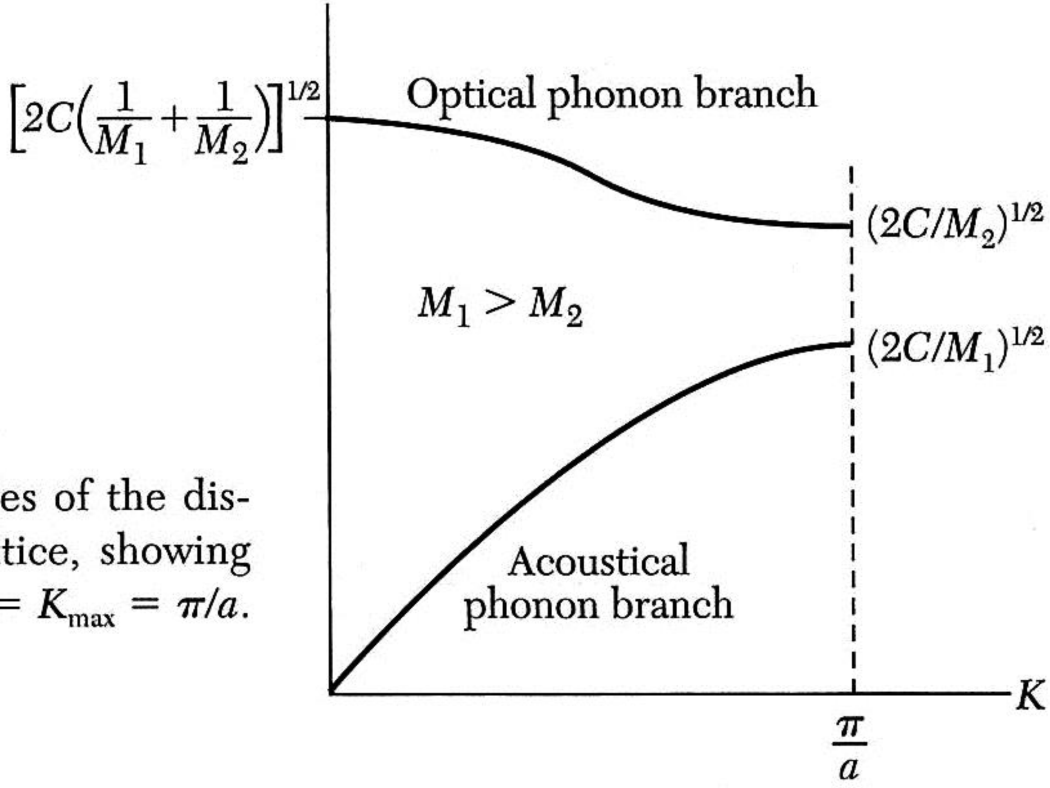


Figure 7 Optical and acoustical branches of the dispersion relation for a diatomic linear lattice, showing the limiting frequencies at $K = 0$ and $K = K_{\max} = \pi/a$. The lattice constant is a.

[111] Phonon Dispersion in Ge

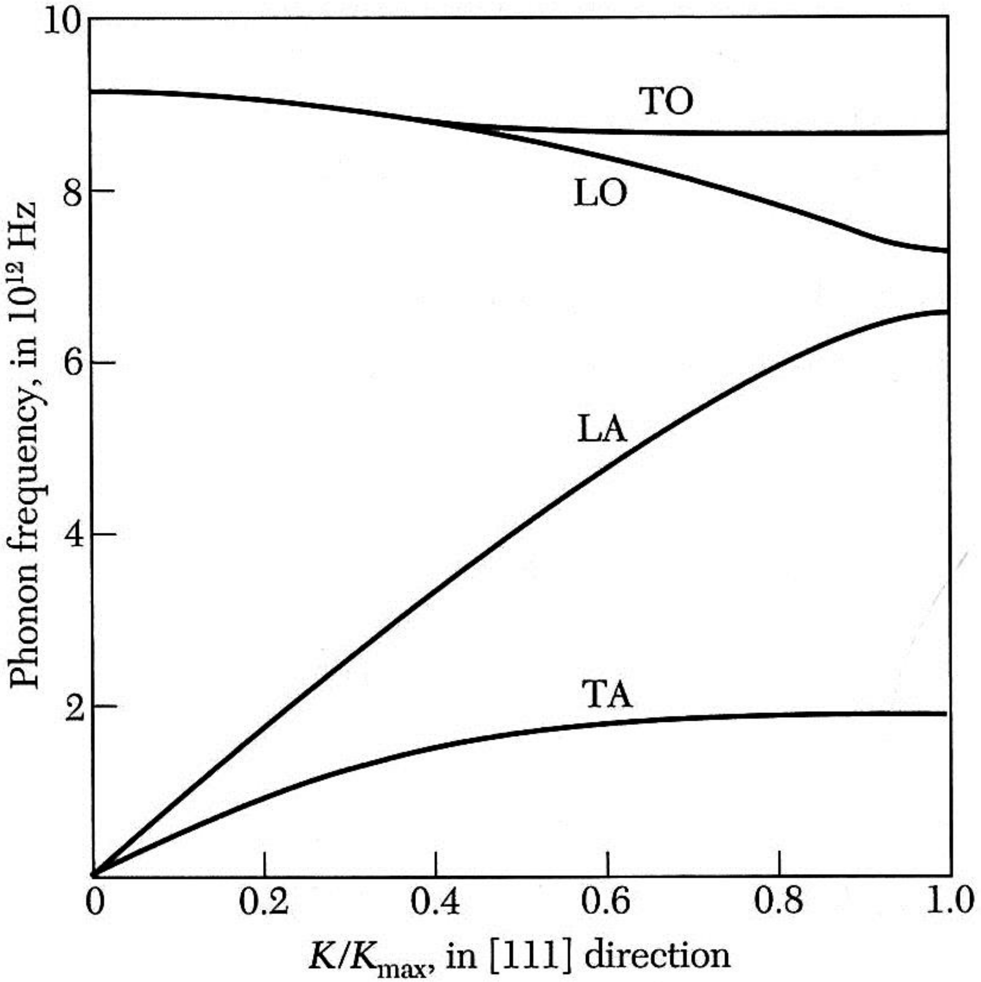


Figure 8a Phonon dispersion relations in the [111] direction in germanium at 80 K. The two TA phonon branches are horizontal at the zone boundary position, $K_{max} = (2\pi/a)(\frac{1}{2}\frac{1}{2}\frac{1}{2})$. The LO and TO branches coincide at $K = 0$; this also is a consequence of the crystal symmetry of Ge. The results were obtained with neutron inelastic scattering by G. Nilsson and G. Nelin.

[111] Phonon Dispersion in KBr

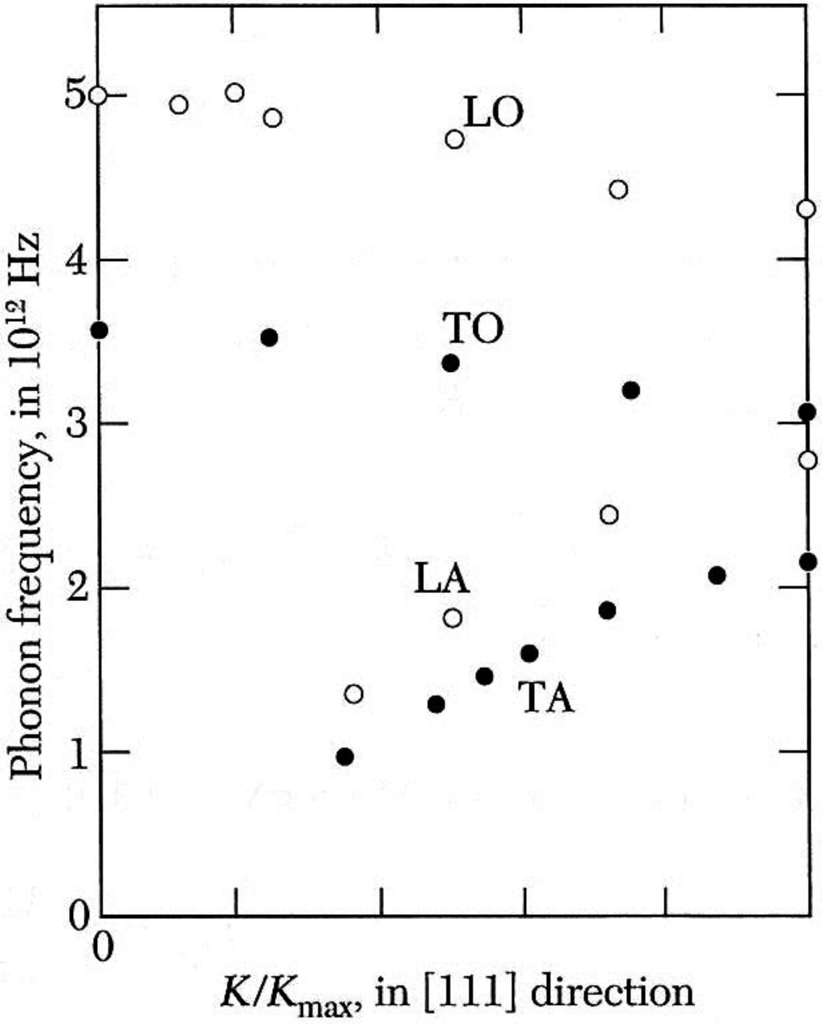


Figure 8b Dispersion curves in the [111] direction in KBr at 90 K, after A. D. B. Woods, B. N. Brockhouse, R. A. Cowley, and W. Cochran. The extrapolation to $K = 0$ of the TO, LO branches are called ω_T, ω_L.

Transverse Optical and Transverse Acoustic Waves of a Diatomic Linear Lattice

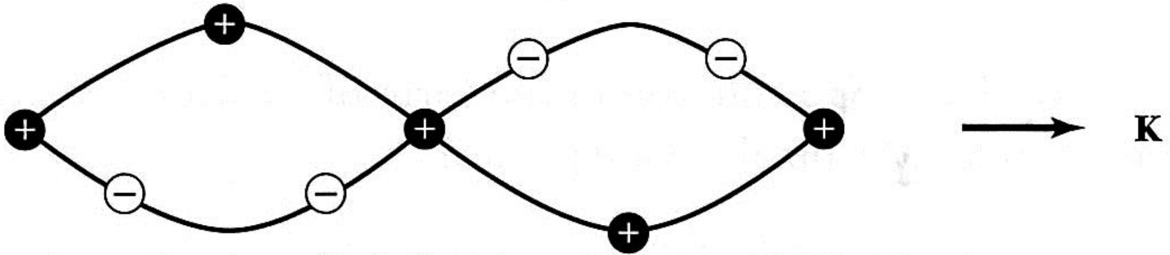
Substituting Eq. 23 to Eq. 20, we get

For *K = 0,* optical branch

$M_1 u + M_2 v = 0$

$$\frac{u}{v} = -\frac{M_2}{M_1} \ . \qquad (26)$$

Center of mass is fixed
like a dipole as easily excited by
E field in the optical wave.

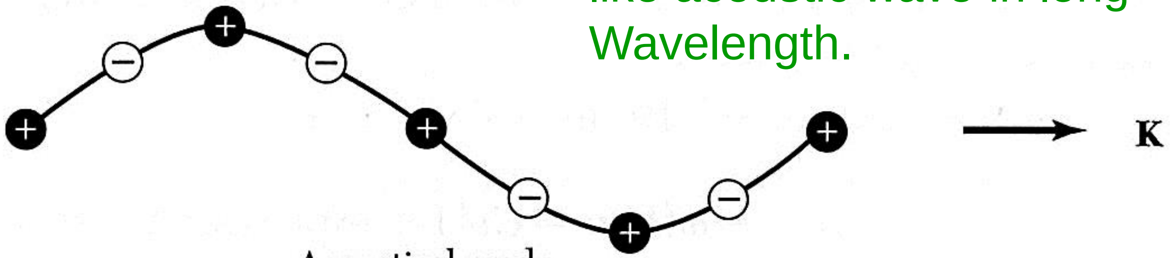


Optical mode

The atoms move in phase
like acoustic wave in long
Wavelength.

For K = 0, acoustic branch, u = v

Figure 10 Transverse optical and transverse acoustical waves in a diatomic linear lattice, illustrated by the particle displacements for the two modes at the same wavelength.



Acoustical mode

Quantization of Elastic Waves

The quantum of lattice vibration energy is called phonon, and the quantum number is denoted as ***n***. The elastic waves in crystals are made of phonons**.**

$$\epsilon = (n + \tfrac{1}{2})\hbar\omega \tag{27}$$

$U = u_o \cos Kx \cos wt$ for a standing wave

The time average kinetic energy is

$$\tfrac{1}{8}\rho V\omega^2 u_0^2 = \tfrac{1}{2}(n + \tfrac{1}{2})\hbar\omega \quad , \tag{28}$$

$$u_0^2 = 4(n + \tfrac{1}{2})\hbar/\rho V\omega \quad . \tag{29}$$

The sign of ω is usually positive, for imaginary ω, the crystal is unstable. An optical mode with ω close to zero is called a soft mode.

Phonon Momentum

- Physical momentum of a crystal is

$$p = M(d/dt)\, \Sigma\, u_s \quad . \tag{30}$$

$$p = M(du/dt) \sum_s \exp(isKa) = M(du/dt)[1 - \exp(iNKa)] \,/\, [1 - \exp(iKa)] \quad , \tag{31}$$

$$\sum_{s=0}^{N-1} x^s = (1 - x^N)/(1 - x) \quad . \tag{32}$$

$$p = M(du/dt) \sum_s \exp(isKa) = 0 \quad . \tag{33}$$

The physical momentum of a crystal is zero.

Phonon Momentum

$$\mathbf{k}' = \mathbf{k} + \mathbf{G} \ , \tag{34}$$

Elastic scattering of photons by a crystal

$$\mathbf{k}' + \underline{\mathbf{K}} = \mathbf{k} + \mathbf{G} \ . \tag{35}$$

For inelastic photon scattering,
it creates a phonon momentum ***K***

$$\mathbf{k}' = \mathbf{k} + \underline{\mathbf{K}} + \mathbf{G} \ . \tag{36}$$

For absorption of a phonon

Inelastic neutron scattering by phonons to obtain ***ω(K)***

$$\mathbf{k} + \mathbf{G} = \mathbf{k}' \pm \mathbf{K} \ , \tag{37}$$

$$\frac{\hbar^2 k^2}{2M_n} = \frac{\hbar^2 k'^2}{2M_n} \pm \hbar\omega \ , \tag{38}$$

Phonon Dispersions of Na in 3-D

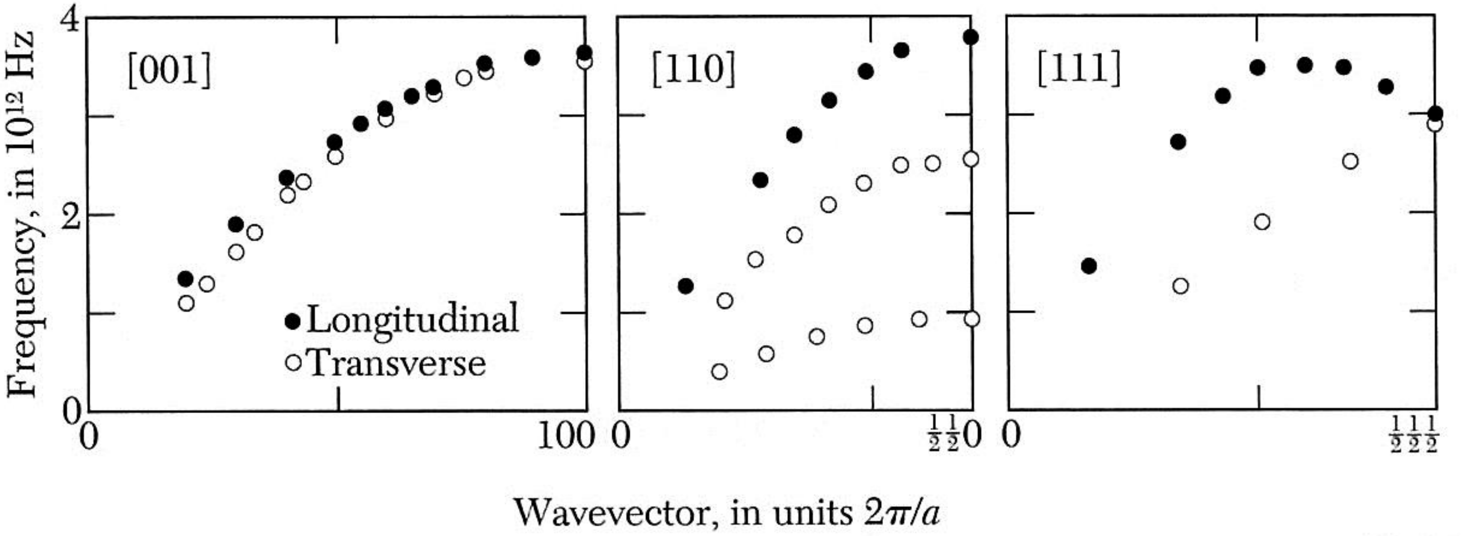


Figure 11 The dispersion curves of sodium for phonons propagating in the [001], [110], and [111] directions at 90 K, as determined by inelastic scattering of neutrons, by Woods, Brockhouse, March and Bowers.

SUMMARY

- The quantum unit of a crystal vibration is a phonon. If the angular frequency is ω, the energy of the phonon is $\hbar\omega$.
- When a phonon of wavevector $\mathbf{K}$ is created by the inelastic scattering of a photon or neutron from wavevector $\mathbf{k}$ to $\mathbf{k}'$, the wavevector selection rule that governs the process is

  $$\mathbf{k} = \mathbf{k}' + \mathbf{K} + \mathbf{G} \quad ,$$

  where $\mathbf{G}$ is a reciprocal lattice vector.
- All elastic waves can be described by wavevectors that lie within the first Brillouin zone in reciprocal space.
- If there are p atoms in the primitive cell, the phonon dispersion relation will have 3 acoustical phonon branches and $3p - 3$ optical phonon branches.