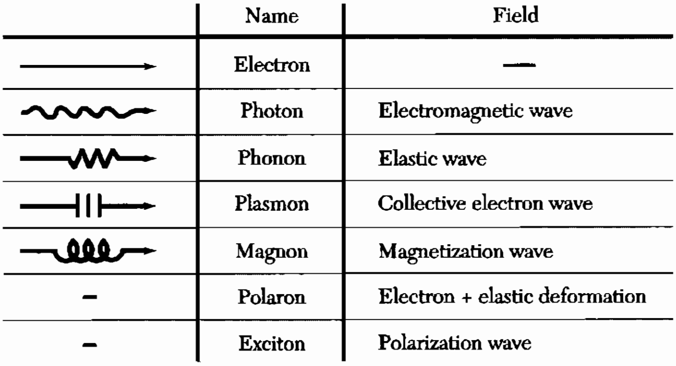
4

Phonons I. Crystal Vibrations

Chapter 5 treats the thermal properties of phonons.



	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.

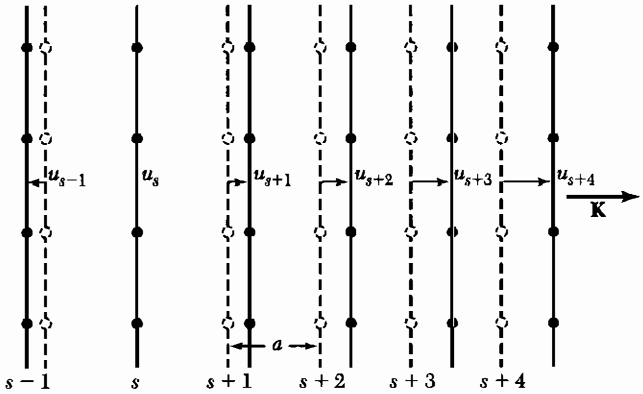


Figure 2 (Dashed lines) Planes of atoms when in equilibrium. (Solid lines) Planes of atoms when displaced as for a longitudinal wave. The coordinate u measures the displacement of the planes.

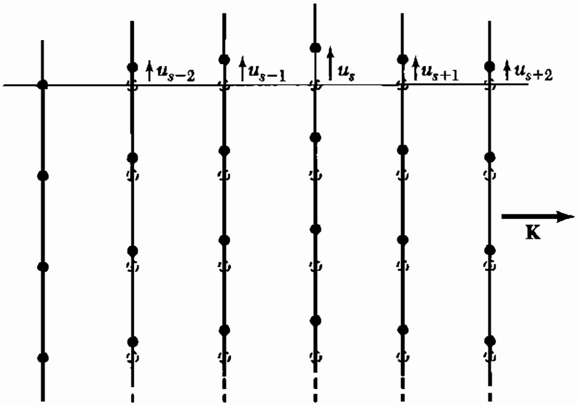


Figure 3 Planes of atoms as displaced during passage of a transverse wave.

VIBRATIONS OF CRYSTALS WITH MONATOMIC BASIS

Consider the elastic vibrations of a crystal with one atom in the primitive cell. We want to find the frequency of an elastic wave in terms of the wavevector that describes the wave and in terms of the elastic constants.

The mathematical solution is simplest in the [100], [110], and [111] propagation directions in cubic crystals. These are the directions of the cube edge, face diagonal, and body diagonal. When a wave propagates along one of these directions, entire planes of atoms move in phase with displacements either parallel or perpendicular to the direction of the wavevector. We can describe with a single coordinate u_s the displacement of the plane s from its equilibrium position. The problem is now one dimensional. For each wavevector there are three modes as solutions for u_s, one of longitudinal polarization (Fig. 2) and two of transverse polarization (Fig. 3).

We assume that the elastic response of the crystal is a linear function of the forces. That is equivalent to the assumption that the elastic energy is a quadratic function of the relative displacement of any two points in the crystal. Terms in the energy that are linear in the displacements will vanish in equilibrium—see the minimum in Fig. 3.6. Cubic and higher-order terms may be neglected for sufficiently small elastic deformations.

We assume that the force on the plane s caused by the displacement of the plane $s + p$ is proportional to the difference $u_{s+p} - u_s$ of their displacements. For brevity we consider only nearest-neighbor interactions, with $p = \pm 1$. The total force on s from planes $s \pm 1$:

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

This expression is linear in the displacements and is of the form of Hooke's law.

The constant C is the **force constant** between nearest-neighbor planes and will differ for longitudinal and transverse waves. It is convenient hereafter to regard C as defined for one atom of the plane, so that F_s is the force on one atom in the plane s.

The equation of motion of an atom in the plane s is

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

where M is the mass of an atom. We look for solutions with all displacements having the time dependence $\exp(-i\omega t)$. Then $d^2u_s/dt^2 = -\omega^2 u_s$, and (2) becomes

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

This is a difference equation in the displacements u and has traveling wave solutions of the form:

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

where a is the spacing between planes and K is the wavevector. The value to use for a will depend on the direction of K.

With (4), we have from (3):

$$-\omega^2 Mu \exp(isKa) = Cu\{\exp[i(s+1)Ka] + \exp[i(s-1)Ka] - 2\exp(isKa)\} \ . \tag{5}$$

We cancel $u \exp(isKa)$ from both sides, to leave

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

With the identity $2 \cos Ka = \exp(iKa) + \exp(-iKa)$, we have the **dispersion relation** $\omega(K)$.

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

The boundary of the first Brillouin zone lies at $K = \pm\pi/a$. We show from (7) that the slope of ω versus K is zero at the zone boundary:

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

at $K = \pm\pi/a$, for here $\sin Ka = \sin(\pm\pi) = 0$. The special significance of phonon wavevectors that lie on the zone boundary is developed in (12) below.

By a trigonometric identity, (7) may be written as

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

A plot of ω versus K is given in Fig. 4.

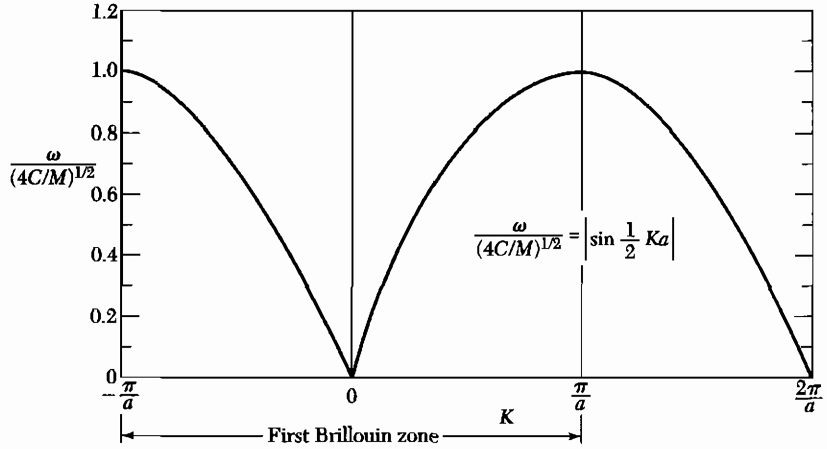


Figure 4 Plot of ω versus K. The region of $K \ll 1/a$ or $\lambda \gg a$ corresponds to the continuum approximation; here ω is directly proportional to K.

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

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

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

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

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

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

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

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

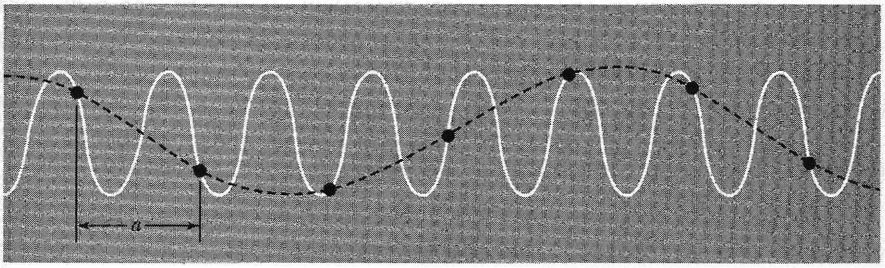


Figure 5 The wave represented by the solid curve conveys no information not given by the dashed curve. Only wavelengths longer than $2a$ are needed to represent the motion.

This is a standing wave: alternate atoms oscillate in opposite phases, because $u_s = \pm 1$ according to whether s is an even or an odd integer. The wave moves neither to the right nor to the left.

This situation is equivalent to Bragg reflection of x-rays: when the Bragg condition is satisfied a traveling wave cannot propagate in a lattice, but through successive reflections back and forth, a standing wave is set up.

The critical value $K_{\max} = \pm\pi/a$ found here satisfies the Bragg condition $2d \sin \theta = n\lambda$: we have $\theta = \frac{1}{2}\pi$, $d = a$, $K = 2\pi/\lambda$, $n = 1$, so that $\lambda = 2a$. With x-rays it is possible to have n equal to other integers besides unity because the amplitude of the electromagnetic wave has a meaning in the space between atoms, but the displacement amplitude of an elastic wave usually has a meaning only at the atoms themselves.

Group Velocity

The transmission velocity of a wave packet is the **group velocity**, given as

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

or

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

the gradient of the frequency with respect to **K**. This is the velocity of energy propagation in the medium.

With the particular dispersion relation (9), the group velocity (Fig. 6) is

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

This is zero at the edge of the zone where $K = \pi/a$. Here the wave is a standing wave, as in (12), and we expect zero net transmission velocity for a standing wave.

Long Wavelength Limit

When $Ka \ll 1$ we expand $\cos Ka \cong 1 - \frac{1}{2}(Ka)^2$, so that the dispersion relation (7) becomes

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

The result that the frequency is directly proportional to the wavevector in the long wavelength limit is equivalent to the statement that the velocity of sound is independent of frequency in this limit. Thus $v = \omega/K$, exactly as in the continuum theory of elastic waves—*in the continuum limit* $Ka \ll 1$.

Derivation of Force Constants from Experiment

In metals the effective forces may be of quite long range and are carried from ion to ion through the conduction electron sea. Interactions have been found between planes of atoms separated by as many as 20 planes. We can make a statement about the range of the forces from the observed experimental

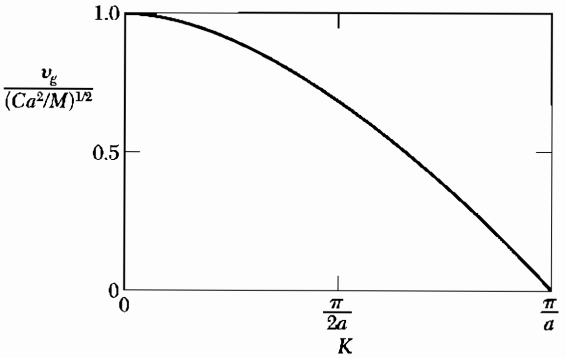


Figure 6 Group velocity v_g versus K, for model of Fig. 4. At the zone boundary $K = \pi/a$ the group velocity is zero.

dispersion relation for ω. The generalization of the dispersion relation (7) to p nearest planes is easily found to be

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

We solve for the interplanar force constants C_p by multiplying both sides by $\cos rKa$, where r is an integer, and integrating over the range of independent values of K:

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

The integral vanishes except for $p = r$. Thus

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

gives the force constant at range pa, for a structure with a monatomic basis.

TWO ATOMS PER PRIMITIVE BASIS

The phonon dispersion relation shows new features in crystals with two or more atoms per primitive basis. Consider, for example, the NaCl or diamond structures, with two atoms in the primitive cell. For each polarization mode in a given propagation direction the dispersion relation ω versus K develops two branches, known as the acoustical and optical branches, as in Fig. 7. We have longitudinal LA and transverse acoustical TA modes, and longitudinal LO and transverse optical TO modes.

If there are p atoms in the primitive cell, there are $3p$ branches to the dispersion relation: 3 acoustical branches and $3p - 3$ optical branches. Thus germanium (Fig. 8a) and KBr (Fig. 8b), each with two atoms in a primitive cell, have six branches: one LA, one LO, two TA, and two TO.

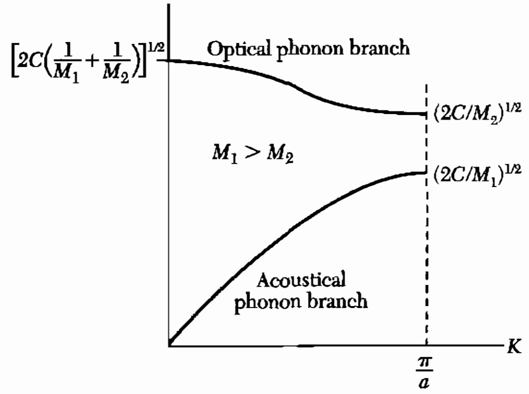


Figure 7 Optical and acoustical branches of the dispersion relation for a diatomic linear lattice, showing the limiting frequencies at $K = 0$ and $K = K_{max} = \pi/a$. The lattice constant is a.

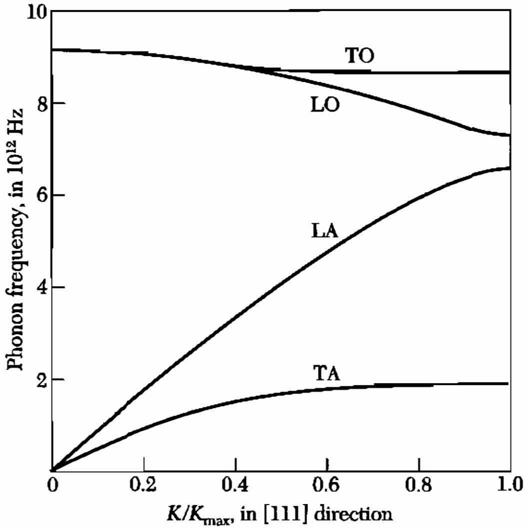


Figure 8a Phonon dispersion relations in the [111] direction in germanium at 80 K. The two TA phonon branches are horizontal at the zone boundary position, $K_{max} = (2\pi/a)(\frac{1}{2}\frac{1}{2}\frac{1}{2})$. The LO and TO branches coincide at $K = 0$; this also is a consequence of the crystal symmetry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

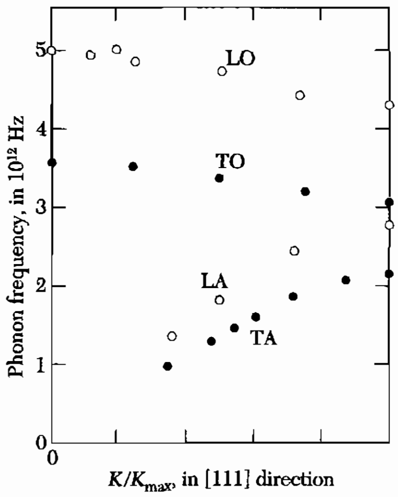


Figure 8b Dispersion curves in the [111] direction in KBr at 90 K, after A. D. B. Woods, B. N. Brockhouse, R. A. Cowley, and W. Cochran. The extrapolation to $K = 0$ of the TO, LO branches are called ω_T, ω_L.

The numerology of the branches follows from the number of degrees of freedom of the atoms. With p atoms in the primitive cell and N primitive cells, there are pN atoms. Each atom has three degrees of freedom, one for each of the x, y, z directions, making a total of $3pN$ degrees of freedom for the crystal. The number of allowed K values in a single branch is just N for one Brillouin zone.[1] Thus the

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[1] We show in Chapter 5 by application of periodic boundary conditions to the modes of the crystal of volume V that there is one $\mathbf{K}$ value in the volume $(2\pi)^3/V$ in Fourier space. The volume of a Brillouin zone is $(2\pi)^3/V_c$, where V_c is the volume of a crystal primitive cell. Thus the number of allowed $\mathbf{K}$ values in a Brillouin zone is V/V_c, which is just N, the number of primitive cells in the crystal.

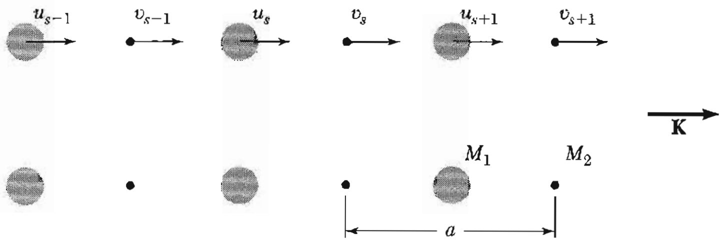


Figure 9 A diatomic crystal structure with masses M_1, M_2 connected by force constant C between adjacent planes. The displacements of atoms M_1 are denoted by u_{s-1}, u_s, u_{s+1}, . . . , and of atoms M_2 by v_{s-1}, v_s, v_{s+1}. The repeat distance is a in the direction of the wavevector K. The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

LA and the two TA branches have a total of $3N$ modes, thereby accounting for $3N$ of the total degrees of freedom. The remaining $(3p-3)N$ degrees of freedom are accommodated by the optical branches.

We consider a cubic crystal where atoms of mass M_1 lie on one set of planes and atoms of mass M_2 lie on planes interleaved between those of the first set (Fig. 9). It is not essential that the masses be different, but either the force constants or the masses will be different if the two atoms of the basis are in nonequivalent sites. Let a denote the repeat distance of the lattice in the direction normal to the lattice planes considered. We treat waves that propagate in a symmetry direction such that a single plane contains only a single type of ion; such directions are [111] in the NaCl structure and [100] in the CsCl structure.

We write the equations of motion under the assumption that each plane interacts only with its nearest-neighbor planes and that the force constants are identical between all pairs of nearest-neighbor planes. We refer to Fig. 9 to obtain

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

We look for a solution in the form of a traveling wave, now with different amplitudes u, v on alternate planes:

$$u_s = u\exp(isKa)\exp(-i\omega t) \ ; \qquad v_2 = v\exp(isKa)\exp(-i\omega t) \ . \tag{19}$$

We define a in Fig. 9 as the distance between nearest identical planes, not nearest-neighbor planes.

On substitution of (19) in (18) we have

$$\begin{aligned} -\omega^2 M_1 u &= Cv[1+\exp(-iKa)] - 2Cu \ ; \\ -\omega^2 M_2 v &= Cu[\exp(iKa)+1] - 2Cv \ . \end{aligned} \tag{20}$$

The homogeneous linear equations have a solution only if the determinant of the coefficients of the unknowns u, v vanishes:

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

or

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

We can solve this equation exactly for ω^2, but it is simpler to examine the limiting cases $Ka \ll 1$ and $Ka = \pm\pi$ at the zone boundary. For small Ka we have $\cos Ka \cong 1 - \frac{1}{2}K^2a^2 + \dots$, and the two roots are

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

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

The extent of the first Brillouin zone is $-\pi/a \leq K \leq \pi/a$, where a is the repeat distance of the lattice. At $K_{\max} = \pm\pi/a$ the roots are

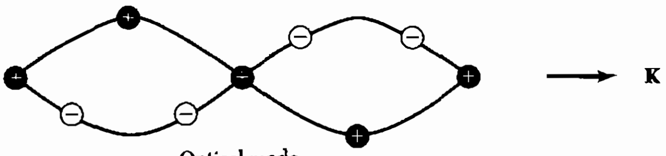
$$\omega^2 = 2C/M_1 \ ; \qquad \omega^2 = 2C/M_2 \ . \tag{25}$$

The dependence of ω on K is shown in Fig. 7 for $M_1 > M_2$.

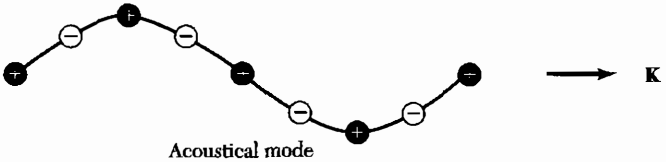
The particle displacements in the transverse acoustical (TA) and transverse optical (TO) branches are shown in Fig. 10. For the optical branch at $K = 0$ we find, on substitution of (23) in (20),

$$\frac{u}{v} = -\frac{M_2}{M_1} \ . \tag{26}$$

The atoms vibrate against each other, but their center of mass is fixed. If the two atoms carry opposite charges, as in Fig. 10, we may excite a motion of this



Optical mode



Acoustical mode

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.

type with the electric field of a light wave, so that the branch is called the optical branch. At a general K the ratio u/v will be complex, as follows from either of the equations (20). Another solution for the amplitude ratio at small K is $u = v$, obtained as the $K = 0$ limit of (24). The atoms (and their center of mass) move together, as in long wavelength acoustical vibrations, whence the term acoustical branch.

Wavelike solutions do not exist for certain frequencies, here between $(2C/M_1)^{1/2}$ and $(2C/M_2)^{1/2}$. This is a characteristic feature of elastic waves in polyatomic lattices. There is a frequency gap at the boundary $K_{\max} = \pm\pi/a$ of the first Brillouin zone.

QUANTIZATON OF ELASTIC WAVES

The energy of a lattice vibration is quantized. The quantum of energy is called a **phonon** in analogy with the photon of the electromagnetic wave. The energy of an elastic mode of angular frequency ω is

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

when the mode is excited to quantum number n; that is, when the mode is occupied by n phonons. The term $\frac{1}{2}\hbar\omega$ is the zero point energy of the mode. It occurs for both phonons and photons as a consequence of their equivalence to a quantum harmonic oscillator of frequency ω, for which the energy eigenvalues are also $(n + \frac{1}{2})\hbar\omega$. The quantum theory of phonons is developed in Appendix C.

We can quantize the mean square phonon amplitude. Consider the standing wave mode of amplitude

$$u = u_0 \cos Kx \cos \omega t \ .$$

Here u is the displacement of a volume element from its equilibrium position at x in the crystal. The energy in the mode, as in any harmonic oscillator, is half kinetic energy and half potential energy, when averaged over time. The kinetic energy density is $\frac{1}{2}\rho(\partial u/\partial t)^2$, where ρ is the mass density. In a crystal of volume V, the volume integral of the kinetic energy is $\frac{1}{4}\rho V\omega^2 u_0^2 \sin^2 \omega t$. The time average kinetic energy is

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

because $<\sin^2 \omega t> = \frac{1}{2}$. The square of the amplitude of the mode is

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

This relates the displacement in a given mode to the phonon occupancy n of the mode.

What is the sign of ω? The equations of motion such as (2) are equations for ω^2, and if this is positive then ω can have either sign, + or −. But the energy of a phonon must be positive, so it is conventional and suitable to view ω as positive. If the crystal structure is unstable, then ω^2 will be negative and ω will be imaginary.

PHONON MOMENTUM

A phonon of wavevector K will interact with particles such as photons, neutrons, and electrons as if it had a momentum $\hbar K$. However, a phonon does not carry physical momentum.

The reason that phonons on a lattice do not carry momentum is that a phonon coordinate (except for $K = 0$) involves relative coordinates of the atoms. Thus in an H_2 molecule the internuclear vibrational coordinate $\mathbf{r}_1 - \mathbf{r}_2$ is a relative coordinate and does not carry linear momentum; the center of mass coordinate $\frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$ corresponds to the uniform mode $K = 0$ and can carry linear momentum.

In crystals there exist wavevector selection rules for allowed transitions between quantum states. We saw in Chapter 2 that the elastic scattering of an x-ray photon by a crystal is governed by the wavevector selection rule

$$\mathbf{k}' = \mathbf{k} + \mathbf{G} \ , \tag{30}$$

where $\mathbf{G}$ is a vector in the reciprocal lattice, $\mathbf{k}$ is the wavevector of the incident photon, and $\mathbf{k}'$ is the wavevector of the scattered photon. In the reflection process the crystal as a whole will recoil with momentum $-\hbar\mathbf{G}$, but this uniform mode momentum is rarely considered explicitly.

Equation (30) is an example of the rule that the total wavevector of interacting waves is conserved in a periodic lattice, with the possible addition of a reciprocal lattice vector $\mathbf{G}$. The true momentum of the whole system always is rigorously conserved. If the scattering of the photon is inelastic, with the creation of a phonon of wavevector $\mathbf{K}$, then the wavevector selection rule becomes

$$\mathbf{k}' + \mathbf{K} = \mathbf{k} + \mathbf{G} \ . \tag{31}$$

If a phonon $\mathbf{K}$ is absorbed in the process, we have instead the relation

$$\mathbf{k}' = \mathbf{k} + \mathbf{K} + \mathbf{G} \ . \tag{32}$$

Relations (31) and (32) are the natural extensions of (30).

INELASTIC SCATTERING BY PHONONS

Phonon dispersion relations $\omega(\mathbf{K})$ are most often determined experimentally by the inelastic scattering of neutrons with the emission or absorption of a phonon. A neutron sees the crystal lattice chiefly by interaction with the nuclei of the atoms. The kinematics of the scattering of a neutron beam by a crystal lattice are described by the general wavevector selection rule:

$$\mathbf{k} + \mathbf{G} = \mathbf{k}' \pm \mathbf{K} \ , \qquad (33)$$

and by the requirement of conservation of energy. Here **K** is the wavevector of the phonon created (+) or absorbed (−) in the scattering process, and **G** is any reciprocal lattice vector. For a phonon we choose **G** such that **K** lies in the first Brillouin zone.

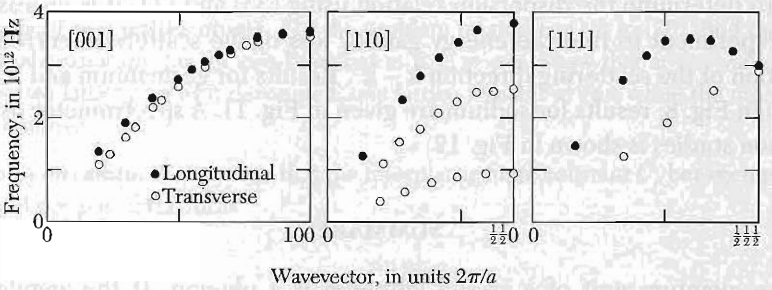


Figure 11 The dispersion curves of sodium for phonons propagating in the [001], [110], and [111] directions at 90 K, as determined by inelastic scattering of neutrons, by Woods, Brockhouse, March and Bowers.

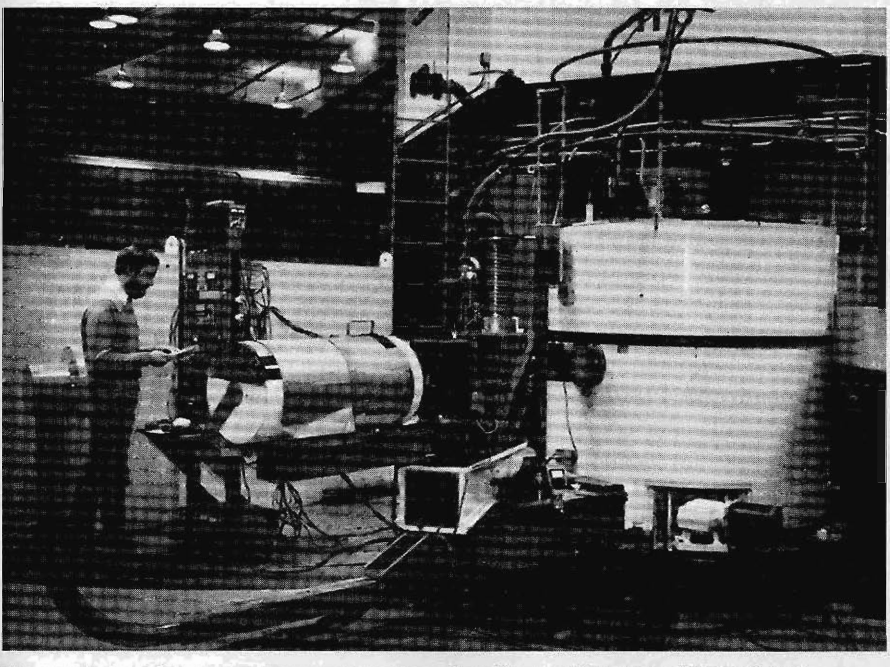


Figure 12 A triple axis neutron spectrometer at Brookhaven. (Courtesy of B. H. Grier.)

The kinetic energy of the incident neutron is $p^2/2M_n$, where M_n is the mass of the neutron. The momentum $\mathbf{p}$ is given by $\hbar\mathbf{k}$, where $\mathbf{k}$ is the wavevector of the neutron. Thus $\hbar^2k^2/2M_n$ is the kinetic energy of the incident neutron. If $\mathbf{k}'$ is the wavevector of the scattered neutron, the energy of the scattered neutron is $\hbar^2k'^2/2M_n$. The statement of conservation of energy is

$$\frac{\hbar^2k^2}{2M_n} = \frac{\hbar^2k'^2}{2M_n} \pm \hbar\omega \ , \tag{34}$$

where $\hbar\omega$ is the energy of the phonon created (+) or absorbed (−) in the process.

To determine the dispersion relation using (33) and (34) it is necessary in the experiment to find the energy gain or loss of the scattered neutrons as a function of the scattering direction $\mathbf{k} - \mathbf{k}'$. Results for germanium and KBr are given in Fig. 8; results for sodium are given in Fig. 11. A spectrometer used for phonon studies is shown in Fig. 12.

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

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

  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.

Problems

1. ***Monatomic linear lattice.*** Consider a longitudinal wave

$$u_s = u\cos(\omega t - sKa)$$

which propagates in a monatomic linear lattice of atoms of mass M, spacing a, and nearest-neighbor interaction C.

(a) Show that the total energy of the wave is

$$E = \tfrac{1}{2}M\sum_s (du_s/dt)^2 + \tfrac{1}{2}C\sum_s (u_s - u_{s+1})^2 \ .$$

where s runs over all atoms.

(b) By substitution of u_s in this expression, show that the time-average total energy per atom is

$$\tfrac{1}{4}M\omega^2u^2 + \tfrac{1}{2}C(1 - \cos Ka)u^2 = \tfrac{1}{2}M\omega^2u^2 \ ,$$

where in the last step we have used the dispersion relation (9) for this problem.

2. ***Continuum wave equation.*** Show that for long wavelengths the equation of motion (2) reduces to the continuum elastic wave equation

$$\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2} \ ,$$

where v is the velocity of sound.

3. ***Basis of two unlike atoms.*** For the problem treated by (18) to (26), find the amplitude ratios u/v for the two branches at $K_{max} = \pi/a$. Show that at this value of K the two lattices act as if decoupled: one lattice remains at rest while the other lattice moves.

4. ***Kohn anomaly.*** We suppose that the interplanar force constant C_p between planes s and $s + p$ is of the form

$$C_p = A\frac{\sin pk_0a}{pa} \ ,$$

where A and k_0 are constants and p runs over all integers. Such a form is expected in metals. Use this and Eq. (16a) to find an expression for ω^2 and also for $\partial\omega^2/\partial K$. Prove that $\partial\omega^2/\partial K$ is infinite when $K = k_0$. Thus a plot of ω^2 versus K or of ω versus K has a vertical tangent at k_0: there is a kink at k_0 in the phonon dispersion relation $\omega(K)$.

5. ***Diatomic chain.*** Consider the normal modes of a linear chain in which the force constants between nearest-neighbor atoms are alternately C and $10C$. Let the masses be equal, and let the nearest-neighbor separation be $a/2$. Find $\omega(K)$ at $K = 0$ and $K = \pi/a$. Sketch in the dispersion relation by eye. This problem simulates a crystal of diatomic molecules such as H_2.

6. ***Atomic vibrations in a metal.*** Consider point ions of mass M and charge e immersed in a uniform sea of conduction electrons. The ions are imagined to be in stable equilibrium when at regular lattice points. If one ion is displaced a small distance r from its equilibrium position, the restoring force is largely due to the electric charge within the sphere of radius r centered at the equilibrium position. Take the number density of ions (or of conduction electrons) as $3/4\pi R^3$, which defines R. (a) Show that the frequency of a single ion set into oscillation is $\omega = (e^2/MR^3)^{1/2}$. (b) Estimate the value of this frequency for sodium, roughly. (c) From (a), (b), and some common sense, estimate the order of magnitude of the velocity of sound in the metal.

*7. ***Soft phonon modes.*** Consider a line of ions of equal mass but alternating in charge, with $e_p = e(-1)^p$ as the charge on the pth ion. The interatomic potential is

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*This problem is rather difficult.

the sum of two contributions: (1) a short-range interaction of force constant $C_{1R} = \gamma$ that acts between nearest neighbors only, and (2) a coulomb interaction between all ions. (a) Show that the contribution of the coulomb interaction to the atomic force constants is $C_{pC} = 2(-1)^p e^2/p^3a^3$, where a is the equilibrium nearest-neighbor distance. (b) From (16a) show that the dispersion relation may be written as

$$\omega^2/\omega_0^2 - \sin^2 \tfrac{1}{2}Ka + \sigma\sum_{p-1}^{\infty}(-1)^p\,(1 - \cos pKa)p^{-3} \ ,$$

where $\omega_0^2 \equiv 4\gamma/M$ and $\sigma = e^2/\gamma a^3$. (c) Show that ω^2 is negative (unstable mode) at the zone boundary $Ka = \pi$ if $\sigma > 0.475$ or $4/7\zeta(3)$, where ζ is a Riemann zeta function. Show further that the speed of sound at small Ka is imaginary if $\sigma > (2 \ln 2)^{-1} = 0.721$. Thus ω^2 goes to zero and the lattice is unstable for some value of Ka in the interval $(0, \pi)$ if $0.475 < \sigma < 0.721$. Notice that the phonon spectrum is not that of a diatomic lattice because the interaction of any ion with its neighbors is the same as that of any other ion.