Lecture notes: Phonons II

Two atoms per primitive basis, quantization & momentum

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The phonon dispersion relation exhibits qualitatively new features in crystals with two or more atoms per primitive basis (such as NaCl, CsCl, diamond, germanium, and KBr). For each polarization mode in a given propagation direction, the dispersion curve $\omega(K)$ splits into two distinct branches: an **acoustical branch** and an **optical branch**.

Consider a three-dimensional crystal composed of N primitive unit cells, with p atoms in each primitive basis:

- **Total number of atoms:** pN.
- **Total vibrational degrees of freedom:** Each atom moves in three spatial dimensions (x, y, z), giving $3pN$ degrees of freedom for the entire crystal.
- **Allowed wavevectors:** Within the First Brillouin Zone, there are N independent allowed values of the wavevector $\mathbf{K}$ per branch.

Dividing the $3pN$ total degrees of freedom by the N wavevectors per branch yields exactly $3p$ **dispersion branches**:

1. 3 **Acoustical branches (**$3N$ **modes):** 1 Longitudinal Acoustic (LA) branch and 2 Transverse Acoustic (TA) branches.

2. $3p-3$ **Optical branches (**$(3p-3)N$ **modes):** For a diatomic basis ($p=2$), there are $3(2)-3=3$ optical branches: 1 Longitudinal Optical (LO) branch and 2 Transverse Optical (TO) branches, making 6 branches in total.

1 Equations of motion for a diatomic lattice

Consider a cubic crystal in which atoms of mass M_1 lie on one set of parallel planes and atoms of mass M_2 lie on alternating interleaved planes (for example, waves propagating along the [111] direction in NaCl or the [100] direction in CsCl). Let a denote the repeat distance between nearest *identical* planes along the direction of wavevector $\mathbf{K}$, and let C be the harmonic force constant between nearest-neighbor planes.

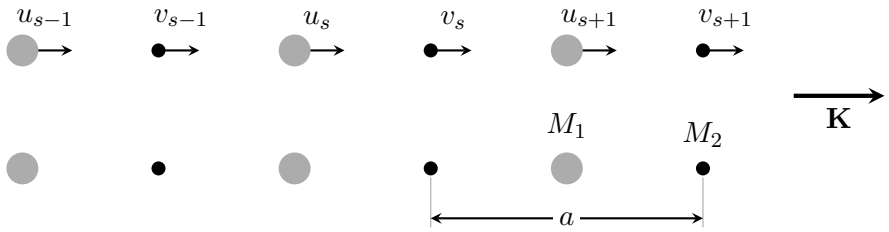


Figure 1: Diatomic crystal planes with masses M_1 and M_2 connected by force constant C. Displacements of M_1 are u_s and of M_2 are v_s; the repeat distance is a.

Denoting the displacement of plane s of mass M_1 by u_s and of plane s of mass M_2 by v_s, the nearest-neighbor restoring forces via Hooke's law are:

$$F_{1,s} = C(v_s - u_s) + C(v_{s-1} - u_s) = C(v_s + v_{s-1} - 2u_s) \tag{1}$$

$$F_{2,s} = C(u_{s+1} - v_s) + C(u_s - v_s) = C(u_{s+1} + u_s - 2v_s) \tag{2}$$

Applying Newton's second law yields the coupled equations of motion:

$$M_1 \frac{d^2 u_s}{dt^2} = C(v_s + v_{s-1} - 2u_s) \tag{3}$$

$$M_2 \frac{d^2 v_s}{dt^2} = C(u_{s+1} + u_s - 2v_s) \tag{4}$$

2 Dispersion Relation $\omega(K)$

We seek harmonic traveling wave solutions with different complex amplitudes u and v on the two sublattices:

$$u_s(t) = u\, e^{i(sKa - \omega t)}, \qquad v_s(t) = v\, e^{i(sKa - \omega t)} \tag{5}$$

Differentiating twice with respect to time gives:

$$\frac{d^2u_s}{dt^2} = -\omega^2 u_s, \qquad \frac{d^2v_s}{dt^2} = -\omega^2 v_s \tag{6}$$

Using spatial phase factors for neighboring planes ($v_{s-1} = v_s e^{-iKa}$ and $u_{s+1} = u_s e^{iKa}$), substituting (5) into (3) and (4), and canceling the common factor $e^{i(sKa-\omega t)}$ yields:

$$-\omega^2 M_1 u = Cv\left(1 + e^{-iKa}\right) - 2Cu \tag{7}$$

$$-\omega^2 M_2 v = Cu\left(e^{iKa} + 1\right) - 2Cv \tag{8}$$

Rearranging (7) and (8) into a homogeneous system of linear equations for u and v:

$$\begin{pmatrix} 2C - M_1\omega^2 & -C\left(1 + e^{-iKa}\right) \\ -C\left(1 + e^{iKa}\right) & 2C - M_2\omega^2 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{9}$$

Nontrivial solutions exist only if the determinant of the coefficient matrix vanishes:

$$\begin{vmatrix} 2C - M_1\omega^2 & -C\left(1 + e^{-iKa}\right) \\ -C\left(1 + e^{iKa}\right) & 2C - M_2\omega^2 \end{vmatrix} = 0 \tag{10}$$

Expanding the determinant step by step:

$$(2C - M_1\omega^2)(2C - M_2\omega^2) - C^2\left(1 + e^{-iKa}\right)\left(1 + e^{iKa}\right) = 0 \tag{11}$$

Using Euler's identity ($e^{iKa} + e^{-iKa} = 2\cos Ka$), the exponential product simplifies to:

$$\left(1 + e^{-iKa}\right)\left(1 + e^{iKa}\right) = 1 + e^{iKa} + e^{-iKa} + 1 = 2 + 2\cos Ka \tag{12}$$

Substituting this back and collecting powers of ω^2:

$$4C^2 - 2C(M_1 + M_2)\omega^2 + M_1M_2\omega^4 - C^2(2 + 2\cos Ka) = 0 \tag{13}$$

$$M_1M_2\omega^4 - 2C(M_1 + M_2)\omega^2 + 2C^2(1 - \cos Ka) = 0 \tag{14}$$

Applying the quadratic formula to (14) and using $1 - \cos Ka = 2\sin^2(Ka/2)$ gives the two dispersion branches:

$$\omega^2(K) = C\left(\frac{1}{M_1} + \frac{1}{M_2}\right) \pm C\sqrt{\left(\frac{1}{M_1} + \frac{1}{M_2}\right)^2 - \frac{4\sin^2(Ka/2)}{M_1M_2}} \tag{15}$$

where the upper sign (+) corresponds to the **optical branch** and the lower sign (−) corresponds to the **acoustical branch**.

2.1 Limiting cases and the phonon band gap

We examine the roots of (14) in two important physical limits:

1. Long-wavelength limit ($Ka \ll 1$)

For small Ka, Taylor expansion gives $\cos Ka \cong 1 - \frac{1}{2}K^2a^2 + \cdots$, so $1 - \cos Ka \cong \frac{1}{2}K^2a^2$. Equation (14) becomes:

$$M_1M_2\omega^4 - 2C(M_1 + M_2)\omega^2 + C^2K^2a^2 \cong 0 \tag{16}$$

- **Optical branch (ω finite as $K \to 0$):** Neglecting the $\mathcal{O}(K^2a^2)$ term yields:

$$M_1M_2\omega^4 \cong 2C(M_1 + M_2)\omega^2 \implies \omega^2 \cong 2C\left(\frac{1}{M_1} + \frac{1}{M_2}\right) \tag{17}$$

- **Acoustical branch ($\omega \to 0$ as $K \to 0$):** Neglecting the $\omega^4 \propto K^4$ term yields:

$$2C(M_1 + M_2)\omega^2 \cong C^2K^2a^2 \implies \omega^2 \cong \frac{\frac{1}{2}C}{M_1 + M_2}K^2a^2 \tag{18}$$

  which describes linear acoustic sound propagation $\omega = vK$ with velocity $v = a\sqrt{\frac{C}{2(M_1+M_2)}}$.

2. First Brillouin zone boundary ($K_{\max} = \pm\pi/a$)

The First Brillouin Zone extends over $-\frac{\pi}{a} \le K \le \frac{\pi}{a}$. At $K_{\max} = \pm\frac{\pi}{a}$, we have $\cos(\pm\pi) = -1$, so $1 - \cos(\pm\pi) = 2$. Substituting into (14):

$$M_1M_2\omega^4 - 2C(M_1 + M_2)\omega^2 + 4C^2 = 0 \tag{19}$$

This factors directly as:

$$(M_1\omega^2 - 2C)(M_2\omega^2 - 2C) = 0 \tag{20}$$

yielding the two zone-boundary frequencies:

$$\omega^2 = \frac{2C}{M_1} \qquad \text{and} \qquad \omega^2 = \frac{2C}{M_2} \tag{21}$$

Assuming $M_1 > M_2$, the upper (optical) branch terminates at $\omega_{\text{opt}}(\pi/a) = \sqrt{2C/M_2}$ and the lower (acoustical) branch terminates at $\omega_{\text{ac}}(\pi/a) = \sqrt{2C/M_1}$. Between $(2C/M_1)^{1/2}$ and $(2C/M_2)^{1/2}$ lies a **forbidden frequency gap** in which no wavelike solutions can propagate through the lattice.

2.2 Amplitude ratio u/v and physical motion

Evaluating equation (7) at $K = 0$ ($e^{-iKa} = 1$) gives:

$$-\omega^2M_1u = 2C(v - u) \tag{22}$$

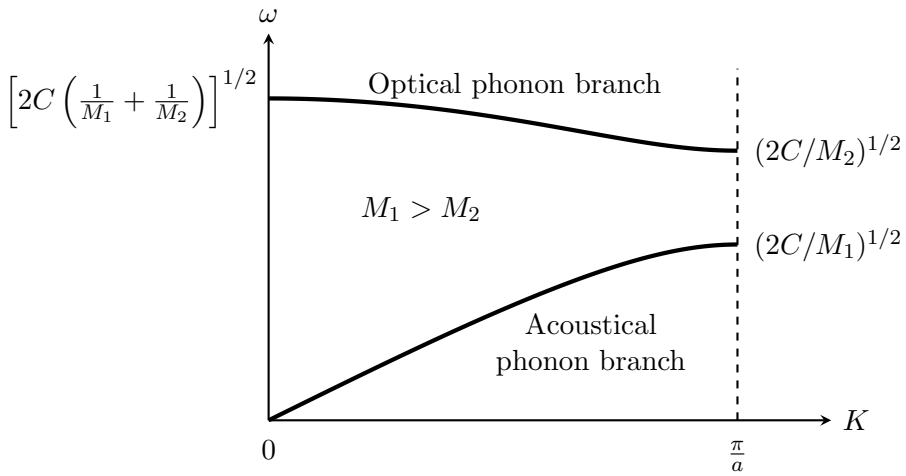


Figure 2: Optical and acoustical dispersion branches for a diatomic linear lattice ($M_1 > M_2$), showing limiting frequencies at $K = 0$ and $K_{\max} = \pi/a$.

- **Optical branch at $K = 0$:** Substituting $\omega^2 = 2C\left(\frac{1}{M_1}+\frac{1}{M_2}\right)$ from (17):

$$-2C\left(\frac{1}{M_1}+\frac{1}{M_2}\right)M_1 u = 2C(v-u) \implies -\left(1+\frac{M_1}{M_2}\right)u = v-u \tag{23}$$

  Canceling $-u$ from both sides yields:

$$\frac{u}{v} = -\frac{M_2}{M_1} \qquad \text{or} \qquad M_1 u + M_2 v = 0 \tag{24}$$

  The two atoms oscillate 180° out of phase against each other while keeping their center of mass stationary. In ionic crystals where the two basis atoms carry opposite charges, this relative motion produces an oscillating electric dipole moment that couples directly with the electric field of infrared light.

- **Acoustical branch as $K \to 0$:** Substituting $\omega \to 0$ gives $0 = 2C(v-u)$, so:

$$u = v \qquad \left(\frac{u}{v} = 1\right) \tag{25}$$

  Both atoms and their center of mass move together in phase with equal amplitude, characteristic of long-wavelength acoustic sound waves.

3 Quantization of elastic waves

The vibrational energy of a crystal lattice is quantized. In direct analogy with the photon of the electromagnetic field, the quantum of energy of an elastic lattice vibration is called a **phonon**. Because each normal mode of angular frequency ω is mathematically equivalent to a quantum harmonic oscillator, its allowed energy eigenvalues are:

$$\epsilon = \left(n+\frac{1}{2}\right)\hbar\omega, \qquad n = 0, 1, 2, \ldots \tag{26}$$

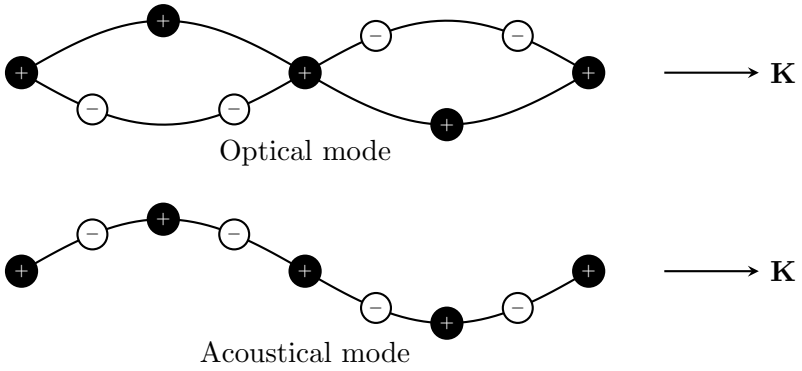


Figure 3: Transverse optical and transverse acoustical waves in a diatomic linear lattice at the same wavelength.

where n is the phonon quantum number (the number of phonons occupying the mode) and $\frac{1}{2}\hbar\omega$ is the zero-point energy of the mode.

Consider a standing elastic wave mode along the x-axis with displacement amplitude u_0:

$$u(x,t) = u_0 \cos(Kx)\cos(\omega t) \tag{27}$$

where $u(x,t)$ denotes the displacement of a volume element from its equilibrium position at x.

The instantaneous kinetic energy density is $\frac{1}{2}\rho\left(\frac{\partial u}{\partial t}\right)^2$, where ρ is the mass density of the crystal. Differentiating $u(x,t)$ with respect to time gives:

$$\frac{\partial u}{\partial t} = -u_0\omega\cos(Kx)\sin(\omega t) \tag{28}$$

Integrating the kinetic energy density over the crystal volume V:

$$T(t) = \int_V \frac{1}{2}\rho\left(\frac{\partial u}{\partial t}\right)^2 dV = \frac{1}{2}\rho u_0^2\omega^2\sin^2(\omega t)\int_V \cos^2(Kx)\,dV \tag{29}$$

Since the spatial average of $\cos^2(Kx)$ over the macroscopic volume V is $\frac{1}{2}$, we have $\int_V \cos^2(Kx)\,dV = \frac{1}{2}V$, so the instantaneous total kinetic energy is:

$$T(t) = \frac{1}{4}\rho V\omega^2 u_0^2\sin^2(\omega t) \tag{30}$$

Taking the time average over an oscillation cycle using $\langle\sin^2(\omega t)\rangle = \frac{1}{2}$:

$$\langle T\rangle = \frac{1}{4}\rho V\omega^2 u_0^2\left(\frac{1}{2}\right) = \frac{1}{8}\rho V\omega^2 u_0^2 \tag{31}$$

In any harmonic oscillator, the time-averaged kinetic energy equals half of the total mode energy ($\langle T\rangle = \frac{1}{2}\epsilon$). Equating this to half of (26):

$$\frac{1}{8}\rho V\omega^2 u_0^2 = \frac{1}{2}\left(n+\frac{1}{2}\right)\hbar\omega \tag{32}$$

Solving for the square of the displacement amplitude u_0^2:

$$u_0^2 = \frac{4\left(n + \frac{1}{2}\right)\hbar}{\rho V \omega} \tag{33}$$

This relation connects the macroscopic displacement amplitude u_0 of an elastic mode directly to its quantum phonon occupancy n.

The lattice equations of motion determine ω^2. When $\omega^2 > 0$, ω can take either a + or − sign. Because the energy of a phonon must be positive, it is standard convention to choose $\omega > 0$. If a crystal structure is dynamically unstable, ω^2 becomes negative and ω becomes imaginary.

4 Phonon momentum

A phonon of wavevector $\mathbf{K}$ interacts with particles such as photons, neutrons, and electrons *as if* it carried momentum $\hbar\mathbf{K}$ (called **crystal momentum**). However, a phonon does **not** carry true physical linear momentum.

- **Molecular analogy:** In an H_2 molecule with atomic coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$, the internal vibrational coordinate $\mathbf{r}_1 - \mathbf{r}_2$ represents relative motion and carries zero linear momentum, whereas the center-of-mass coordinate $\frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$ corresponds to uniform translation ($\mathbf{K} = 0$) and carries true linear momentum.
- **Explicit lattice proof:** For a 1D lattice of N identical atoms of mass M with lattice spacing a and displacement $u_s(t) = u\, e^{i(sKa - \omega t)}$, the total physical momentum of the crystal is:

$$P = \sum_{s=0}^{N-1} M \frac{du_s}{dt} = -i\omega M u\, e^{-i\omega t} \sum_{s=0}^{N-1} e^{isKa} \tag{34}$$

  Under periodic boundary conditions ($e^{iNKa} = 1$), the geometric sum vanishes for every non-zero wavevector $K \neq 0$ inside the First Brillouin Zone:

$$\sum_{s=0}^{N-1} e^{isKa} = \frac{1 - e^{iNKa}}{1 - e^{iKa}} = 0 \implies P = 0 \qquad (K \neq 0) \tag{35}$$

  Only the uniform mode $K = 0$ moves all atoms together in phase ($P = -i\omega N M u\, e^{-i\omega t} \neq 0$).

Although individual phonons ($K \neq 0$) carry no physical momentum, total momentum of the interacting system is strictly conserved and manifests as **wavevector selection rules** in periodic crystals:

1. **Elastic X-ray scattering (Bragg diffraction):**

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

where $\mathbf{k}$ and $\mathbf{k}'$ are the incident and scattered photon wavevectors, and $\mathbf{G}$ is a reciprocal lattice vector. During reflection, the crystal as a whole recoils with physical momentum $-\hbar\mathbf{G}$.

2. **Inelastic scattering with phonon creation (emission):** When an incident particle ($\mathbf{k}$) scatters into state $\mathbf{k}'$ while creating a phonon of wavevector $\mathbf{K}$:

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

3. **Inelastic scattering with phonon absorption:** When an incident particle ($\mathbf{k}$) absorbs a phonon of wavevector $\mathbf{K}$ and scatters into state $\mathbf{k}'$:

$$\mathbf{k}' = \mathbf{k} + \mathbf{K} + \mathbf{G} \tag{38}$$

Relations (37) and (38) generalize the Bragg condition (36) to inelastic processes, allowing phonon dispersion relations $\omega(\mathbf{K})$ to be measured experimentally via inelastic neutron scattering.

Note: These lecture notes were prepared with the assistance of AI educational tools (Gemini) for pedagogical structuring, step-by-step algebraic typesetting, and diagram generation.