Lecture notes: Phonons I

Vibrations of crystals with monatomic basis

Dr. Mohammad Abdur Rashid
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just.edu.bd/t/rashid

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Consider a one-dimensional array of identical atoms, each of mass M, separated by equilibrium interplanar distance a. Let u_s denote the displacement of plane s from its equilibrium position. Under the harmonic approximation, the elastic response of the crystal is quadratic in relative displacements, yielding linear restoring forces. Assuming interactions between nearest-neighbor planes ($s \pm 1$) with force constant C:

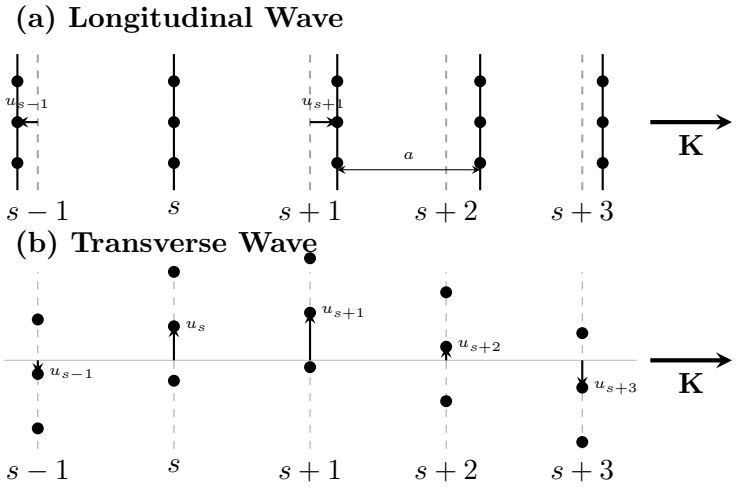


Figure 1: Atomic plane displacements for (a) longitudinal waves (displacements parallel to **K**) and (b) transverse waves (displacements perpendicular to **K**).

- Force on plane s due to displacement of plane $s+1$:

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

- Force on plane s due to displacement of plane $s-1$:

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

Summing these force contributions gives the total restoring force F_s acting on plane s:

$$F_s = F_{s+1\to s} + F_{s-1\to s} = C(u_{s+1} - u_s) + C(u_{s-1} - u_s) = C(u_{s+1} + u_{s-1} - 2u_s) \tag{3}$$

Applying Newton's second law ($F_s = M\frac{d^2u_s}{dt^2}$) to atom s yields the fundamental equation of motion:

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

1 Dispersion Relation $\omega(K)$

We look for traveling wave solutions in which displacements vary harmonically in time with angular frequency ω and spatial wavevector K.

Assume a trial solution of the form:

$$u_s(t) = u \cdot e^{i(sKa-\omega t)} \tag{5}$$

where u is the wave amplitude and sa is the equilibrium coordinate of plane s.

Differentiating $u_s(t)$ twice with respect to time t:

$$\frac{du_s}{dt} = \frac{d}{dt}\left[u\, e^{i(sKa-\omega t)}\right] = (-i\omega)\, u\, e^{i(sKa-\omega t)} = -i\omega u_s \tag{6}$$

$$\frac{d^2u_s}{dt^2} = \frac{d}{dt}\left[-i\omega u_s\right] = (-i\omega)^2 u\, e^{i(sKa-\omega t)} = -\omega^2 u_s \tag{7}$$

Substituting $\frac{d^2u_s}{dt^2} = -\omega^2 u_s$ into the equation of motion gives:

$$-M\omega^2 u_s = C(u_{s+1} + u_{s-1} - 2u_s) \tag{8}$$

Express the displacements of neighboring planes u_{s+1} and u_{s-1} in terms of u_s:

$$u_{s+1} = u\, e^{i((s+1)Ka-\omega t)} = u\, e^{i(sKa-\omega t)} \cdot e^{iKa} = u_s\, e^{iKa} \tag{9}$$

$$u_{s-1} = u\, e^{i((s-1)Ka-\omega t)} = u\, e^{i(sKa-\omega t)} \cdot e^{-iKa} = u_s\, e^{-iKa} \tag{10}$$

Substituting these back into the differential equation yields:

$$-M\omega^2 u_s = C\left(u_s e^{iKa} + u_s e^{-iKa} - 2u_s\right) \tag{11}$$

Factoring out u_s:

$$-M\omega^2 u_s = C u_s\left(e^{iKa} + e^{-iKa} - 2\right) \tag{12}$$

Assuming non-zero displacement amplitude ($u \neq 0$), we divide both sides by u_s:

$$-M\omega^2 = C\left(e^{iKa} + e^{-iKa} - 2\right) \tag{13}$$

Multiplying through by -1:

$$M\omega^2 = C\left(2 - e^{iKa} - e^{-iKa}\right) \tag{14}$$

Using Euler's identity ($e^{i\theta} + e^{-i\theta} = 2\cos\theta$), we substitute $e^{iKa} + e^{-iKa} = 2\cos(Ka)$:

$$M\omega^2 = C\left(2 - 2\cos(Ka)\right) = 2C\left(1 - \cos(Ka)\right) \tag{15}$$

Applying the trigonometric identity $1 - \cos\theta = 2\sin^2\left(\frac{\theta}{2}\right)$:

$$M\omega^2 = 2C\left[2\sin^2\left(\frac{Ka}{2}\right)\right] = 4C\sin^2\left(\frac{Ka}{2}\right) \tag{16}$$

Dividing by M:

$$\omega^2 = \frac{4C}{M}\sin^2\left(\frac{Ka}{2}\right) \tag{17}$$

Taking the positive square root ($\omega \geq 0$) yields the explicit **Dispersion Relation**:

$$\omega(K) = 2\sqrt{\frac{C}{M}}\left|\sin\left(\frac{Ka}{2}\right)\right| \tag{18}$$

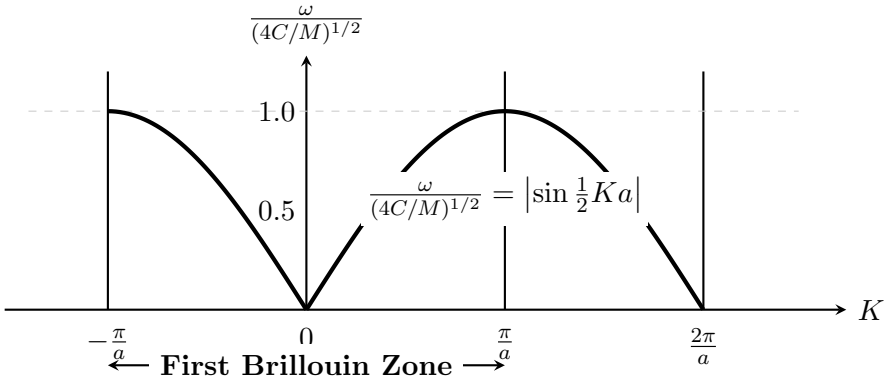


Figure 2: Phonon dispersion relation $\omega(K)$ for a 1D monatomic lattice. The region $-\pi/a < K \leq \pi/a$ defines the First Brillouin Zone.

2 First Brillouin Zone & Boundary Physics

2.1 Wavevector Redundancy

The displacement ratio between adjacent planes is:

$$\frac{u_{s+1}}{u_s} = \frac{u\, e^{i(s+1)Ka}}{u\, e^{isKa}} = e^{iKa} \tag{19}$$

If K is shifted by an integer multiple of a reciprocal lattice vector $G = \frac{2\pi n}{a}$ ($n \in \mathbb{Z}$):

$$\frac{u_{s+1}}{u_s} = e^{i\left(K+\frac{2\pi n}{a}\right)a} = e^{iKa+i2\pi n} = e^{iKa} \cdot e^{i2\pi n} = e^{iKa} \cdot 1 = e^{iKa} \tag{20}$$

Because wavevectors differing by $\frac{2\pi n}{a}$ describe identical atomic motions, all physically independent wavevectors lie inside the **First Brillouin Zone (FBZ)**:

$$-\frac{\pi}{a} < K \leq \frac{\pi}{a} \tag{21}$$

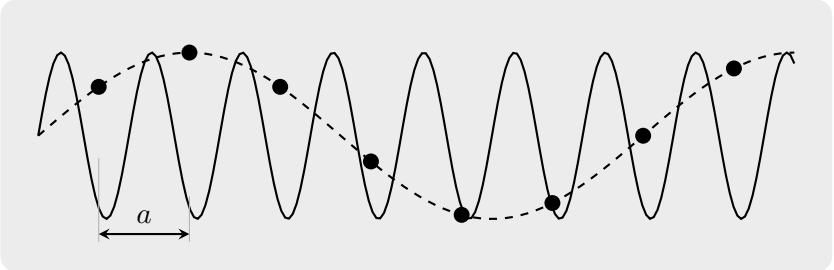


Figure 3: Illustration of wavevector aliasing: the solid high-frequency curve ($\lambda < 2a$) passes through the exact same atomic positions as the dashed curve ($\lambda > 2a$). Only wavelengths $\lambda \geq 2a$ within the First Brillouin Zone represent distinct physical motions.

2.2 Physics at the Zone Boundaries ($K = \pm\pi/a$)

At the zone edge $K = \frac{\pi}{a}$:

$$u_s = u\, e^{is\pi} = u(-1)^s \tag{22}$$

The ratio of displacements of adjacent planes becomes:

$$\frac{u_{s+1}}{u_s} = \frac{u(-1)^{s+1}}{u(-1)^s} = -1 \tag{23}$$

Key physical consequences:

1. **Opposing Phase Oscillations:** Adjacent atomic planes move strictly 180° out of phase ($u_{s+1} = -u_s$).
2. **Maximum Frequency:** At $K = \pm\pi/a$, $|\sin(\pi/2)| = 1$, giving $\omega_{\max} = 2\sqrt{\frac{C}{M}}$.
3. **Standing Waves:** Wavelength $\lambda = \frac{2\pi}{K} = 2a$ satisfies the Bragg condition $2a = \lambda$, creating a standing wave that does not propagate.

3 Group Velocity & Continuum Limit

Group velocity v_g measures the velocity of wave packet propagation and energy transmission:

$$v_g = \frac{d\omega}{dK} \tag{24}$$

Differentiating $\omega(K) = 2\sqrt{\frac{C}{M}}\sin\left(\frac{Ka}{2}\right)$ for $0 \le Ka \le \pi$:

$$v_g = \frac{d}{dK}\left[2\sqrt{\frac{C}{M}}\sin\left(\frac{Ka}{2}\right)\right] \tag{25}$$

$$= 2\sqrt{\frac{C}{M}}\cdot\cos\left(\frac{Ka}{2}\right)\cdot\frac{d}{dK}\left(\frac{Ka}{2}\right) \tag{26}$$

$$= 2\sqrt{\frac{C}{M}}\cdot\frac{a}{2}\cos\left(\frac{Ka}{2}\right) \tag{27}$$

$$v_g(K) = a\sqrt{\frac{C}{M}}\cos\left(\frac{Ka}{2}\right) \tag{28}$$

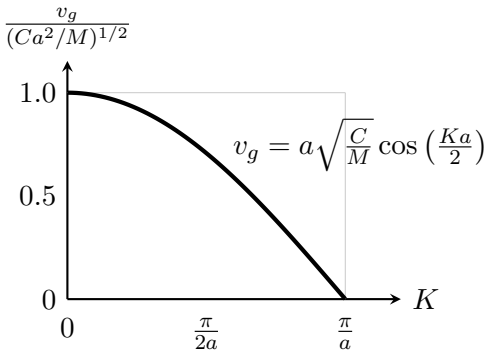


Figure 4: Group velocity v_g as a function of wavevector K. Note that $v_g = 0$ at the zone boundary $K = \pi/a$, confirming standing wave formation.

3.1 Behavior at Zone Edge

Evaluating at $K = \frac{\pi}{a}$:

$$v_g\left(\frac{\pi}{a}\right) = a\sqrt{\frac{C}{M}}\cos\left(\frac{\pi}{2}\right) = 0 \tag{29}$$

Zero group velocity at the zone edge confirms zero net energy transport for standing waves.

3.2 Long-Wavelength (Continuum) Limit ($Ka \ll 1$)

For long wavelengths ($\lambda \gg a \implies Ka \ll 1$), apply Taylor expansion $\sin x \approx x$:

$$\omega(K) \approx 2\sqrt{\frac{C}{M}}\left(\frac{Ka}{2}\right) = \left(a\sqrt{\frac{C}{M}}\right)K \tag{30}$$

The phase velocity v (speed of sound) is:

$$v = \frac{\omega}{K} = a\sqrt{\frac{C}{M}} \tag{31}$$

In this limit, sound speed is independent of frequency, matching continuum elasticity theory.

4 Extension to p-th Nearest Neighbors & Force Constant Extraction

When plane interactions extend beyond nearest neighbors to p-th neighbors with force constants C_p:

$$M\frac{d^2u_s}{dt^2} = \sum_{p>0} C_p(u_{s+p} + u_{s-p} - 2u_s) \tag{32}$$

Substituting $u_s = u\, e^{i(sKa-\omega t)}$ gives:

$$-M\omega^2 = \sum_{p>0} C_p \left(e^{ipKa} + e^{-ipKa} - 2\right) = \sum_{p>0} C_p \left(2\cos(pKa) - 2\right) \tag{33}$$

$$\omega^2(K) = \frac{2}{M} \sum_{p>0} C_p \left(1 - \cos(pKa)\right) \tag{34}$$

4.1 Orthogonality Proof to Extract C_p

Multiply both sides by $\cos(rKa)$ ($r \in \mathbb{Z}^+$) and integrate over the First Brillouin Zone $K \in [-\pi/a, \pi/a]$:

$$\int_{-\pi/a}^{\pi/a} \omega^2(K) \cos(rKa)\, dK = \frac{2}{M} \sum_{p>0} C_p \int_{-\pi/a}^{\pi/a} (1 - \cos(pKa)) \cos(rKa)\, dK \tag{35}$$

Splitting the integral on the right-hand side:

$$\int_{-\pi/a}^{\pi/a} (1 - \cos(pKa)) \cos(rKa)\, dK = \underbrace{\int_{-\pi/a}^{\pi/a} \cos(rKa)\, dK}_{=0 \text{ for } r>0} - \int_{-\pi/a}^{\pi/a} \cos(pKa) \cos(rKa)\, dK \tag{36}$$

By cosine orthogonality:

$$\int_{-\pi/a}^{\pi/a} \cos(pKa) \cos(rKa)\, dK = \frac{\pi}{a} \delta_{p,r} \tag{37}$$

Thus, the sum collapses to a single non-zero term when $p = r$:

$$\int_{-\pi/a}^{\pi/a} \omega^2(K) \cos(rKa)\, dK = \frac{2}{M} C_r \left(-\frac{\pi}{a}\right) = -\frac{2\pi C_r}{Ma} \tag{38}$$

Rearranging for the force constant C_p:

$$C_p = -\frac{Ma}{2\pi} \int_{-\pi/a}^{\pi/a} \omega^2(K) \cos(pKa)\, dK \tag{39}$$

This formula allows interplanar force constants C_p at range pa to be directly extracted from experimentally measured phonon dispersion curves $\omega(K)$.

5 Branch count and physical origin of modes

For a crystal lattice with p atoms per primitive unit cell in d spatial dimensions, the total number of dispersion branches is $d \times p$:

- **1D Monatomic Chain ($p = 1, d = 1$):** Contains only **1 acoustic branch** per polarization mode. The number of optical branches is $p - 1 = 0$.
- **3D Monatomic Crystal ($p = 1, d = 3$):** Contains **3 acoustic branches** (1 LA + 2 TA). The number of optical branches is $3p - 3 = 3(1) - 3 = 0$.
- **Diatomic or Polyatomic Lattices ($p \geq 2$):** Possess 3 acoustic branches and $3p - 3$ optical branches.

5.1 Distinction between Acoustic and Optical branches

The names *Acoustic* and *Optical* originate from how atoms move relative to one another at long wavelengths ($K \to 0$) and how those vibrations interact with sound waves versus light. Optical modes require out-of-phase oscillation between at least two distinct atoms within the same primitive unit cell. Since a monatomic lattice has no internal basis degrees of freedom, optical phonon branches cannot exist.

5.1.1 Acoustic Branches

In an acoustic branch, adjacent atoms within the primitive unit cell oscillate **in phase** at long wavelengths ($K \to 0$).

- **Frequency limit:** $\omega \to 0$ as $K \to 0$.
- **Physical picture:** Near $K = 0$, the dispersion relation is linear ($\omega = vK$). This describes elastic sound waves propagating through the crystal continuum at sound speed v, giving rise to the name *acoustic phonons*.

5.1.2 Optical Branches

In an optical branch, adjacent atoms within the primitive unit cell move **out of phase** (180° relative to one another).

- **Frequency limit:** $\omega(0) > 0$ (remains finite at the zone center).
- **Physical picture:** In polar or ionic crystals (e.g., NaCl, KBr), out-of-phase displacement of oppositely charged ions produces an oscillating electric dipole moment. This dipole moment couples directly with the electric field of incoming *infrared light*, allowing direct optical absorption/excitation. Hence, these modes are named *optical phonons*.

Table 1: Comparison of Acoustic and Optical Branches

Feature	**Acoustic Branch**	**Optical Branch**
Relative Motion ($K \to 0$)	In phase (together)	Out of phase (opposing)
Frequency at $K = 0$	$\omega = 0$	$\omega(0) > 0$
Physical Behavior	Elastic sound wave	Inter-atomic relative vibration
Light Coupling	Weak / Indirect	Strong IR absorption/reflection

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.