Chapter 4

Phonons I: Crystal Vibrations

PHYS 432

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- **VIBRATIONS OF CRYSTALS WITH MONATOMIC BASIS**
  - **First Brillouin zone**
  - **Group velocity and Phase velocity**
  - **Long wavelength limit**
  - **Derivation of force constants from experiment**

- **TWO ATOMS PER PRIMITIVE BASIS**

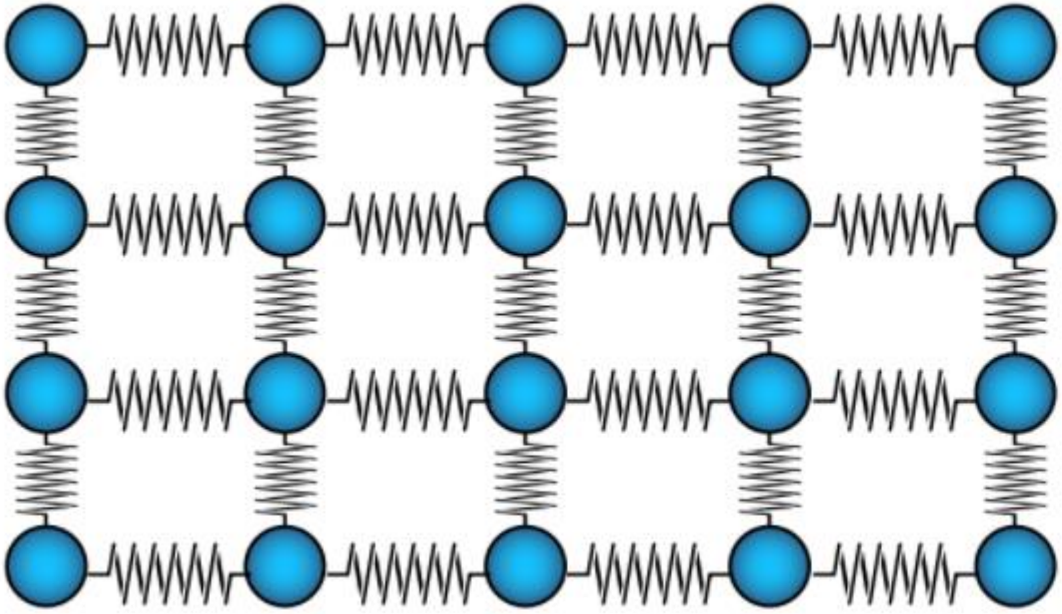
- **QUANTIZATION OF ELASTIC WAVES**

- **PHONON MOMENTUM**

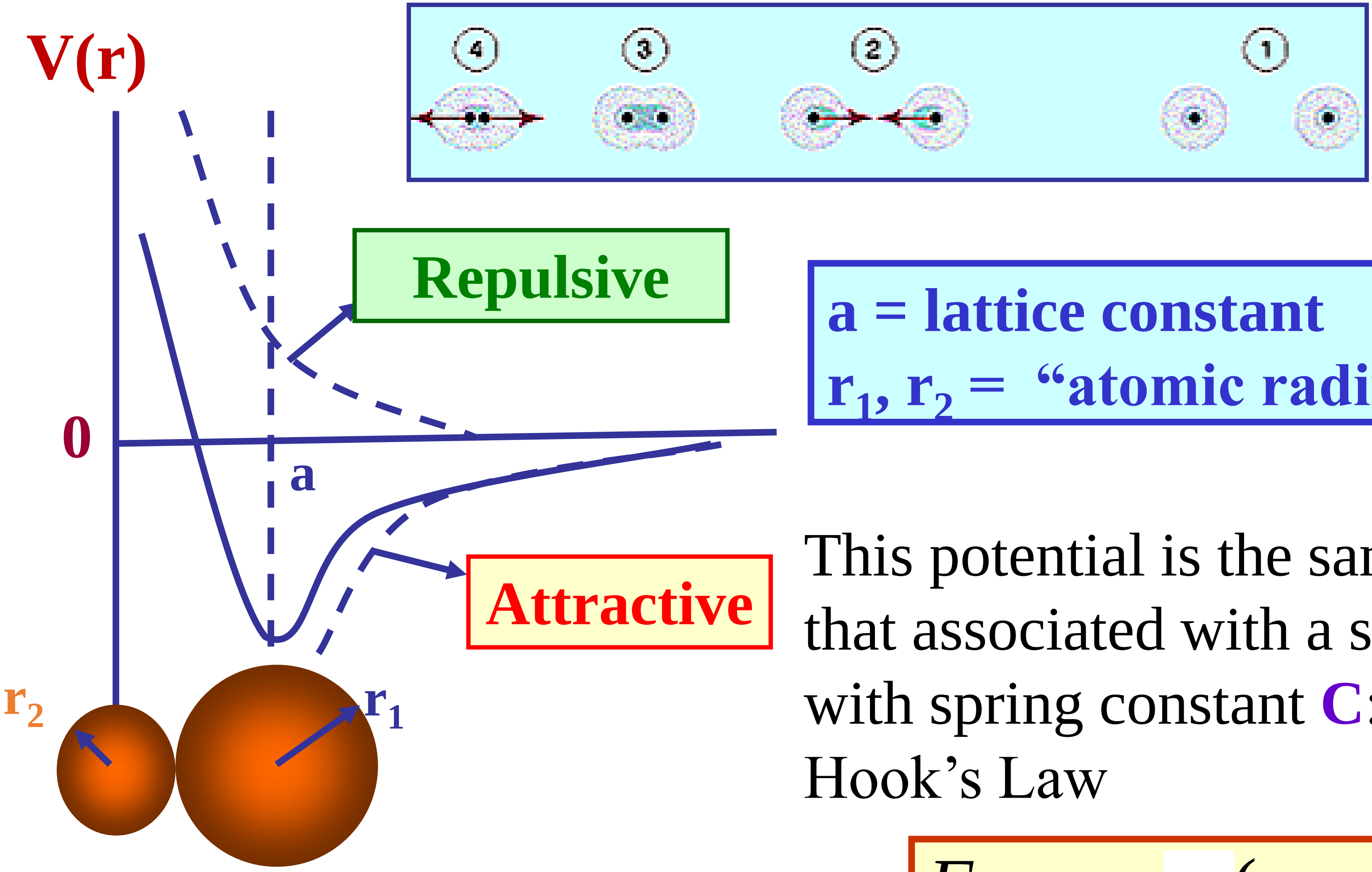
- **INELASTIC SCATTERING BY PHONONS**

VIBRATIONS OF CRYSTALS

- Consider the bonds between any two atoms are like springs with spring constants C’s.



- Consider a ***typical interatomic potential*** as is illustrated in the figure:



a = lattice constant
r_1, r_2 = "atomic radii"

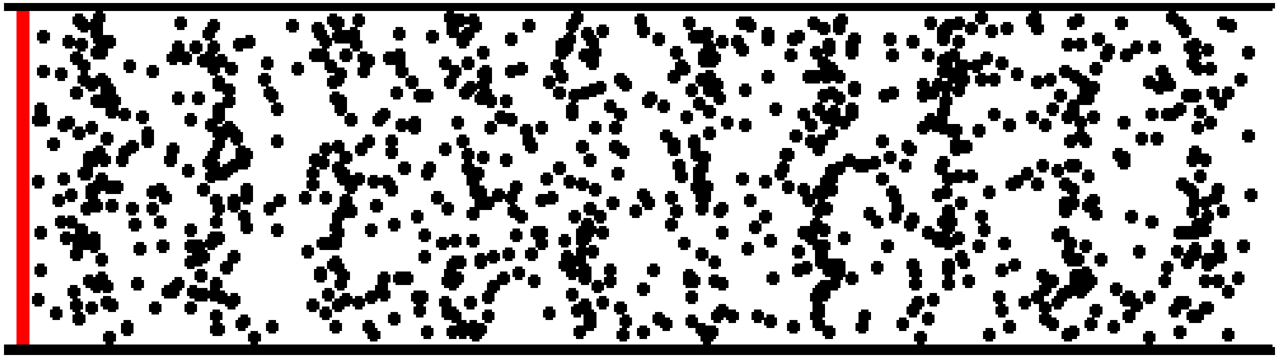
This potential is the same as that associated with a spring with spring constant **C**: Hook's Law

$$Force = c\,(r-a)$$

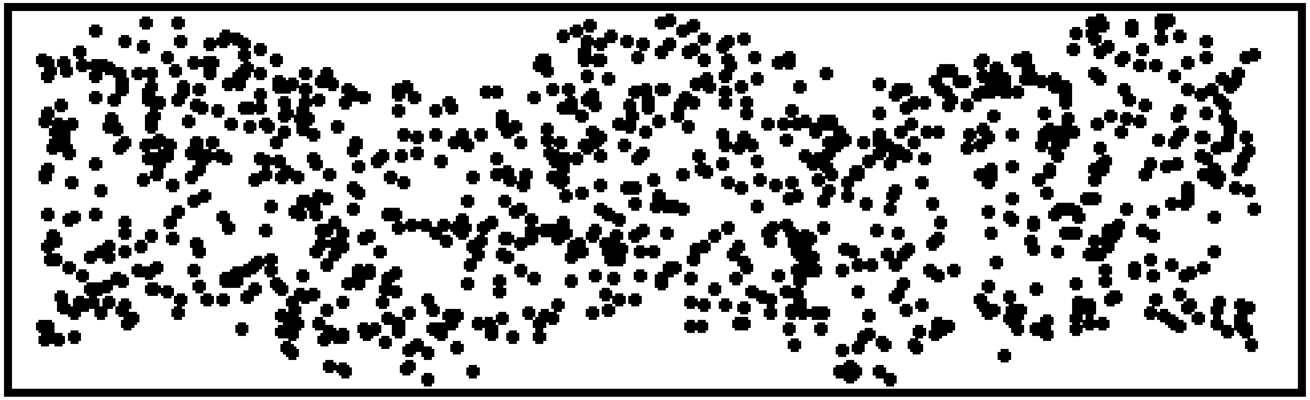
VIBRATIONS OF CRYSTALS

- We will be discussing two kinds of elastic waves: Longitudinal and transverse waves

Longitudinal Waves



Transverse Waves



Phonons

- A phonon is the quantum mechanical description of an elementary vibrational motion in which a lattice of atoms or molecules uniformly oscillates at a single frequency (normal mode).

- The name *phonon* comes from the Greek word *φωνή* (phonē), which translates as *sound* or *voice* because long-wavelength phonons give rise to sound.

- The energy of each mode is quantized, the unit of quantum energy is $\hbar\omega$. Since the modes are elastic waves, we have, in fact, quantized the elastic energy of sound waves.

- The procedure is closely analogous to that used in quantizing the energy of an electromagnetic field, in which the corpuscular nature of the field is expressed by introducing the photon.

- In the present case, the particle-like entity which carries the unit energy of the elastic field in a particular mode is called a phonon. The energy of the phonon is therefore given by $\epsilon = \hbar\omega$.

Comparison of Phonons & Photons

PHONONS

- Quantized normal modes of lattice vibrations. The energies & momenta of phonons are quantized

$$E_{phonon} = \frac{h v_s}{\lambda}$$

$$p_{phonon} = \frac{h}{\lambda}$$

Phonon Wavelength:

$\lambda_{phonon} \approx a \approx 10^{-10}$ m

PHOTONS

- Quantized normal modes of electromagnetic waves. The energies & momenta of photons are quantized

$$E_{photon} = \frac{hc}{\lambda}$$

$$p_{photon} = \frac{h}{\lambda}$$

(visible) **Photon Wavelength:**

$\lambda_{photon} \approx 10^{-6}$ m >> a

Conservation of Phonons

- Since the energy per phonon is equal to $\epsilon = \hbar\omega$, and at a given temperature T in an elastic mode of oscillation the average number of phonons in the mode is given by Planck distribution function.

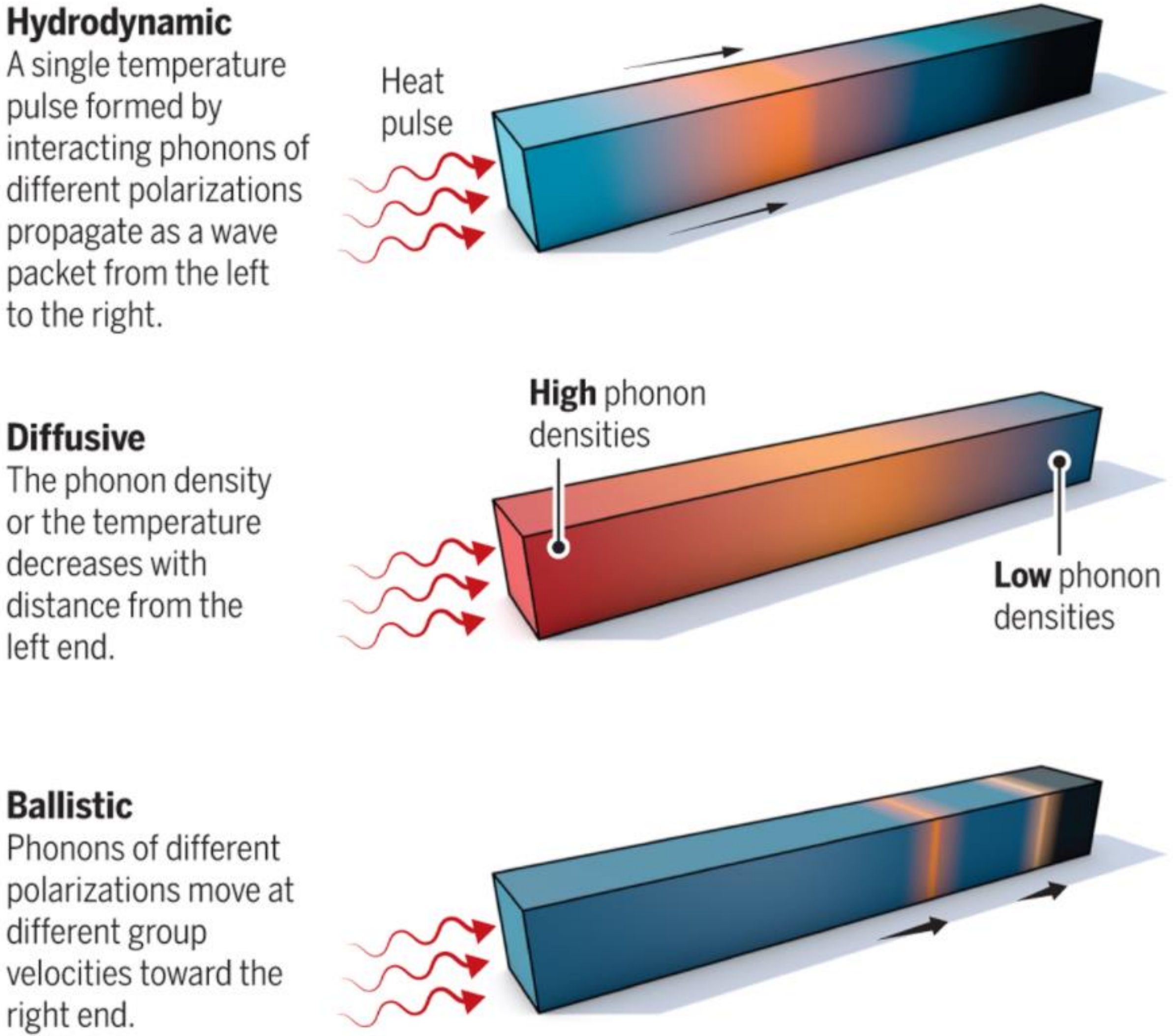
$$\bar{n} = \frac{1}{e^{\hbar\omega/kT} - 1}$$

- This number depends on the temperature; at $T = 0$, $\bar{n} = 0$, but as T increases, $\bar{n}$ also increases, eventually reaching the value $\bar{n} \simeq kT/\hbar\omega$ at high temperatures.

- Here we see an interesting point: Phonons are created simply by raising the temperature, and therefore their number in the system is not conserved.

Phonons

- Phonons propagate heat energy and transmit sound in solids.
- The low-frequency vibrations correspond to sound, while higher frequencies correspond to heat.



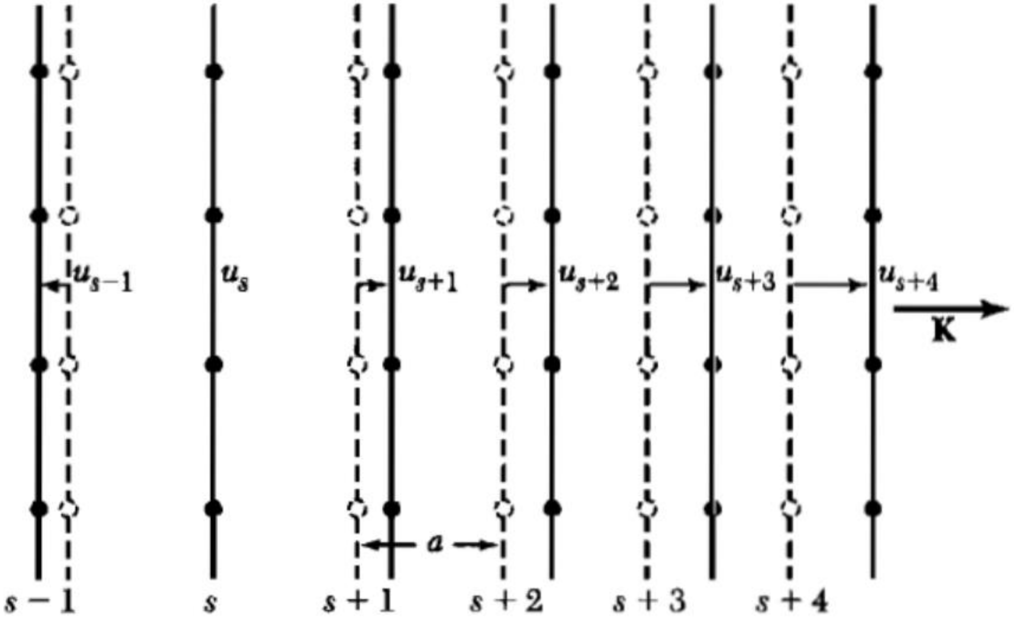
Hydrodynamic
A single temperature pulse formed by interacting phonons of different polarizations propagate as a wave packet from the left to the right.

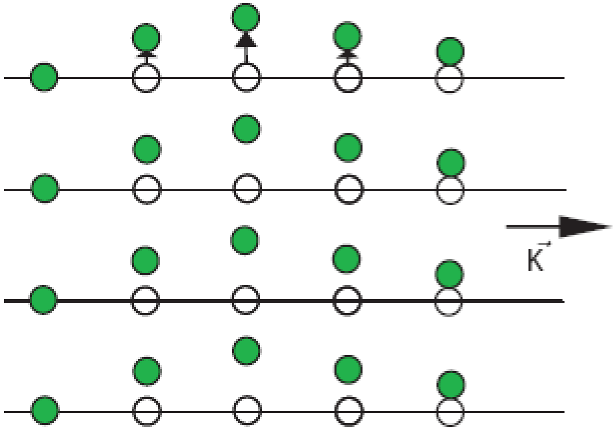
Diffusive
The phonon density or the temperature decreases with distance from the left end.

Ballistic
Phonons of different polarizations move at different group velocities toward the right end.

https://www.science.org/doi/10.1126/science.aax2319

Longitudinal and transverse waves

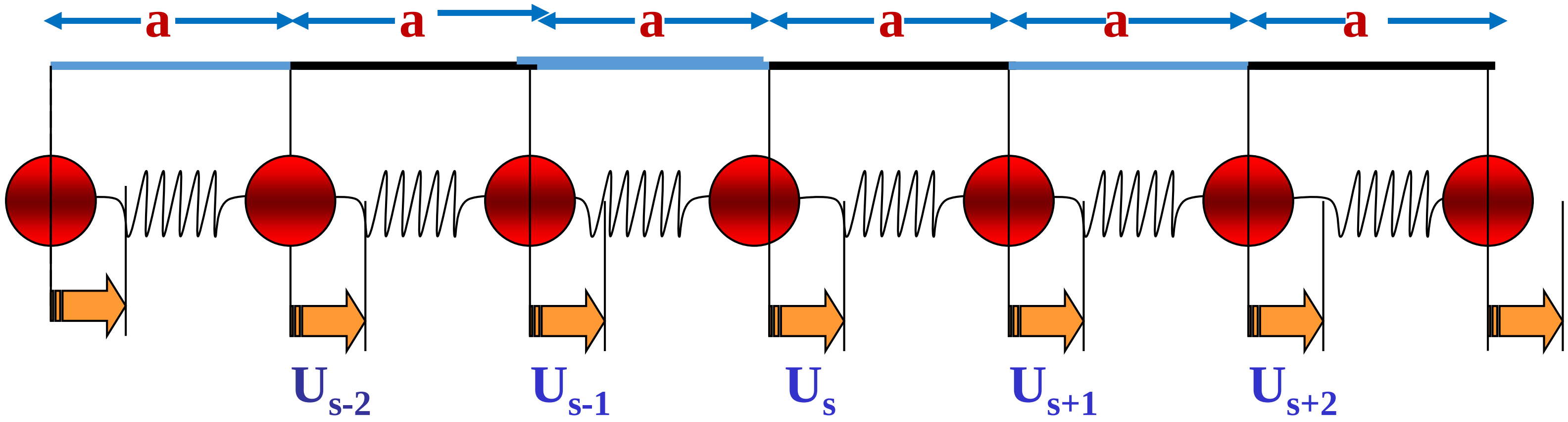




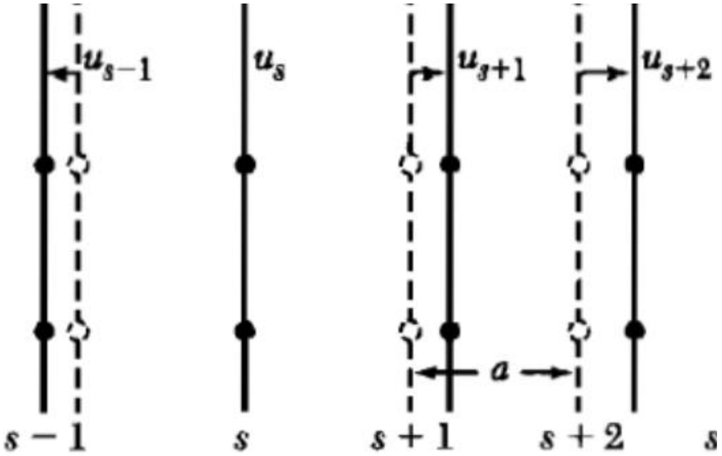
One Dimensional Model # 1:

The Monatomic Chain

- This is the simplest possible solid. Assume that the chain contains a large number **($N \to \infty$)** of atoms with identical masses **m**. Let the lattice constant is **a**.
- Assume that the atoms move only in a direction parallel to the chain. Assume that only nearest-neighbors interact with each other (the forces are short-ranged).



Longitudinal and transverse waves



For small elastic deformations, the restoring forces are linear and given by Hook's law:

$$\vec{F} = -C\vec{x}$$

where C is the spring constant and *x* is the displacement. Here the vector ***x*** is the difference of the displacements.

The two forces from the nearest neighbor planes s+1 and s-1 acting on the central plan s are

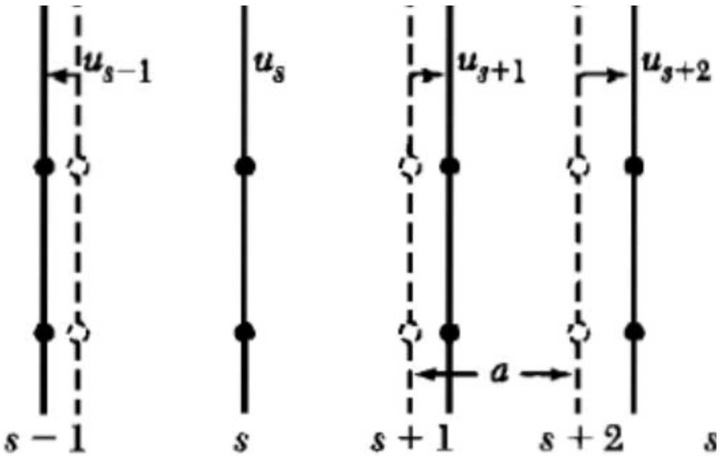
$$F_r = -C(u_{s+1} - u_s)$$

$$F_l = -C(u_s - u_{s-1}).$$

Longitudinal and transverse waves

$$F_s = F_l - F_r$$

$$\vec{F}_s = C(u_{s+1} - u_s) + C(u_{s-1} - u_s)$$



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 planes.

The equation of motion of an atom of mass M in the plane s is.

$$M\frac{d^2U_s}{dt^2} = C[u_{s+1} + u_{s-1} - 2u_s]$$

Assume all displacements have the same frequency of dependence (normal modes) $\exp(-i\omega t)$, then the equation of motion has solutions of the following form.

$$u_{s\pm1} = u\exp[i(K(s\pm1)a - \omega t)]$$

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

$$-M\omega^2 u e^{i(Ksa-\omega t)} = C\left[u e^{i(K(s+1)a-\omega t)} + u e^{i(K(s-1)a-\omega t)} - 2u e^{i(Ksa-\omega t)}\right]$$

$$-M\omega^2 = C\left[e^{iKa} + e^{-iKa} - 2\right]$$

We can use the identity $2cos(Ka) = e^{iKa} + e^{-iKa}$, we can have the dispersion relation ω(*K*)

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

As the boundary of the first Brillouin zone lies at *K* = ±π/*a*, so we can show that slope of ω versus *K* is zero at the zone boundary:

$$\frac{d\omega^2}{dK} = \frac{2Ca}{M}\sin Ka = 0$$

Longitudinal and transverse waves

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

We can write the above equation by using trigonometric identity:

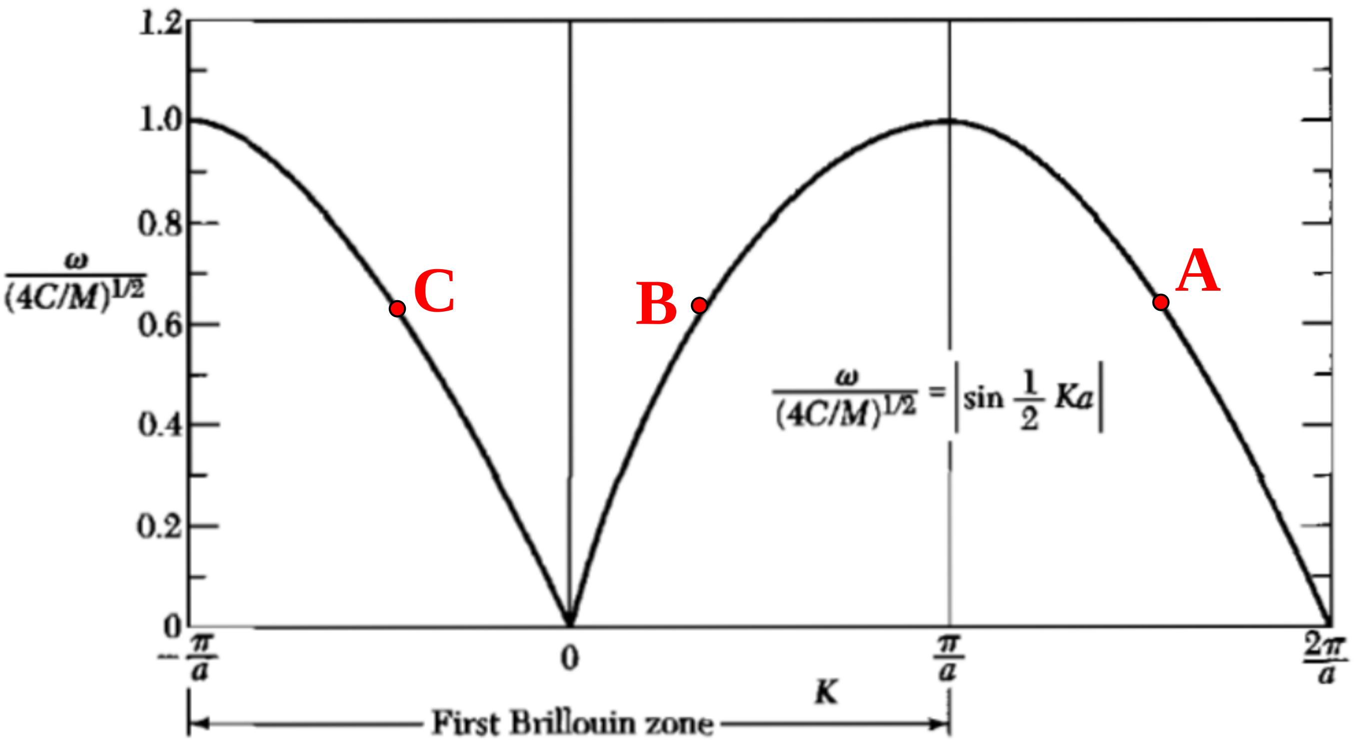
$$\omega^2 = \frac{4C}{M}\sin^2\left(\frac{Ka}{2}\right)$$

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

This is the solution to the normal mode eigenvalue problem for the monatomic chain.

This is the ***dispersion relation*** for an elastic wave of wave vector K and of frequency ω.

“***Phonon Dispersion Relations***” or ***Normal Mode Frequencies*** or **ω** versus **K** relation for the monatomic chain.



- Because of **BZ** periodicity with a period of **2π/a**, **only the first BZ** is needed. Points **A, B** & **C** correspond to the same frequency. They all have the same instantaneous atomic displacements.

- What is the ***physical significance*** of these results?

- For the monatomic chain, the only allowed vibrational frequencies **ω** must be related to the wavenumber **K = (2π/λ)** or the wavelength **λ** by the following equation.

$$\omega = \sqrt{\frac{4C}{M}}\sin(\tfrac{Ka}{2})$$

- This result is often called the ***"Phonon Dispersion Relation"*** for the chain.

- We started from the Newton's 2nd law equations of motion for N *COUPLED harmonic oscillators*. If one atom starts vibration, it does not continue with constant amplitude, but transfers energy to the others in a complicated way. That is, the vibrations of individual atoms are not simple harmonic because of this exchange of energy among them.

- On the other hand, our solutions represent the oscillations of N *UNCOUPLED simple harmonic* oscillators i.e. the dispersion relation is for a single atom.

$$\omega = \sqrt{\frac{4C}{M}}\sin(\tfrac{Ka}{2})$$

- A normal mode of an oscillating system is the motion in which all parts of the system move sinusoidally with the same frequency and with a fixed phase relation.

- These vibrations are called the *Normal Modes* of the system. They are due to the *collective property of the system* and not a property of any of the individual atoms. Each mode represented by ω(k) *oscillates independently of the other modes*. Also, it can be shown that the *number of modes is the same as the original number of equations N*. Proof of this is given in the following topic.

- **First Brillouin Zone**
- **Group velocity and phase velocity**
- **Long wavelength limit of the monoatomic phonon dispersion relation.**
- **Derivation of force constants from experiment**
- **Two atoms per primitive basis**

First Brillouin Zone

- What range of K are physically significant? **Only those in the first Brillouin zone.**

- Since planes are oscillating with $u_s = ue^{i(Ksa-\omega t)}$, the ratio of the displacements of two successive planes is given by

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

- The range -π to +π for the phase *Ka* covers all the independent values of the exponential.

- If $Ka = \pm\pi$, the $\frac{u_{s+1}}{u_s} = -1$, it means that the two planes are oscillating completely out of phase.

- If $K = 0$, the $\frac{u_{s+1}}{u_s} = 1$, it means that the two planes are oscillating in phase.

- Thus all possible oscillations are covered in the range of $-\pi \leq Ka \leq +\pi$.

First Brillouin Zone

- This range is the first Brillouine zone of the linear lattice. The value of K outside of the first Brillouin zone merely reproduce lattice motions described by the values within the limits $\pm\pi/a$.

- If we suppose K lies outside of the first Brillouin zone, but a related wavevector K' defined as $K' = K - 2\pi n/a$ lies within the first zone where n is an integer.

$$u_s = ue^{iK'a} = ue^{iKa}e^{i2\pi n} = ue^{iKa}$$

First Brillouin Zone

At the boundaries, $K_{max} = \pm\pi/a$ of the Brillouin zone, the solution

$$\boxed{u_s = ue^{i(Ksa)}}$$

doesn’t represent a travelling wave, but a standing wave (See the group velocity).

At the zone boundaries [$sK_{max}\, a = \pm\, s\pi$], so

$$\boxed{u_s = ue^{i(\pm s\pi)} = u(-1)^s}$$

This is a standing wave; alternate atoms oscillate in the opposite phases because $u_s = \pm 1$ according to whether s is even or odd.

The wave moves neither to the right nor to the left.

First Brillouin Zone

- The value of K outside of the first Brillouin zone merely reproduce lattice motions described by the values within the limits $\pm\pi/a$.

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

- At the zone boundary: $K = \pm\pi/a$, it satisfies $2d\sin\theta = n\lambda$, $\theta = \pi/2$, $d = a$, $K = 2\pi/\lambda$, $n = 1$ so that $\lambda = 2a$.

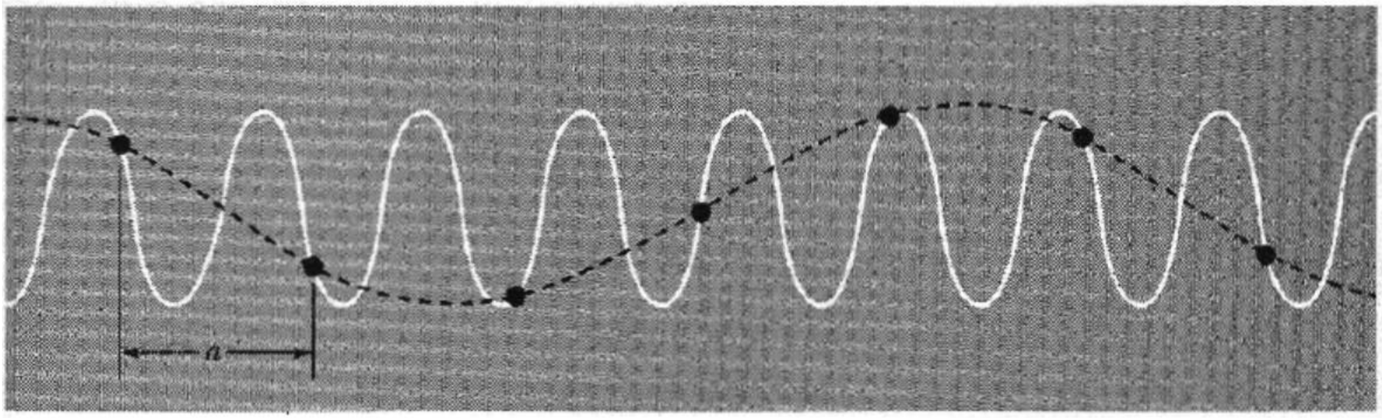


Figure 5 The wave represented by the solid curve conveys no information not given by the dashed curve. Only wavelengths longer than $2a$ are needed to represent the motion.

First Brillouin Zone

- The number of allowed K values in a single branch is just N for one Brillouin zone. (It comes from the fact that if a crystal has volume V that there is one K value in the volume $[(2\pi)^3/V]$ in reciprocal space. The volume of a Brillouin zone is $[(2\pi)^3/V_C]$, where V_C is the volume of a primitive cell. Thus the number of allowed K values in a Brillouin zone is V/V_C, which is just N, the number of primitive cells in the crystal.)

Long wavelength Limit

Consider long wavelength such as $\lambda \to \infty$, it implies that K goes to zero, which means that “crystal" looks like a continuous medium to the wave.

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

When Ka << 1, using Taylor series we expand $\sin(Ka/2) \equiv Ka/2 - (Ka/2)^3/3! + \dots$, so the dispersion relation would become:

$$\omega^2 = \left(C/M\right)K^2a^2 \qquad \frac{\omega}{K} = \sqrt{\frac{C}{M}}a$$

$$v_p = \frac{\omega}{K} = \sqrt{\frac{Ca}{M/a}} = \sqrt{\frac{F}{M/a}} = \sqrt{\frac{Force}{linear\ mass\ density}}$$

velocity of sound in a medium

Here frequency is proportional to the wave vector, which means the velocity of sound is independent of frequency.

Group Velocity and Phase Velocity

- For arbitrary dispersion relations, phase velocity (v_p) and group velocity (v_g) are given by

$$v_p = \frac{\omega}{K}, \qquad v_g = \frac{d\omega}{dK}.$$

- The physical distinction between these velocities is that v_p is the velocity of propagation for a pure wave of an exactly specified frequency ω and a wavevector K.

- The v_g, describes the velocity of a wave pulse whose average frequency and wavevector are specified by ω and K.

- Since energy and momentum are transmitted, in practice, via pulses rather than by pure waves, group velocity is physically more significant.

Group Velocity

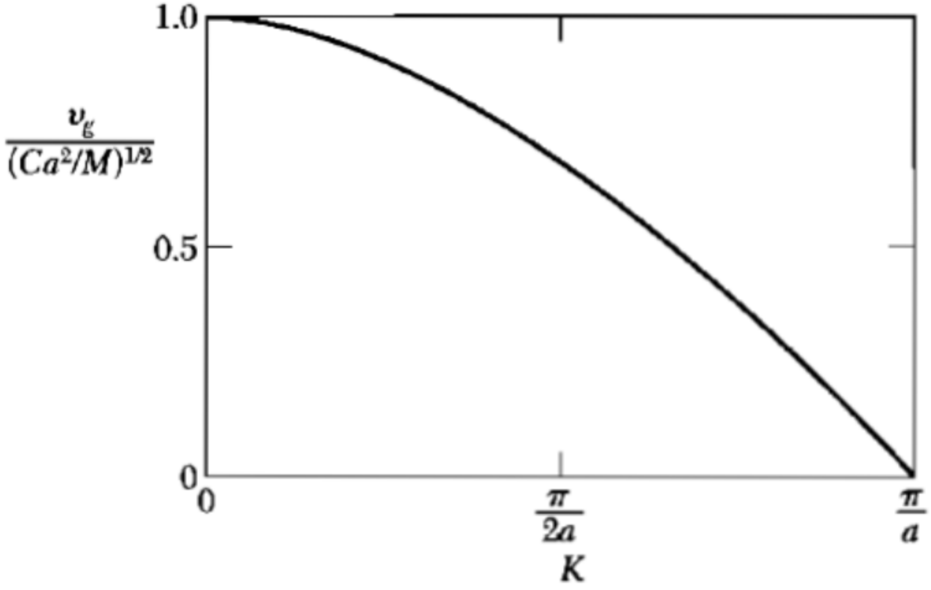
The transmission velocity of a wave packet is the group velocity, given as:

$$v_g = {d\omega}/{dK}$$

This is the velocity of energy propagation in a medium.

$$\omega = \sqrt{\frac{4C}{M}}\sin(\tfrac{Ka}{2})$$

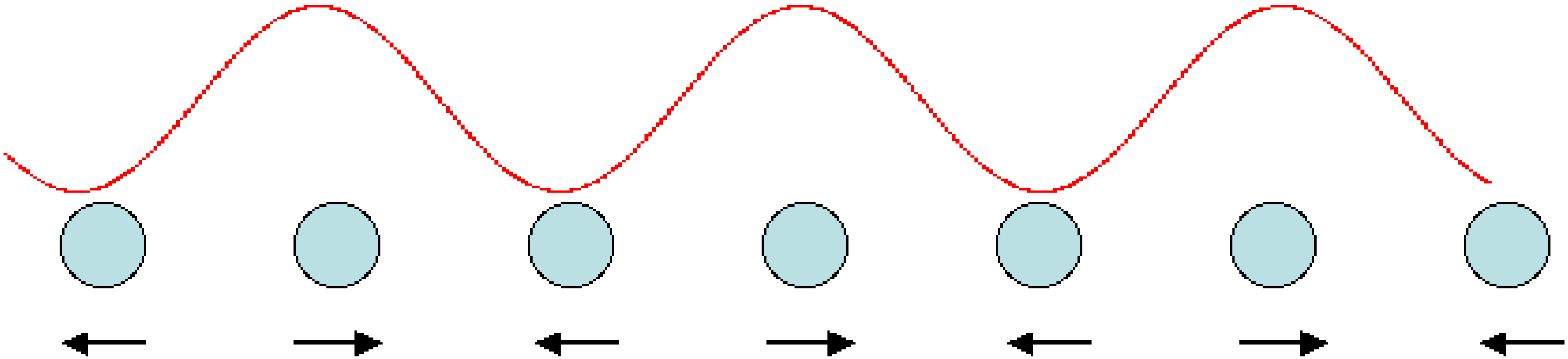
$$v_g = \frac{d\omega}{dK} = \sqrt{\frac{Ca^2}{M}}\cos(\tfrac{Ka}{2})$$

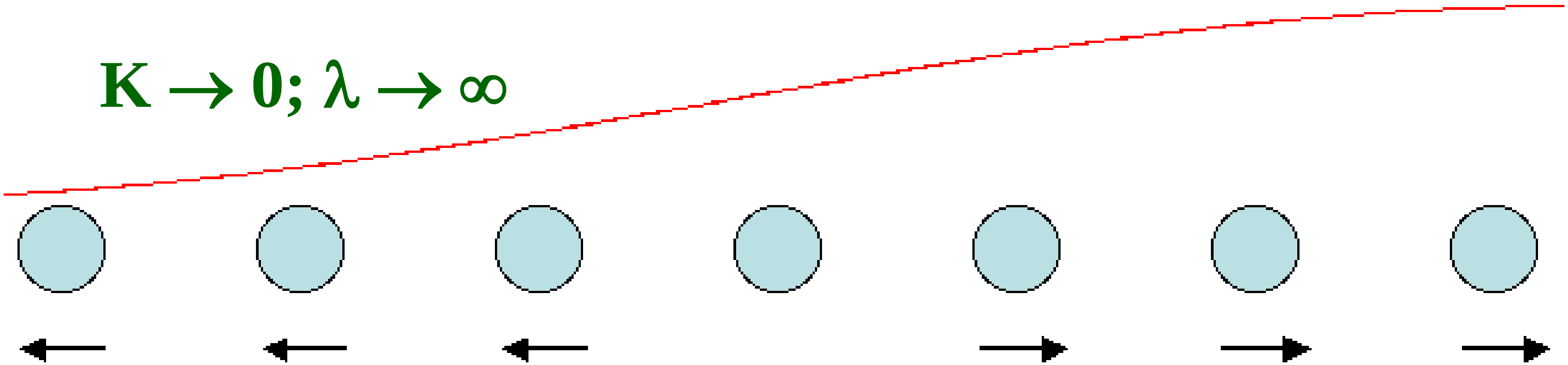


This is zero at the edge of the zone, where K = ± π/*a*.
No energy transfer – standing wave

The Monatomic Chain

$$K = (\pi/a) = (2\pi/\lambda);\ \lambda = 2a$$





$K \to 0;\ \lambda \to \infty$

Derivation of Force Constant 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 dispersion relation for ω. The generalization of the dispersion relation

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

is to *p* nearest planes is easily found to be

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

- We want to determine the value of C_p.
- Multiplying both sides by $\cos(\gamma ka)$, where γ is an integer.

$$\int_{-\pi/a}^{\pi/a} \frac{M}{2} \omega_k^2 \cos(\gamma Ka)\, dK = C_p \left\{ \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \cos(\gamma Ka)\, dK - \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \cos(\gamma Ka) \cos(pKa)\, dK \right\}$$

$$\int_{-\pi/a}^{\pi/a} \frac{M}{2} \omega_k^2 \cos(\gamma K a)\, dK = C_p \left\{ 0 - \frac{1}{2} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} [\cos((\gamma + p)Ka) - 1]\, dK \right\}$$

For $\gamma = p$, the integral vanishes

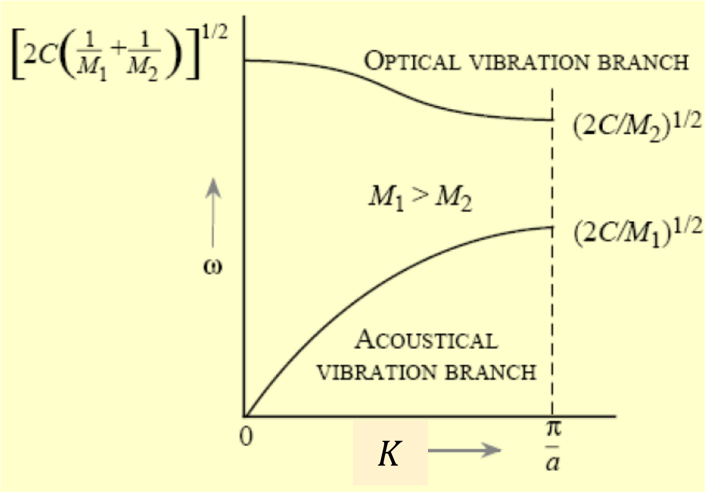
$$\int_{-\pi/a}^{\pi/a} \frac{M}{2} \omega_k^2 \cos(pKa)\, dK = C_p \left\{ 0 - 0 + \frac{1}{2} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dK \right\}$$

$$\int_{-\pi/a}^{\pi/a} \frac{M}{2} \omega_k^2 \cos(pKa)\, dK = C_p \left\{ \frac{2\pi}{2a} \right\}$$

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

Phonons in Diatomic Crystals

- The phonon dispersion relation shows new features in crystals with two or more atoms per primitive cell. For example, the NaCl or diamond have two atoms in the primitive cell.
- For each polarization mode in a given propagation direction the dispersion relation develops two branches acoustical (low frequency) and optical (high frequency).
- 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.



Optical Phonons can interact with light

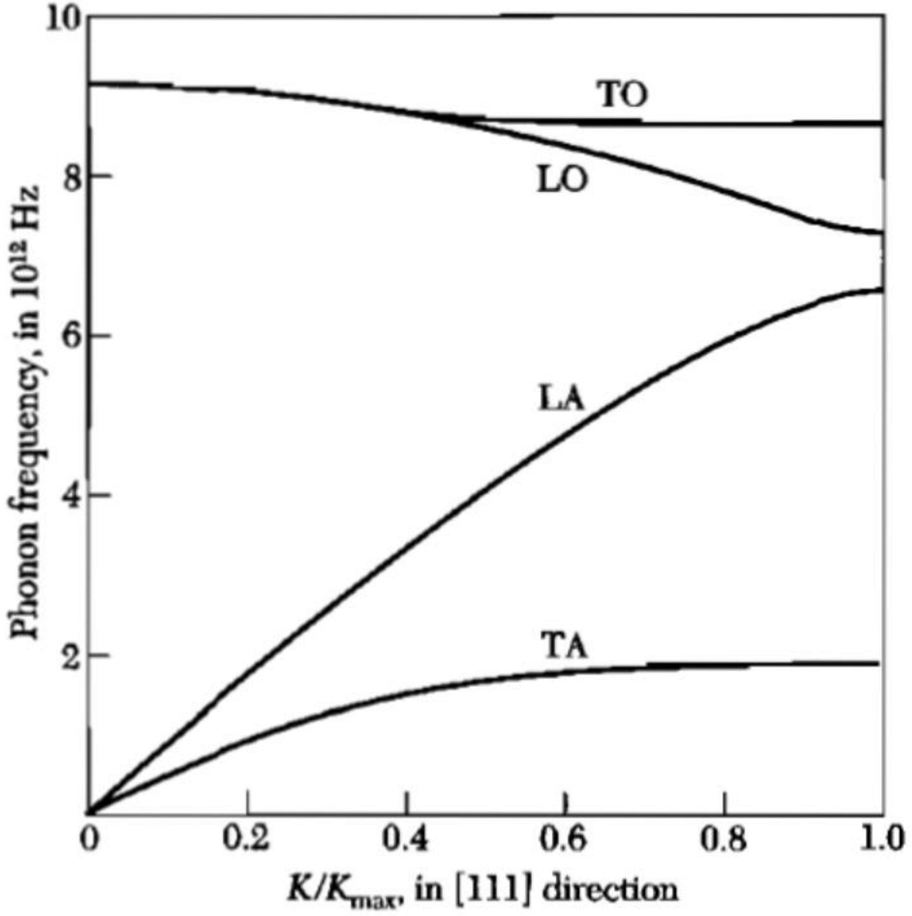
For diamond Optical phonon frequency is ≈ 1300 cm^{-1}

λ≈ 7700 nm
(far-IR)

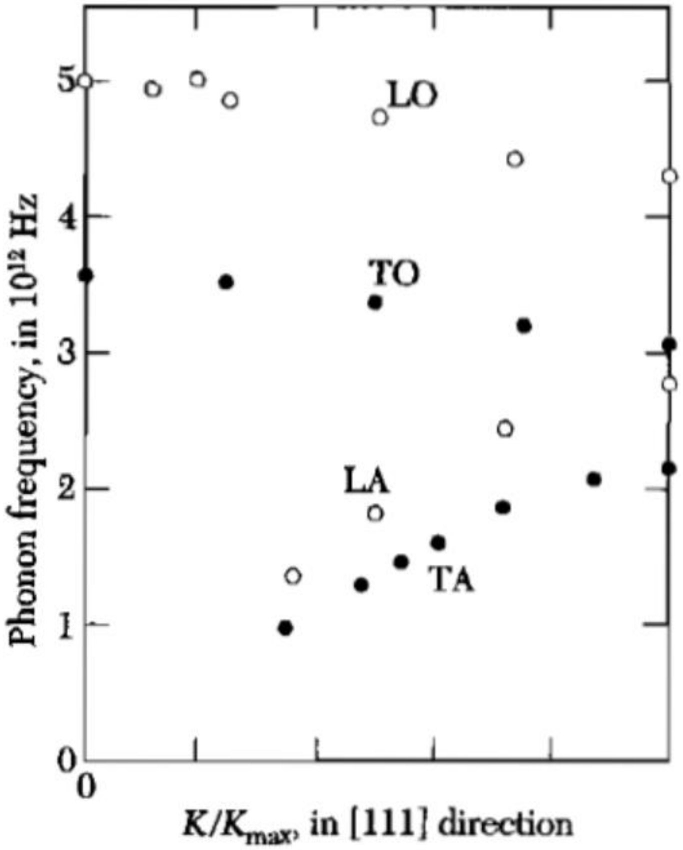
Phonons in Diatomic Crystals

- Thus Germanium and KBr each with two atoms in the primitive cell, have six branches: one LA, one LO, two TA, and two TO

Germanium: diamond crystal structure



KBr: rock salt (NaCl) crystal structure

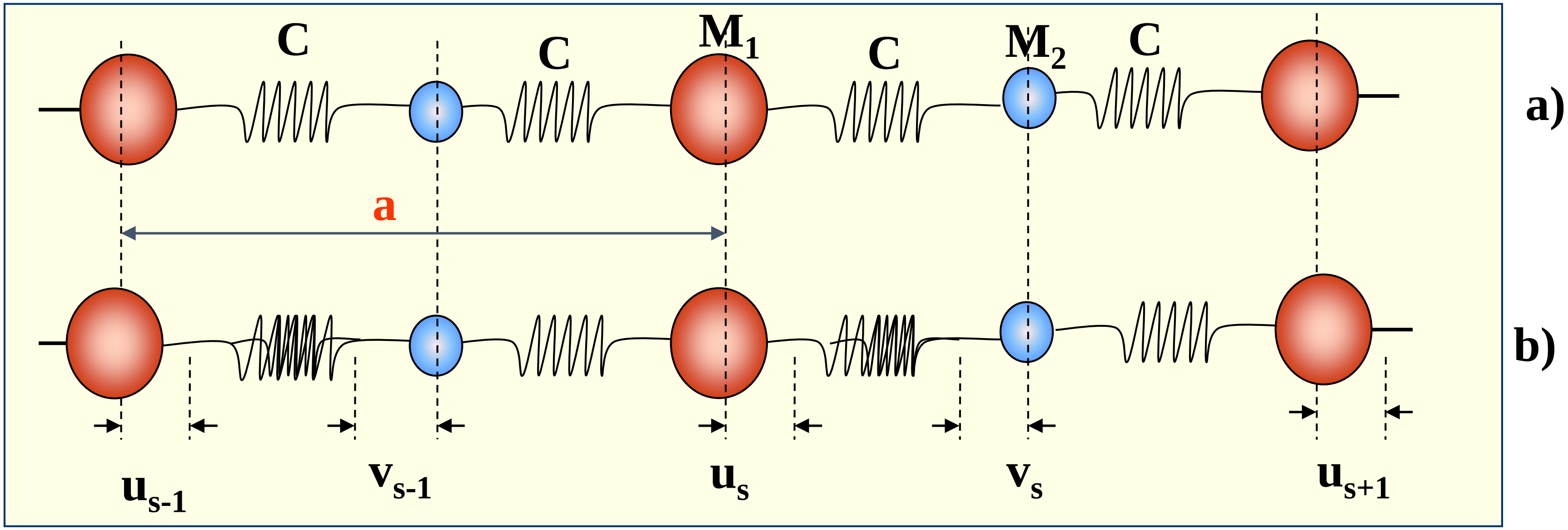


Phonons in Diatomic Crystals

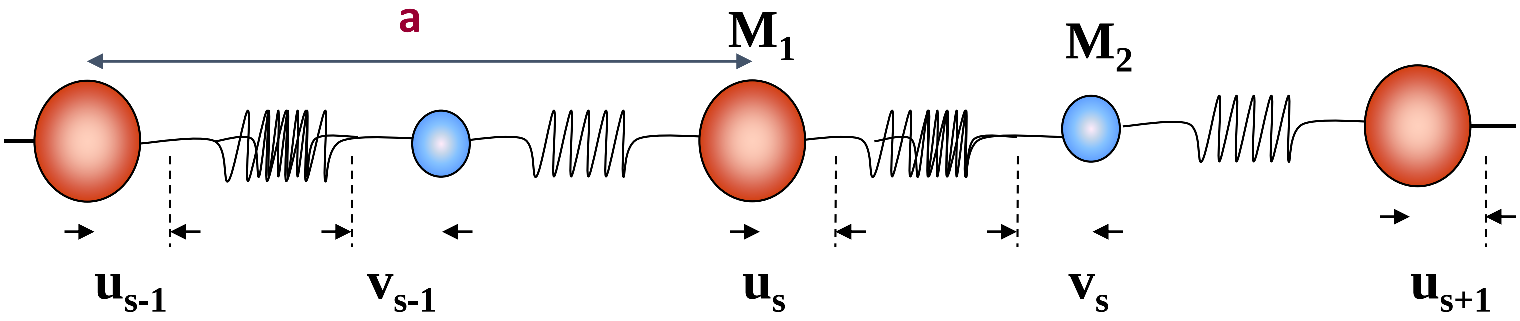
- The numerology of the branches follows from the number of degrees of freedom of the atoms.
- With p atoms in the primitive cell and N primitive cells, there are pN atoms.
- Each atom has three degrees of freedom, one for each of the x, y, z directions, making a total of 3pN degrees of freedom for the crystal.
- Thus one longitudinal acoustical (LA) and the two transverse acoustical (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 (longitudinal optical LO and transverse optical TO).

- Two atoms per primitive basis
- Dispersion Relations for Optical and Acoustical Branches
- Quantization of Elastic Waves
- Phonon Momentum

- Consider a ***Diatomic Chain*** with nearest-neighbor interaction in the form of **Hooke's Law** (**$F = -Cx$**). This is equivalent to a spring-block model with two different types of atoms of masses, **M_1** & **M_2** connected by identical springs of spring constant **C**.



- This is the simplest possible model of a diatomic crystal. **a** is the repeat distance, so, the nearest-neighbor separation is **(½)a**



- This model is complicated due to the presence of 2 different atom types, which, in general, move in opposite directions.

- The ***GOAL*** is to find the dispersion relation **ω(K)** for this model. There are 2 atom types, with masses **M_1** & **M_2**, so there will be ***2 equations of motion***, one for **M_1** & one for **M_2**.

$$M_1 \frac{d^2u_s}{dt^2} = C(v_s + v_{s-1} - 2u_s)$$ ← **Equation of Motion for M_1**

$$M_2 \frac{d^2v_s}{dt^2} = C(u_{s+1} + u_s - 2v_s)$$ ← **Equation of Motion for M_2**

Model for Diatomic Crystals

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

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

The solution can be of the form of travelling waves:

$$u_s = ue^{i(sKa - \omega t)} \qquad v_s = ve^{i(sKa - \omega t)}$$

By substituting the solution back in the above equations:

$$-\omega^2 M_1 u = Cv[1 + e^{-iKa}] - 2Cu$$

$$-\omega^2 M_2 v = Cu[1 + e^{iKa}] - 2Cv$$

By writing these equations in the determinant form:

$$\begin{vmatrix} 2C - M_1\omega^2 & -C[1+e^{iKa}] \\ -C[1+e^{iKa}] & 2C - M_2\omega^2 \end{vmatrix} = 0$$

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

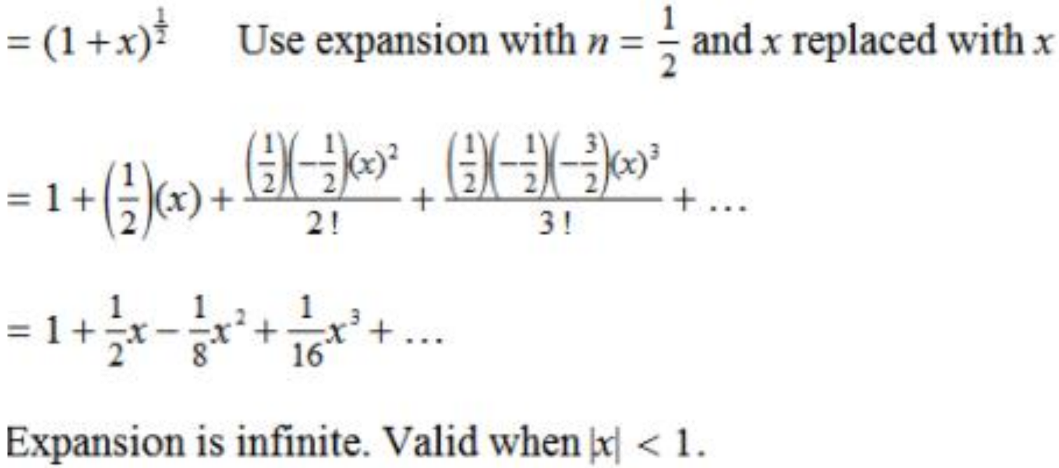
This equation is a quadratic equation and can be solved exactly for ω^2, but it is simpler to examine the two limiting cases: K*a* << 1 and K*a* = ±π.

(i) If K*a* << 1 then cos(K*a*) = 1 – ½ K^2a^2 + ….

$$M_1M_2\omega^4 - 2C(M_1 + M_2)\omega^2 + C^2K^2a^2 = 0$$

$$M_1M_2\omega^4 - 2C(M_1+M_2)\omega^2 + C^2K^2a^2 = 0$$

$$\omega^2 = \frac{2C(M_1+M_2) \pm \sqrt{4C^2(M_1+M_2)^2 - 4M_1M_2C^2K^2a^2}}{2M_1M_2}$$



$= (1+x)^{\frac{1}{2}}$ Use expansion with $n = \frac{1}{2}$ and x replaced with x

$$= 1 + \left(\frac{1}{2}\right)(x) + \frac{\left(\frac{1}{2}\right)\left(-\frac{1}{2}\right)(x)^2}{2\,!} + \frac{\left(\frac{1}{2}\right)\left(-\frac{1}{2}\right)\left(-\frac{3}{2}\right)(x)^3}{3\,!} + \ldots$$

$$= 1 + \frac{1}{2}x - \frac{1}{8}x^2 + \frac{1}{16}x^3 + \ldots$$

Expansion is infinite. Valid when $|x| < 1$.

$$\frac{M_1M_2K^2a^2}{(M_1+M_2)^2} \ll 1$$

$$\omega_+^2 \cong \frac{4C(M_1+M_2)}{2M_1M_2} = 2C\left(\frac{1}{M_1} + \frac{1}{M_2}\right)$$

Optical branch

$$\omega_-^2 \cong \frac{2C(M_1 + M_2)}{2M_1 M_2} \frac{M_1 M_2 K^2 a^2}{2(M_1 + M_2)^2} = \frac{CK^2 a^2}{2(M_1 + M_2)}$$

$$\omega_-^2 \cong \frac{\frac{C}{2} K^2 a^2}{(M_1 + M_2)}$$

Acoustical branch

- Since the chain contains **N** unit cells, there will be **2N normal modes** of vibration, because there are **2N** atoms and **2N** equations of motion for masses **M_1** & **M_2**.

Second limiting case: K*a* = ± π.

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

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

$$\omega^2 = \frac{2C(M_1 + M_2) \pm \sqrt{4C^2(M_1 + M_2)^2 - 16M_1M_2C^2}}{2M_1M_2}$$

$$\omega^2 = \frac{2C(M_1 + M_2) \pm 2C\sqrt{(M_1 + M_2)^2 - 4M_1M_2}}{2M_1M_2}$$

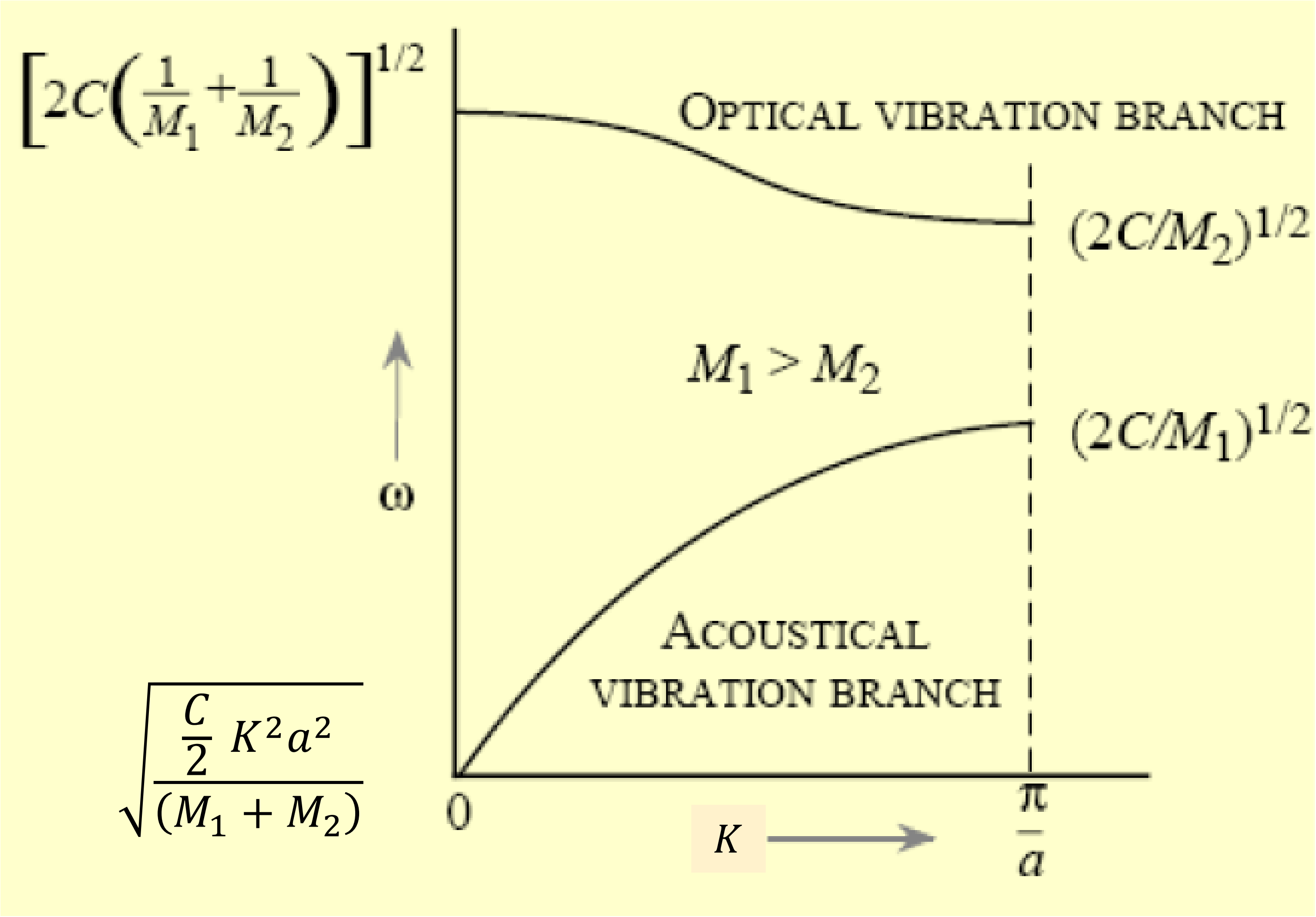
$$\omega^2 = \frac{2C(M_1 + M_2) \pm 2C\sqrt{(M_1 - M_2)^2}}{2M_1M_2}$$

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

$$\omega_+^2 = \frac{2C}{M_2}$$ Optical branch

$$\omega_-^2 = \frac{2C}{M_1}$$ Acoustical branch

Model for Diatomic Crystals



Transverse optical waves at K = 0

If we substitute the value of ω's (optical branch) in the equations of motion then for K= 0, we can get:

$$-\omega^2 M_1 u = Cv[1+e^{-iKa}]-2Cu$$

Equation of Motion for M_1

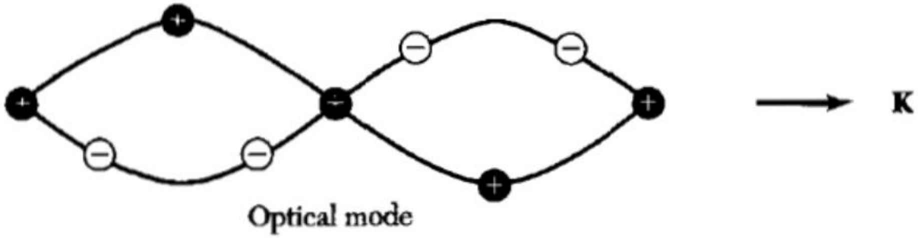
$$\omega_+^2 = 2C\left(\frac{1}{M_1}+\frac{1}{M_2}\right)$$

$$-\omega^2 M_1 u = 2Cv - 2Cu$$

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

$$-2u - 2\left(\frac{M_1}{M_2}\right)u = 2v - 2u$$

$$\frac{M_2}{M_1} = -\frac{u}{v}$$



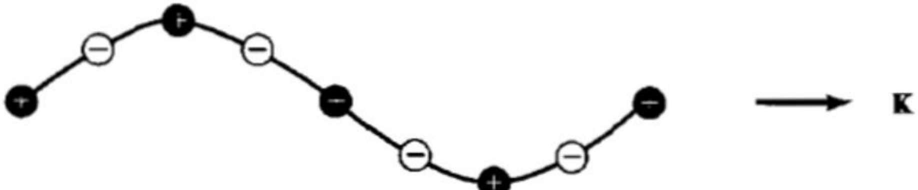
Optical mode

If the atoms are of opposite charge then it can be excited with the electric field of the light waves, hence the branch is called optical branch.

Transverse Acoustical waves at K = 0

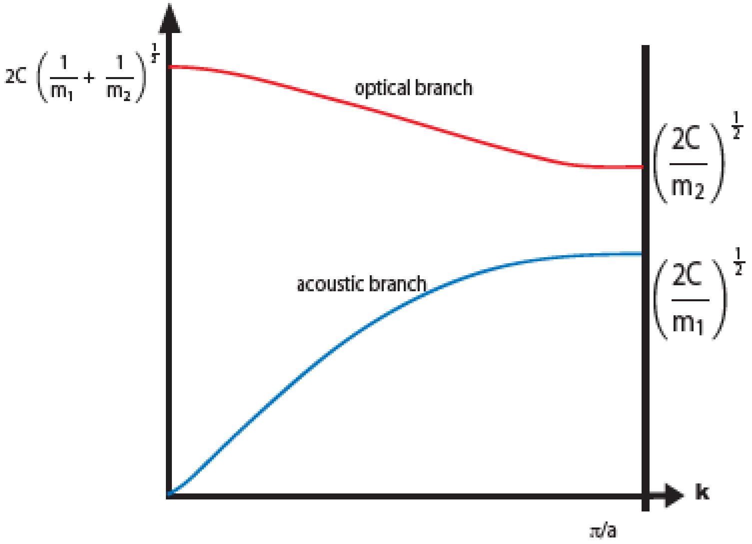
If we substitute the value of ω's (acoustical branch) in displacement equations then for K=0, we can get:

$$u = v$$



Acoustical mode

Here atoms and their center of mass move together, as it happens in the longitudinal (acoustic) waves, so the term acoustical branch

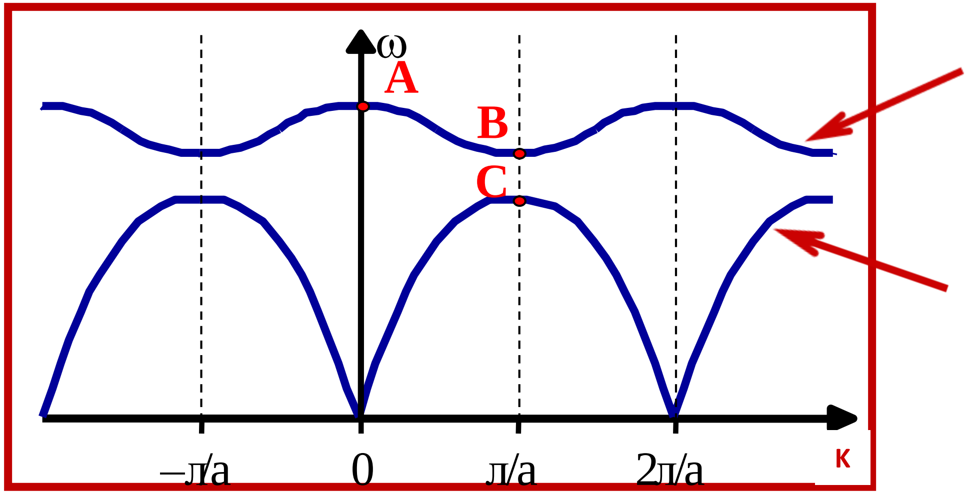


Wavelike solution does not exist for certain frequencies, here between $(2C/M_1)^{1/2}$ and $(2C/M_2)^{1/2}$.

This is a characteristic feature of elastic waves in polyatomic lattices.

Solutions to the Normal Mode Eigenvalue Problem

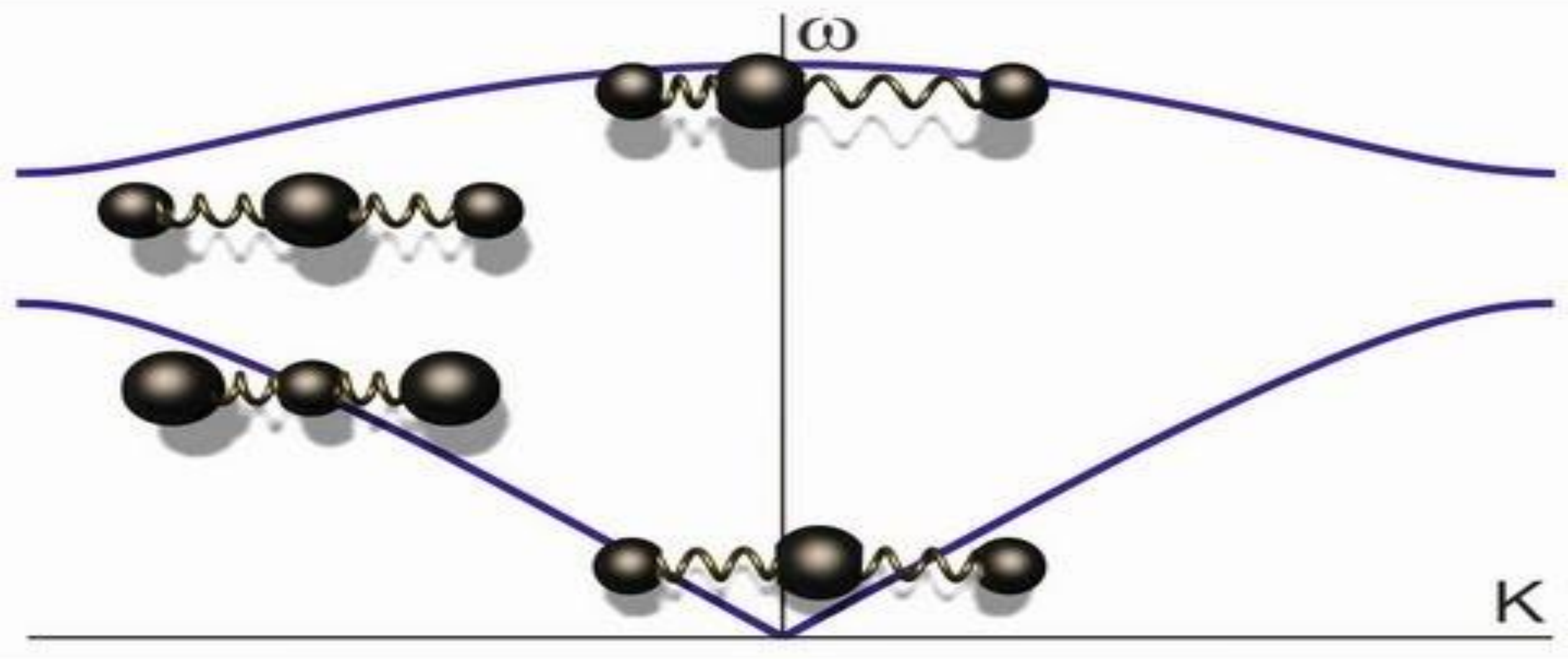
ω(K) for the Diatomic Chain



ω_+ = “Optic” Modes

ω_- = “Acoustic” Modes

- From an analysis of the displacements, it can be shown that, at point **A**, **the two atoms are oscillating 180° out of phase**, with their center of mass at rest. Also, at point **B**, the lighter mass is oscillating & heavier mass is at rest, while at point **C**, heavier mass is oscillating & lighter mass is at rest.



https://www.youtube.com/watch?v=M4WQs_U1nmU

Acoustic & Optic Branches

- Despite the fact that diatomic chain model is one-dimensional, it's results for the vibrational normal modes ω contain considerable qualitative physics that carries over to the observed vibrational frequencies for many real materials.

- So, much of the physics contained in the diatomic chain results can teach us something about the physics contained in the normal modes of many real materials.

- In particular, ALL MATERIALS with 2 atoms per unit cell are observed to have two very different kinds of vibrational normal modes, which are called The Acoustic Branch & The Optic Branch

Quantization of Elastic Waves

- Phonons is a quantum mechanical particle, such particles are often called ***"Quasiparticles".***

Examples of ***other* Quasiparticles**:

- **Photons:** Quantized Normal Modes of electromagnetic waves.
- **Rotons:** Quantized Normal Modes of molecular rotational excitations.
- **Magnons:** Quantized Normal Modes of magnetic excitations in magnetic solids
- **Excitons:** Quantized Normal Modes of electron-hole pairs
- **Polaritons:** Quantized Normal Modes of electric polarization excitations in solids

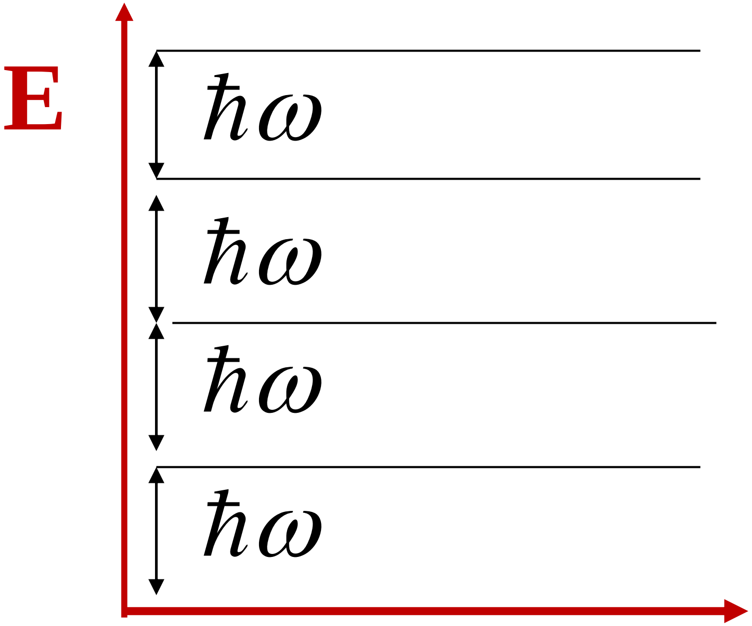
+ *Many* Others!!!

Quantization of Elastic Waves

- The energy of a lattice vibration is quantized and the quantum of energy is called PHONON
- The energy of an elastic mode of angular frequency ω is

$$E = \left(n + \frac{1}{2}\right)\hbar\omega$$

n = 0,1,2,3,..



The energy levels are equally spaced!

- Often, we consider **E** as being constructed by adding **n** excitation quanta of energy ħω to the ground state.

$$E_0 = \frac{1}{2}\hbar\omega$$

Oscillator Ground State (or "zero point") Energy.

- If the system makes a transition from a lower energy level to a higher energy level, it is always true that the change in energy is an integer multiple of ħω.

Phonon Absorption or Emission

$$\Delta E = (n - n')\,\hbar\omega$$

n & n′ = integers

- In complicated processes, such as phonons interacting with electrons or photons, it is known that

The number of phonons is NOT conserved.

That is, phonons can be created & destroyed during such interactions. **BOSONS**

Quantization of Elastic Waves

- **Quantizing the phonon amplitude:**

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

$$u = u_o \cos(Kx)\cos(\omega t)$$

Energy in the mode, as in any harmonic oscillator, is half kinetic and half potential, when averaged over time. The kinetic energy density give by: $\frac{1}{2}\ \rho \left(\frac{\partial u}{\partial t}\right)^2$, where ρ is the mass density.

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

$$\frac{K.E}{V} = \frac{1}{2}\ \rho \left(\frac{\partial u}{\partial t}\right)^2 = \frac{1}{2}\ \rho\ (u_0 \cos(Kx) \sin(\omega t)\, \omega)^2$$

Quantization of Elastic Waves

- In a crystal of volume V, the volume integral of the K.E is

$$K.E = \frac{1}{2}\rho\ (u_0 \sin(\omega t)\ \omega)^2 \int_{-\pi/K}^{\pi/K} x^2 dx\ d\Phi d cos(\theta)\ (\cos(Kx))^2$$

$$K.E = \frac{1}{4}\rho\ (u_0 \sin(\omega t)\ \omega)^2 \left(\frac{4}{3}\pi x^3\right)$$

- The time average of the kinetic energy is

$$< K.E >= \frac{1}{4}\rho\ (u_0\omega)^2 < sin^2(\omega t) > V$$

$$< K.E >= \frac{1}{8}\rho\ (u_0\omega)^2 V$$

Quantization of Elastic Waves

The time averaged KE is:

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

The square of the amplitude of the mode is:

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

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

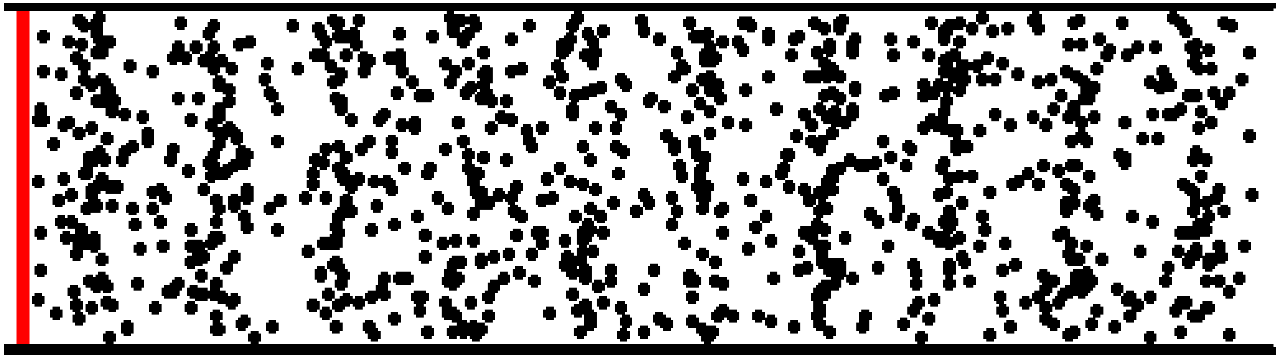
For a stable crystal structure ω should always be positive. For unstable crystal structure ω will be imaginary.

Phonon Momentum

- A phonon of wavevector K will interact with particles such as photons, neutrons, and electrons as if it had a momentum ħK.

- However, a phonon does not carry physical momentum.

- For example a neutron can interact with the crystal and start a wave by transferring momentum to the lattice. This momentum is transferred to the whole lattice, but the atoms themselves are not being translated permanently from their equilibrium positions.



Phonon Momentum

- In crystals there exist wavevector selection rules for allowed transitions between quantum states.

- For elastic scattering of x-ray photon by a crystal x-ray photon by a crystal is governed by the wavevector selection rule

$$\boldsymbol{k}' = \boldsymbol{k} + \boldsymbol{G}$$

where $\boldsymbol{G}$ is a vector in the reciprocal lattice, $\boldsymbol{k}$ is the wavevector of the incident photon, and $\boldsymbol{k'}$is the wavevector of the scattered photon.

- In the reflection process the crystal as a whole will recoil with momentum $-\hbar\boldsymbol{G}$, but this uniform mode momentum is rarely considered explicitly.

Phonon Momentum

- The true momentum of the whole system always rigorously conserved. If the scattering of the photon is inelastic, with the **creation of a phonon** of wavevector K, then the wavevector selection rule becomes

$$\boldsymbol{k}' + \boldsymbol{K} = \boldsymbol{k} + \boldsymbol{G}$$

- If a **phonon K is absorbed** in the process, we have instead the relation

$$\boldsymbol{k}' = \boldsymbol{k} + \boldsymbol{K} + \boldsymbol{G}$$

- These two relations are the natural extensions of the equation shown on the previous slide.

Inelastic Scattering by Phonons

- Phonon dispersion relations ω(K) are most often determined experimentally by the inelastic scattering of neutrons with the emission or absorption of phonon.

- In an inelastic scattering the total momentum is conserved, but the kinetic energy before and after the scattering will be different.

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

- M_n is the mass of neutron, $\hbar\omega$ is the energy of phonon, and the (+) and (-) signs represent phonon creation and absorption in the process.