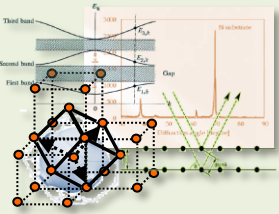


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Solid State Physics Phys(471)

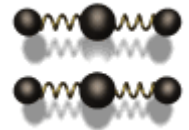
Lecture 9-11



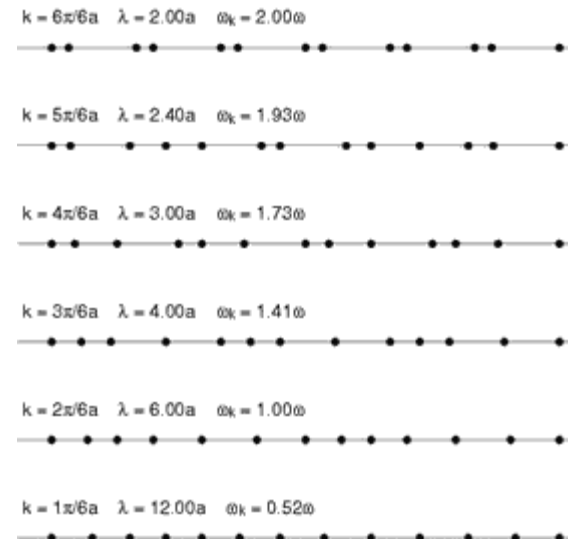
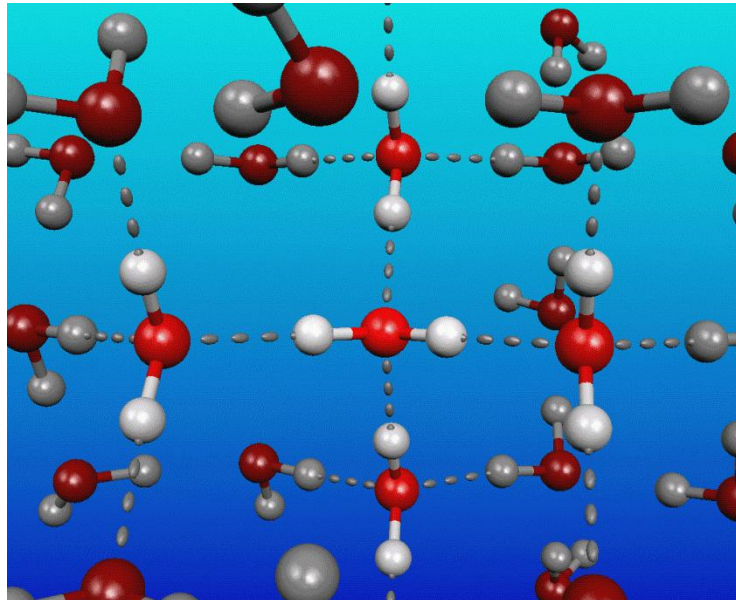
LATTICE VIBRATIONS

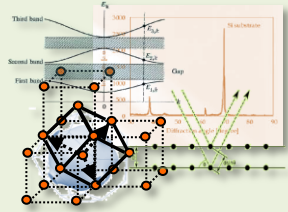
➤ Atoms in lattice are not stationary even at $T = 0\text{K}$. They vibrate about particular equilibrium positions (**zero-point energy**).

➤ For $T > 0\text{K}$, vibration amplitude increases as atoms gain thermal energy.



➤ At low frequencies ($f < 1\text{THz}$), long wavelength $\lambda \sim 50\text{\AA}$, one can treat solid as continuum, **i.e.** ignore discrete nature.





LATTICE VIBRATIONS

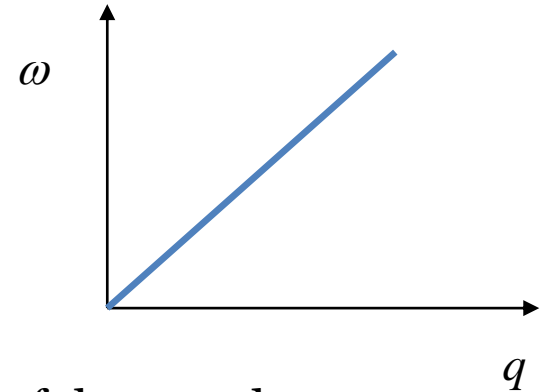
Continuum Model

Propagation of an *elastic wave* in a sample of long bar follows the *dispersion relation* :

$$\omega = v_s q$$

Where v_s is the wave velocity (sound velocity) which equal in this case to

$$v_s = \sqrt{Y / \rho}$$



Y & ρ are *Young's modulus* and density of the sample.

Note that the v is independent of λ for an elastic medium!

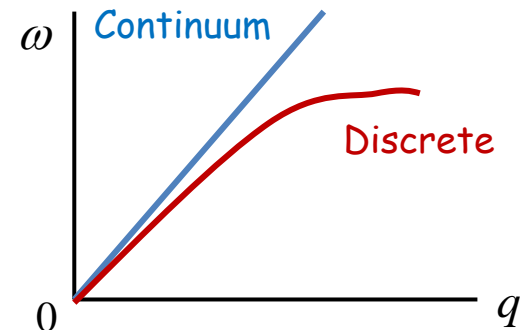
Discrete Lattice

By contrast to a continuous solid, a real solid is not uniform on an atomic scale, and thus it will exhibit dispersion.

I.e. v now depends on λ .

As the λ decreases and q increases, the atoms begin to scatter the wave, and hence to decrease its velocity.

Thus, one expects the dispersion relation to be as shown

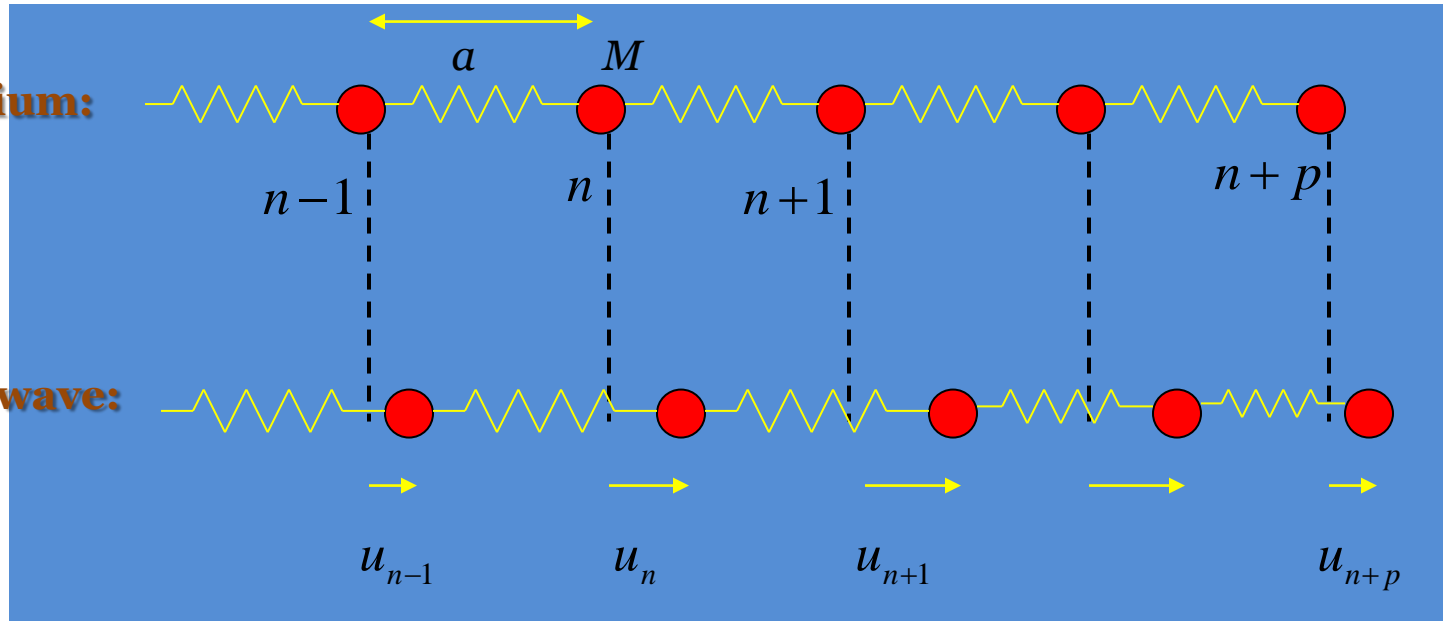


LATTICE VIBRATIONS

Monatomic Chain

Consider **1D** chain of identical atoms each of mass M , where atoms joined to nearest neighbors by 'spring' of force constant α , and spacing a apart.

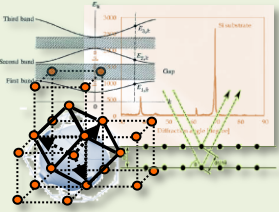
At equilibrium:



For atom n ,

$$F_n = M \frac{\partial^2 u_n}{\partial t^2} = \sum_p \alpha_p (u_{n+p} - u_n)$$

Where p is atom label and α_p is force constant for atom p .



LATTICE VIBRATIONS

Look for wavelike solution: $u_n = Ae^{i(qX_n - \omega t)}$

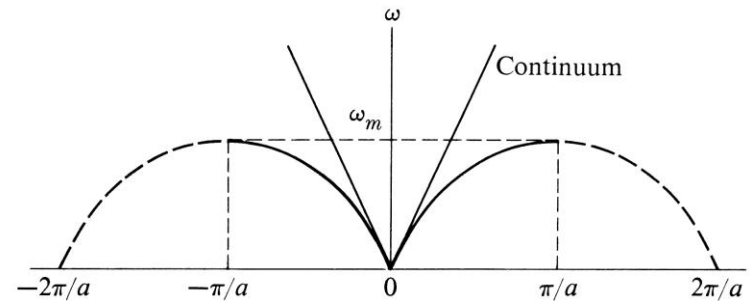
Where $X_n = na$ is the equilibrium position .

Substitute into eq. of motion get:

$$\omega^2 = \frac{4\alpha}{M} \sin^2 \frac{1}{2} qa$$

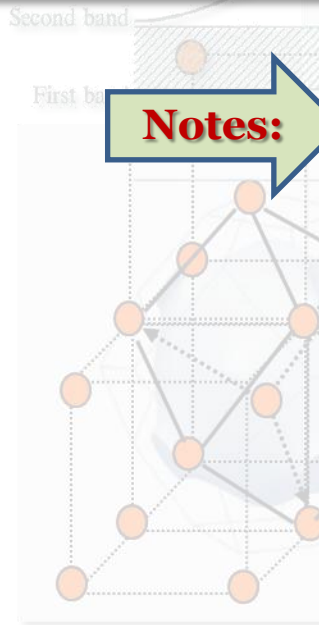
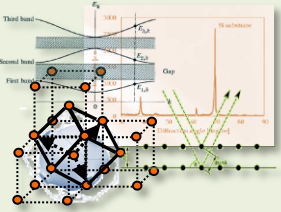
Hence, the **Dispersion relation** , which Determines how wave vector q is related to ω , in **1D** is :

$$\omega = \omega_m \left| \sin \frac{1}{2} qa \right|$$



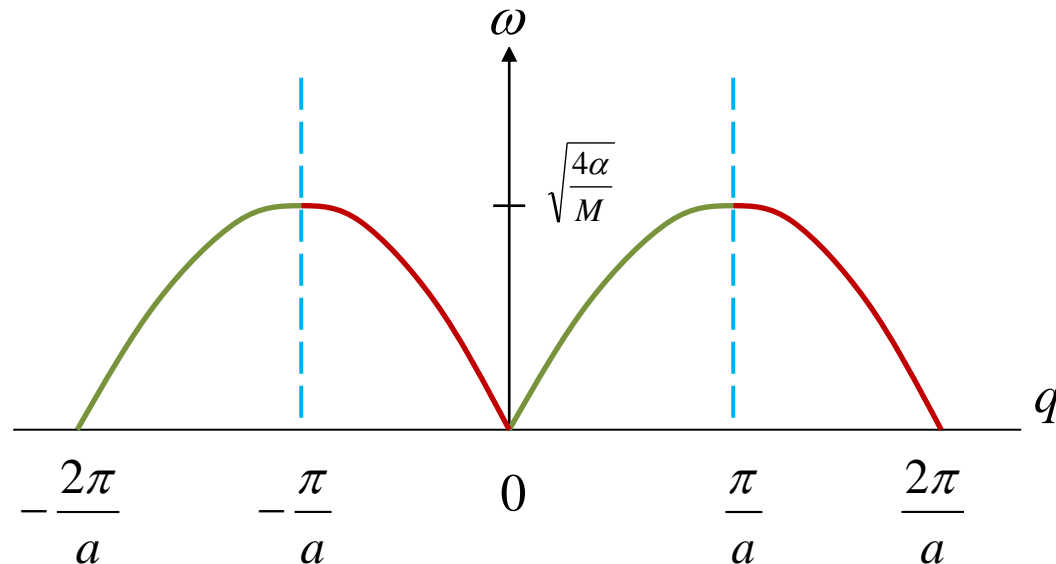
Where $\omega_m = (4\alpha/M)^{1/2}$.

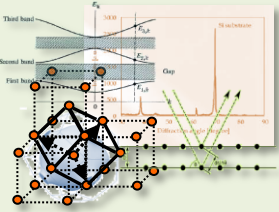
LATTICE VIBRATIONS



Notes:

- ω is periodic in q & all values of ω contained in range: $-\pi/a < q < \pi/a$.
- Range of q related to **1st Brillouin zone**. Values of q outside range have no physical meaning.
- N does not appear in dispersion relation, **i.e.** equations of motion of all atoms lead to the same algebraic relation between ω and θ .





LATTICE VIBRATIONS

1- Long wavelength limit:

As $q \rightarrow 0$, $\sin \theta = \theta$, and then

$$\omega = \frac{\omega_m a}{2} q$$

Or;

$$v_s = \frac{\omega_m a}{2}$$



Using $v_s = \sqrt{Y / \rho}$

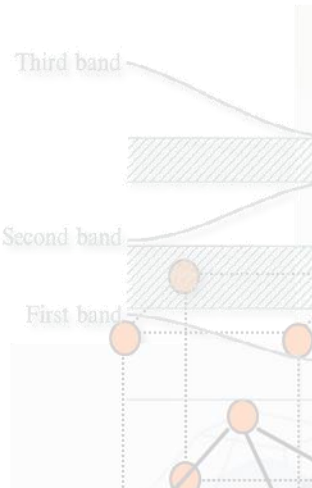
$$\alpha = Ya$$

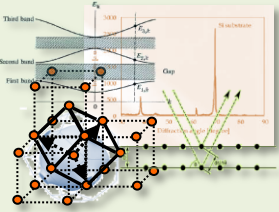
2- Short wavelength limit:

As q increases, the dispersion relation begins to deviate from the straight line.

It will saturate at $q = \pi/a$ with maximum frequency

$$\omega_m = \sqrt{\frac{4\alpha}{M}}$$

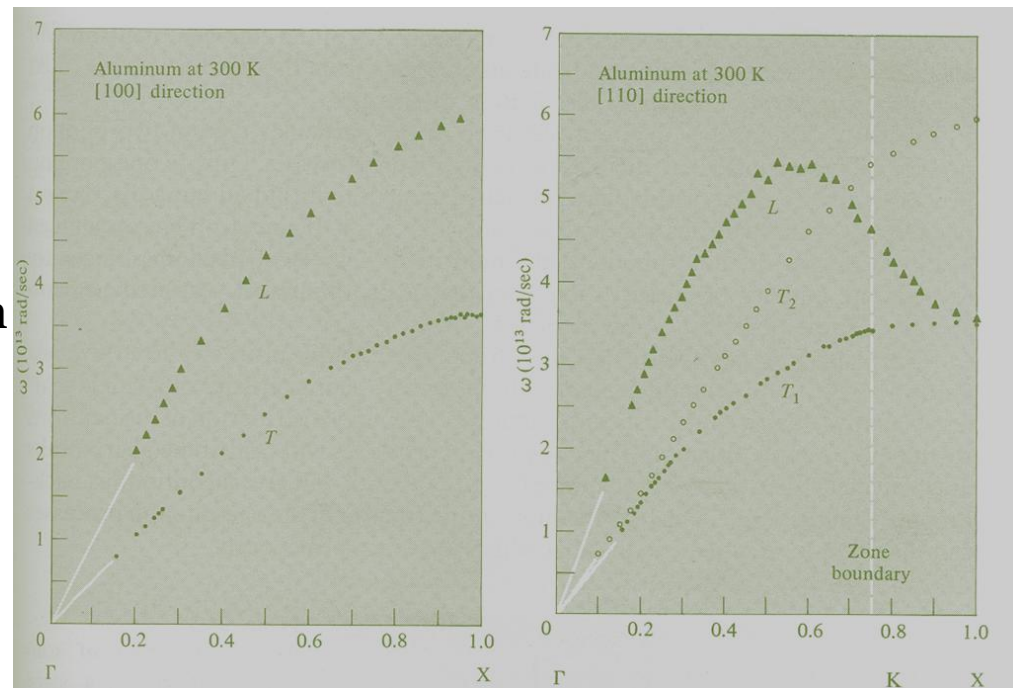




LATTICE VIBRATIONS

In a **3-D** atomic lattice we expect to observe **3** different **branches** of the **dispersion relation**, since there are **two** mutually perpendicular **transverse** wave patterns in addition to **the one longitudinal** pattern we have considered.

Along different directions in the reciprocal lattice the shape of the dispersion relation is different. But note the similarity to the simple **1-D** result we found.

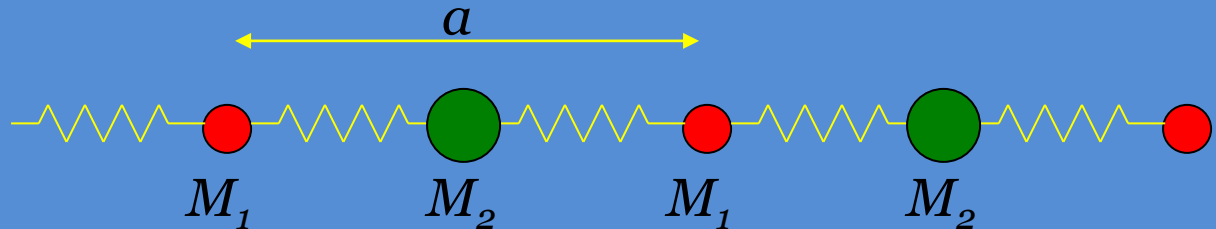


LATTICE VIBRATIONS

Diatomic Chain

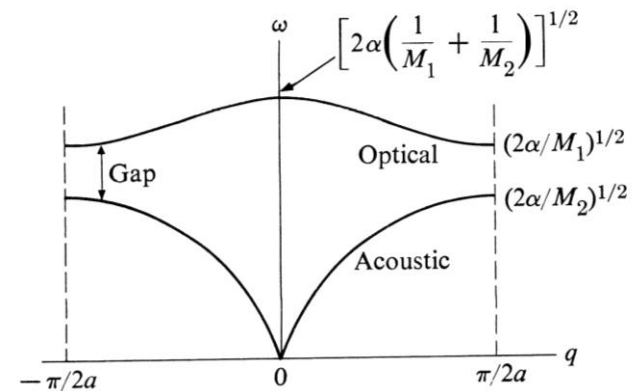
Consider a linear diatomic chain of atoms (**1D** model for a crystal like **NaCl**) with masses M_1 , M_2 and a force constant α .

At equilibrium:

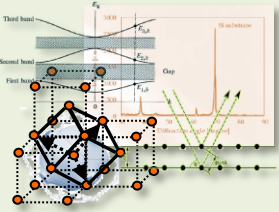


Applying Newton's second law gives a dispersion relation with two "branches":

What if $M_1 = M_2$?



$$\omega^2 = \alpha \left(\frac{1}{M_1} + \frac{1}{M_2} \right) \pm \alpha \sqrt{\left(\frac{1}{M_1} + \frac{1}{M_2} \right)^2 - \frac{4 \sin^2(qa)}{M_1 M_2}}$$

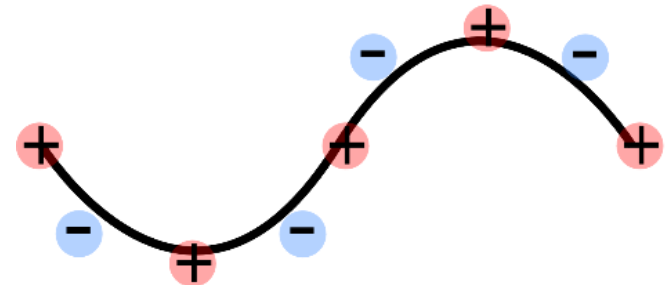


LATTICE VIBRATIONS

Acoustic modes

$\omega_-(q)$ $\omega \rightarrow 0$ as $q \rightarrow 0$ (M_1 and M_2 move **in phase**)

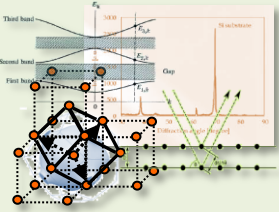
One Longitudinal (LA) and two Transverse (TA) modes.



Optical modes

$\omega_+(q)$ $\omega \rightarrow \omega_{\max}$ as $q \rightarrow 0$ (M_1 and M_2 move **out of phase**)

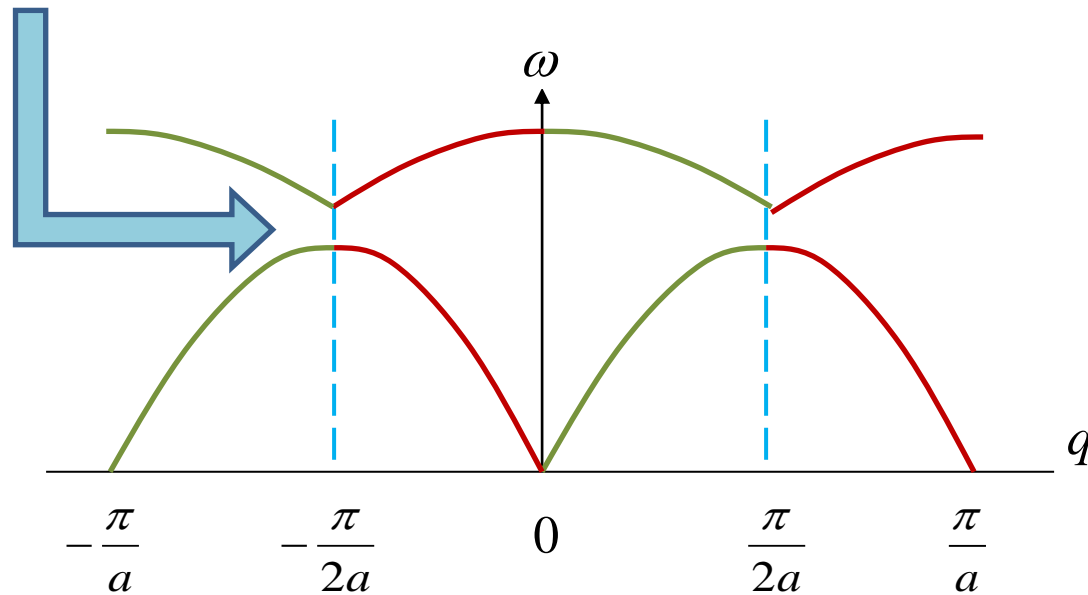
One Longitudinal (LO) and two Transverse (TO) modes.



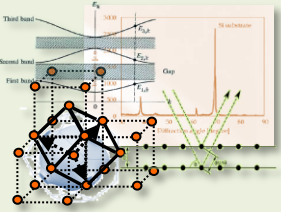
LATTICE VIBRATIONS

Notes:

- ω is periodic in q & all values of ω contained in range:
 $-\pi/2a < q < \pi/2a$.
- Range of q related to half of **1st Brillouin zone**.
- The gap indicates the allowed frequencies (**Band-pass Filter**).

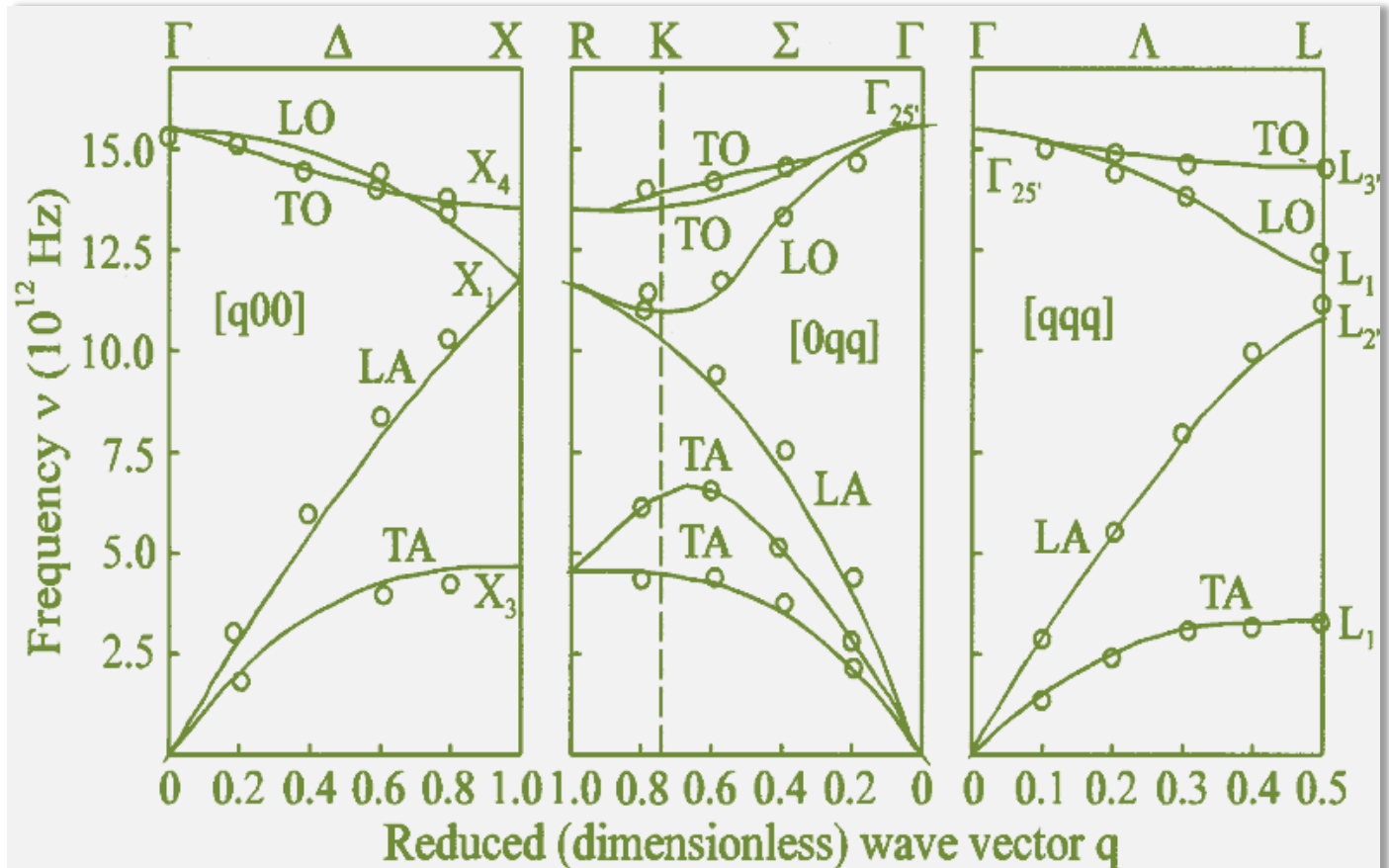


- Generalize to crystals with s different atoms in unit cell; **3 acoustic branches** & **3(s - 1) optical branches**; (s-1) LO and 2(s-1) TO.

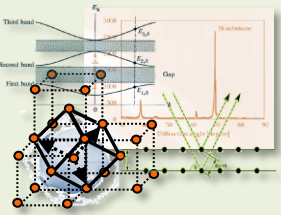


LATTICE VIBRATIONS

Dispersion Relation in GaAs (3D)



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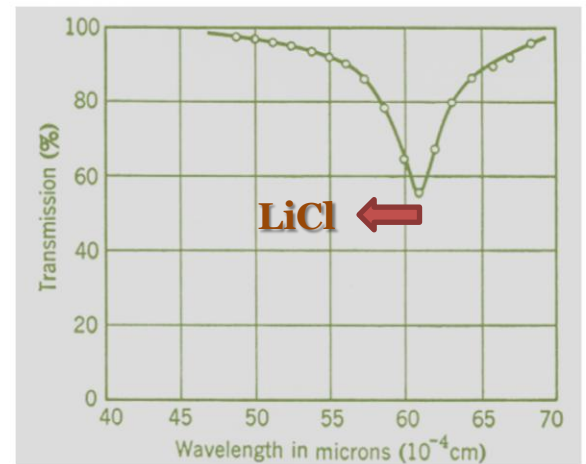
The **optical modes** generally have frequencies near $\omega = 10^{13} \text{ s}^{-1}$, which is in the range of **infrared radiation** of the electromagnetic spectrum. Thus, when **IR** radiation is incident upon such a lattice it should be strongly absorbed in this band of frequencies.

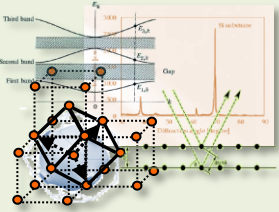
At right is a transmission spectrum for **IR** radiation incident upon a very thin **NaCl** film. Note the sharp minimum in transmission (maximum in absorption) at a wavelength of about $61 \times 10^{-4} \text{ cm}$, or $61 \times 10^{-6} \text{ m}$. This corresponds to a frequency $\omega = 4.9 \times 10^{12} \text{ s}^{-1}$.

Since,
$$\omega \propto 1/\sqrt{M}$$

If instead we measured this spectrum for **LiCl**, we would expect the peak to shift to higher frequency (lower wavelength) because

$$M_{\text{Li}} < M_{\text{Na}}.$$





LATTICE VIBRATIONS

Phonons:

The **energy of lattice vibration** is quantized, and *the quantum of this energy* is called a **phonon**, in analogy to photons the quantum of the electromagnetic waves.

The **energy** of phonon is: $\varepsilon = \hbar\omega$

With a **momentum** equal to: $p = \hbar q$

The **number of phonons** is given by **Bose-Einstein** distribution:

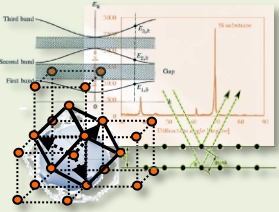
$$n = \frac{1}{e^{\hbar\omega / KT} - 1}$$

This number depends on temperature ,

at $T=0 \Rightarrow n=0$

at very high temperature, \Rightarrow

$$n = \frac{KT}{\hbar\omega}$$



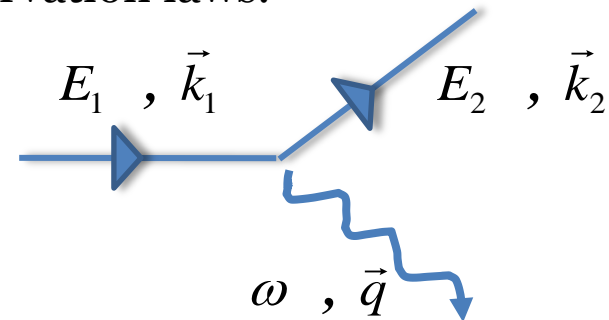
LATTICE VIBRATIONS

The phonon dispersion curves $\omega(\mathbf{K})$ are determined via inelastic scattering of neutrons with the emission or absorption of a phonon

Interaction of phonons with other excitation (or with themselves) governed by conservation laws.

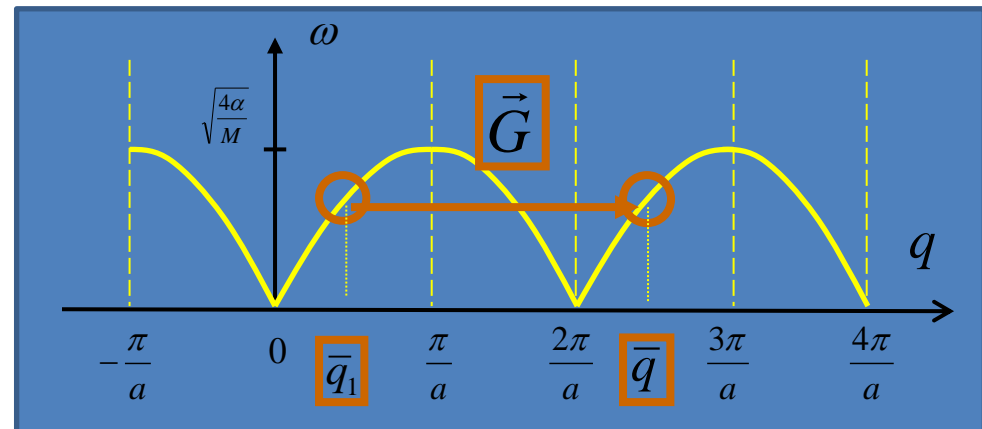
$$E_1 - E_2 = \hbar\omega$$

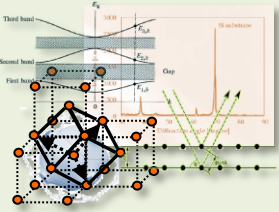
$$\vec{k}_1 - \vec{k}_2 = \vec{q}$$



Fact:

The number of phonons in a system is not conserved.





LATTICE VIBRATIONS

Density of States

In order to calculate physical properties of solids, the **no. of modes in a given frequency** (or energy, or q -space) **range** is required.

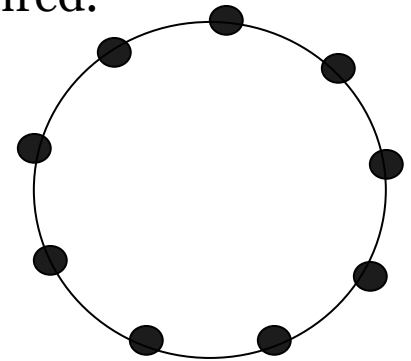
1D density of States

A 'better' way of obtaining this is to apply the *periodic boundary condition*:

$$u(x=L) = u(x=0)$$

$$e^{iqL} = 1$$

$$qL = n2\pi, \quad \text{ie. } q = n2\pi/L$$



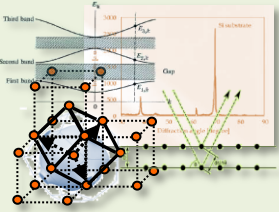
$$q = -6\pi/L \quad -4\pi/L \quad -2\pi/L \quad 0 \quad 2\pi/L \quad 4\pi/L \quad 6\pi/L$$

Thus, 'length' occupied by one mode in q -space is $2\pi/L$.

Hence the No. of modes in the range $dq \longrightarrow dq / \frac{2\pi}{L}$

Since there is **the same No. of states** in $g(q)dq$ & $g(\omega)d\omega$, then

$$g(\omega)d(\omega) = g(q)d(q) = \frac{L}{2\pi} dq \quad \longrightarrow \quad g(\omega) = \frac{L}{2\pi} \frac{dq}{d\omega}$$



LATTICE VIBRATIONS

Since the modes lying in(**-ve**) q-region must be included as well, then:

$$g(\omega) = \frac{L}{\pi} \frac{dq}{d\omega}$$



$$g(\omega) = \frac{L}{\pi} \frac{1}{v_g}$$

Note the relation between the density of states and the group velocity.

At long wavelength limit:

$$\omega = v_s q, \quad \text{ie. } d\omega/dq = v_s$$

and hence,

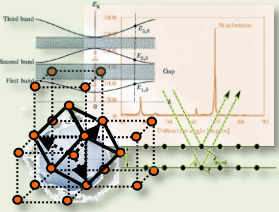
$$g(\omega) = \frac{L}{\pi} \frac{1}{v_s}$$

At Dispersive region:

$$\omega = \omega_m \left| \sin \frac{1}{2} qa \right|$$

and hence,

$$g(\omega) = \frac{2L}{\pi a \omega_m} [\cos(qa/2)]^{-1}$$



LATTICE VIBRATIONS

3D density of States

Volume occupied by one mode in q -space is:

$$(2\pi/L)^3 = (8\pi^3)/V$$

Thus, No. of modes contained in a small spherical shell in q -space is:

$$4\pi q^2 dq / 8\pi^3 / V$$

Hence, density of states in ω -space is

$$g(\omega) = \frac{V}{8\pi^3} 4\pi q^2 \frac{dq}{d\omega}$$

$$g(\omega) = \frac{V}{2\pi^2} q^2 \frac{dq}{d\omega}$$

This is the density of state if we assume that each value of q associated with one single mode. But, in fact for each q there are **3** modes (**1** longitudinal & **2** transverse), then

$$g(\omega) = \frac{3V}{2\pi^2} q^2 \frac{dq}{d\omega}$$