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Crystal Structure : Lattice Vibration, Phonons,Phonon Spectrum, Brillouin Zone
Solved Problems

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Lattice Vibration

Lattice Vibration is the oscillations of atoms in a solid about the equilibrium position. For a crystal, the equilibrium positions form a regular **lattice**, due to the fact that the atoms are bound to neighboring atoms. The **vibration** of these neighboring atoms is not independent of each other.

Lattice vibrations can explain sound velocity, thermal properties, elastic properties and optical properties of materials. Lattice Vibration is the oscillations of atoms in a solid about the equilibrium position. For a crystal, the equilibrium positions form a regular lattice, due to the fact that the atoms are bound to neighboring atoms. The vibration of these neighboring atoms is not independent of each other. A regular lattice with harmonic forces between atoms and normal modes of vibrations are called lattice waves. Lattice waves range from low frequencies to high frequencies on the order of 1,013 Hz or even higher [4][4]. However, the wavelengths at extremely high frequencies are of the order of inter atomic spacing. Due to the shortness of these wavelengths, the motion of the neighboring atoms is uncorrelated; with each atom moving about its average position in three dimensions with average vibrational energy, which is usually 3kT, with ‘kk’ representing the Boltzmann constant and 'TT' the absolute temperature. Lattice vibrations can also interact with free electrons in a conducting solid which gives rise to electrical resistance .

Optical Properties of Lattice Vibrations:

- Compared to the static lattice model that deals with the average positions of atoms in a crystal; lattice dynamics works towards extending the concept of crystal lattice to an array of atoms with finite masses capable of motion. The motion of masses is a superposition of vibrations of atoms around the equilibrium sites induced by the interaction with neighboring atoms. The collective vibration of the atoms within the crystal forms a wave of allowed wavelength and amplitude. For example, as we know that light is said to be a wave motion composed of photons, we can also think of the normal modes of vibration in a solid as being a particle. One major problem with Lattice dynamics is that is hard to find the normal modes of vibration of the crystal. However, lattice dynamic, offers two different ways of finding the dispersion relation within the lattice.

Phonons:

- Almost all solids with the exception of amorphous solids and glasses have periodic arrays of atoms which form a crystal lattice. The existence of the periodic crystal lattice in solid materials provides a medium for characteristic vibrations. Between the lattice spacing, there are quantized vibrational modes called a phonon. The study of phonon is an important part of solid state physics, as they play an essential role in the physical properties of solids, the thermal and electrical conductivity of the materials. The long wavelength property of phonon also gives attributes to sounds in solids. Phonons are also a quantum mechanical version of a special type of vibrational motion. This type of vibrational motion is called a normal mode (elementary blocks of lattice vibration), which is a pattern of motion in which all parts of the system move in a sinusoidal fashion, with the same frequency. An example of a normal mode is a standing wave, which is a continuous form of normal mode and all space elements, (x, y and Z co-ordinates) are oscillating at the same frequencies, and phase but different amplitude.

Types of Phonons:

- Optical Phonons:
- Optical phonon are quantized modes of lattice vibrations when two or more charged particles in a primitive cell move in opposite directions with the center of mass at rest. This mode has highest energy for wavelength infinity or k=0.,when the two lattices move in opposing direction of each other.
- Acoustic Phonons:
- Acoustical phonons are phonons whose frequency which goes to zero in the limit of small kk. Let’s consider monatomic a linear chain of identical atoms of mass ‘M’ spaced at a distance ‘aa’, the lattice constant, connected by invisible Hook's law springs and longitudinal deformations.

Phonon Spectrum:

- Optical phonons have a non-zero frequency at the Brillouin zone center and show no dispersion near that long wavelength limit. This is because they correspond to a mode of vibration where positive and negative ions at adjacent lattice sites swing against each other, creating a time-varying electrical dipole moment. Optical phonons that interact in this way with light are called *infrared active*. Optical phonons that are *Raman active* can also interact indirectly with light, through Raman scattering. Optical phonons are often abbreviated as LO and TO phonons, for the longitudinal and transverse modes respectively; the splitting between LO and TO frequencies is often described accurately by the Lyddane–Sachs–Teller relation.
- When measuring optical phonon energy experimentally, optical phonon frequencies are sometimes given in spectroscopic wavenumber notation, where the symbol ω represents ordinary frequency (not angular frequency), and is expressed in units of cm^{-1}. The value is obtained by dividing the frequency by the speed of light in vacuum. In other words, the wavenumber in cm^{-1} units corresponds to the inverse of the wavelength of a photon in vacuum, that has the same frequency as the measured phonon.

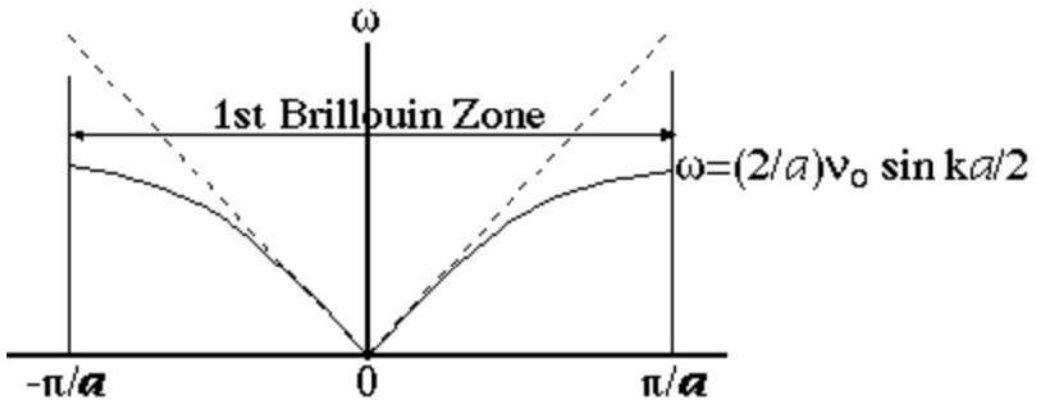


Fig 1.

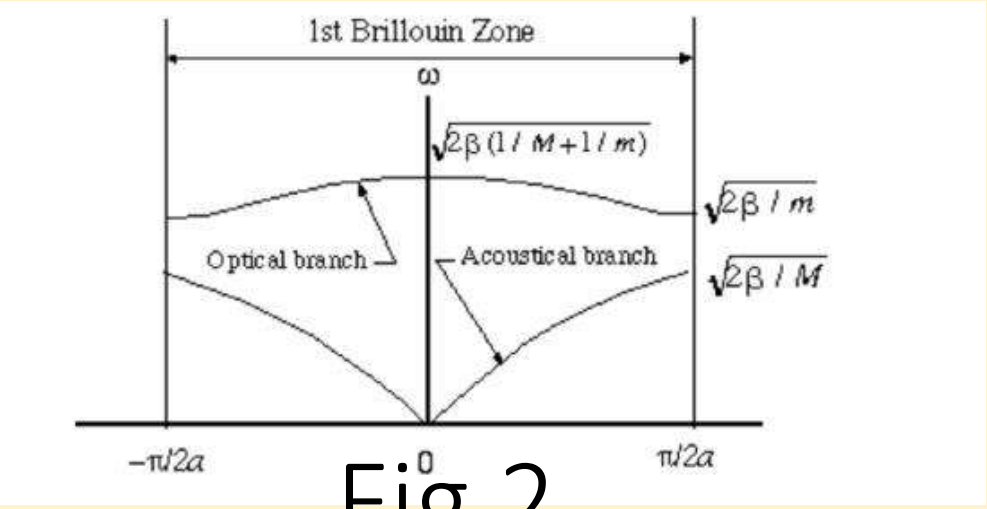


Fig 2

The force on atom 'n' will be given by its displacement and the displacement of its nearest neighbors:

$$F_n = \beta(U_{n+1} - 2U_n + U_{n-1}) \quad (8)$$

The equation of motion is:

$$M\frac{\partial^2 U_n}{\partial t^2} = \beta(U_{n+1} - 2U_n + U_{n-1}) \quad (9)$$

where β is a spring constant.

With wave solution

$$U_n = U_{no}e^{[i(kna\pm\omega t)]} \quad (10)$$

If $U_{no} = U_o$ and has a definite amplitude.

Substitute Equations 7 into Equations 5 and 6 we obtain phonon's dispersion relation for linear monatomic chain as follows:

$$\omega = \pm\sqrt{\frac{4\beta}{M}}\sin\left(\frac{ka}{2}\right) \quad (11)$$

with dispersion curve as fig 1

Let's consider a lattice with two kinds of atoms with masses m and M. The equations of motion are:

$$m\frac{\partial^2 U_{2n}}{\partial^2 t} = \beta(U_{2n+1} - 2U_{2n} + U_{2n-1}) \quad (3)$$

$$m\frac{\partial^2 U_{2n+1}}{\partial^2 t} = \beta(U_{2n+2} - 2U_{2n+1} + U_{2n}) \quad (4)$$

for atom with masses 'm' and 'M' respectively

$$U_{2n} = Ae^{i(2nka\pm\omega t)} \quad (5)$$

$$U_{2n+1} = Ae^{i((2n+1)ka\pm\omega t)} \quad (6)$$

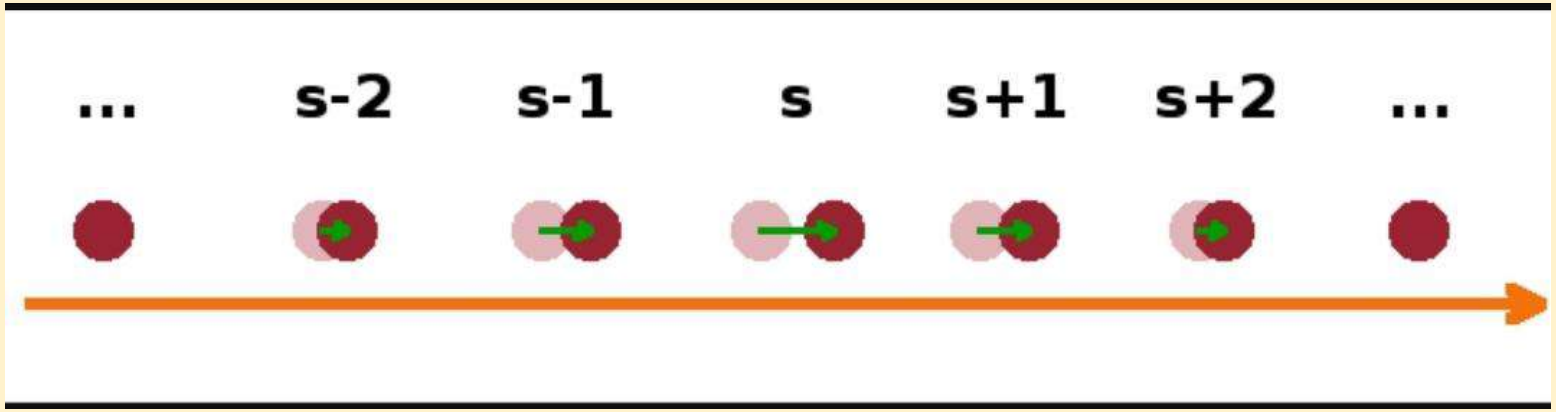
The solution of the diatomic lattice is

$$\omega^2 = \beta\left(\frac{1}{m}+\frac{1}{M}\right) \pm \beta\sqrt{\left(\frac{1}{m}+\frac{1}{M}\right)^2 - \frac{4\sin^2 ka}{Mm}} \quad (7)$$

The plot of the solution is plotted in fig−2

Monoatomic Chain:

- The *monatomic chain* model represents a crystal in one dimension where all atoms are identical, equally spaced in equilibrium and connected by bonds of equal strength. The mass of an atom is mm, the *spring constant*, CC, describes the strength of the bond between atoms, and we enumerate the atoms along the chain using a variable ss as a counter. The coordinate of atom ss along the chain is xsxs.
- The force FsFs acting on an atom ss at any given moment is the product of its mass and its acceleration:
- Fs=md2xsdt2Fs=md2xsdt2
- As long as the displacement of the atom is *elastic, i.e.* no permanent deformation takes place, we can apply *Hooke's law* and express the force as the displacement times the spring constant, CC. Since the neighbouring atoms s−1s−1 and s+1s+1 are also displaced from their equilibrium position, we need to consider the relative displacement between pairs:.

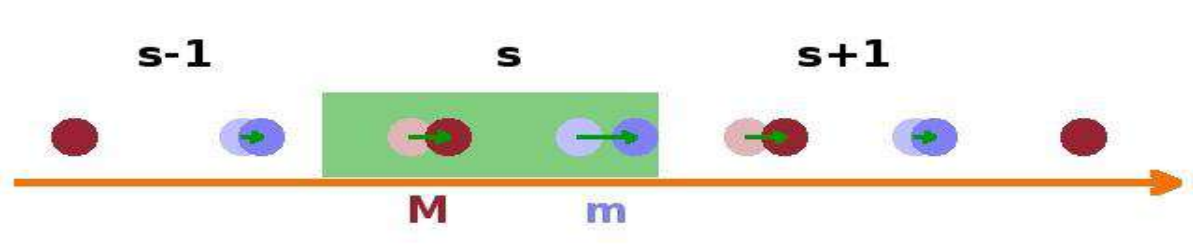


Diatomic Chain:

The *monatomic chain* is a one-dimensional model representing the situation in a crystal with a *primitive lattice*, *i.e.* with only a single atom in the unit cell. An extension of the model to a more realistic *three-dimensional case* is achieved by replacing the wavenumber, kk, with a wave vector, $\vec{k}$ k→, with three components for the different directions of (reciprocal) space. At the same time, the lattice constant, aa, is replaced with a unit cell vector, $\vec{r}$ r→, with three components for the three directions of real space.

In the same way, we can use a one-dimensional *diatomic chain* model to represent *centred lattices*, where more than one atom is present in the unit cell. To preserve generality, we have to distinguish the two atoms and assign different masses to them: The positions of the two atom types are denoted by uu (shown in red) and vv (blue) and their masses by MM and mm. We assume the spring constants for all bonds to be equal, CC. Instead of individual atoms, the loop variable ss is now used to count unit cells (green), and the lattice parameter aa is now the distance between two *identical* atoms.

As in the monatomic case, we calculate the forces acting on atoms as a consequence of relative displacements between neighbours, taking account of the fact that neighbours are now of a different type and mass. For a 'red' atom of mass MM, the force FuFu is the difference of its own displacement usus relative to its two neighbours, the 'blue' atoms in the same unit cell, vs, and in the adjacent unit cell to the left, vs−1.



Few Important links:

1. https://youtu.be/w89t53jfV5Y
2. https://youtu.be/DiuuFUIx4xU
3. https://youtu.be/JfWkNebSCG4
4. https://youtu.be/LYBPFYwWQmM
5. https://youtu.be/eK4jX9BHJrw