

Phonons

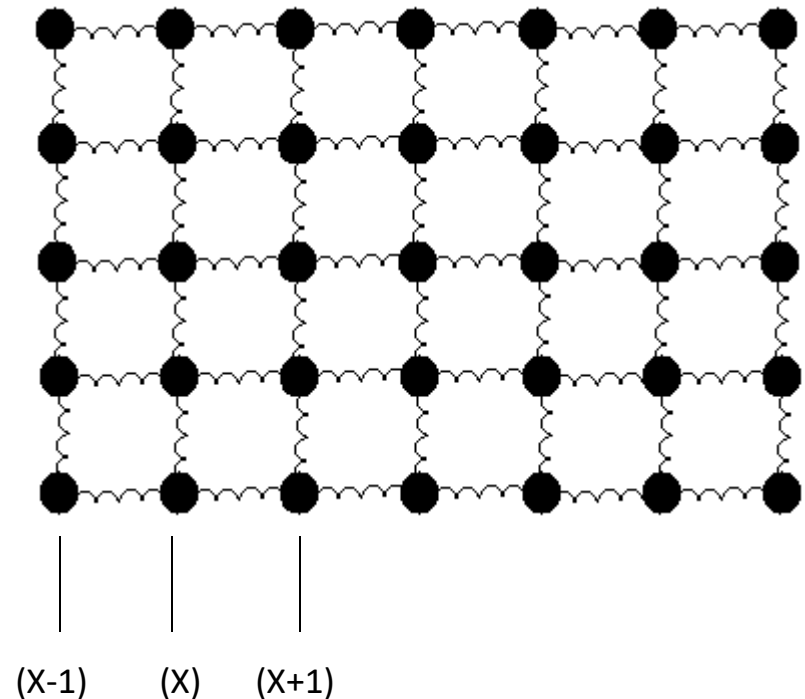
Packets of sound found present in the lattice as it vibrates ... but the lattice vibration cannot be heard.

Unlike static lattice model, which deals with average positions of atoms in a crystal, lattice dynamics extends the concept of crystal lattice to an array of atoms with finite masses that are capable of motion. This motion is not random but is a superposition of vibrations of atoms around their equilibrium sites due to the interaction with neighbor atoms. A collective vibration of atoms in the crystal forms a wave of allowed *wavelength* and *amplitude*. Just as light is a wave motion that is considered as composed of particles called photons, we can think of the normal modes of vibration in a solid as being particle-like.

Quantum of lattice vibration is called the *phonon*.

Uniform Solid Material

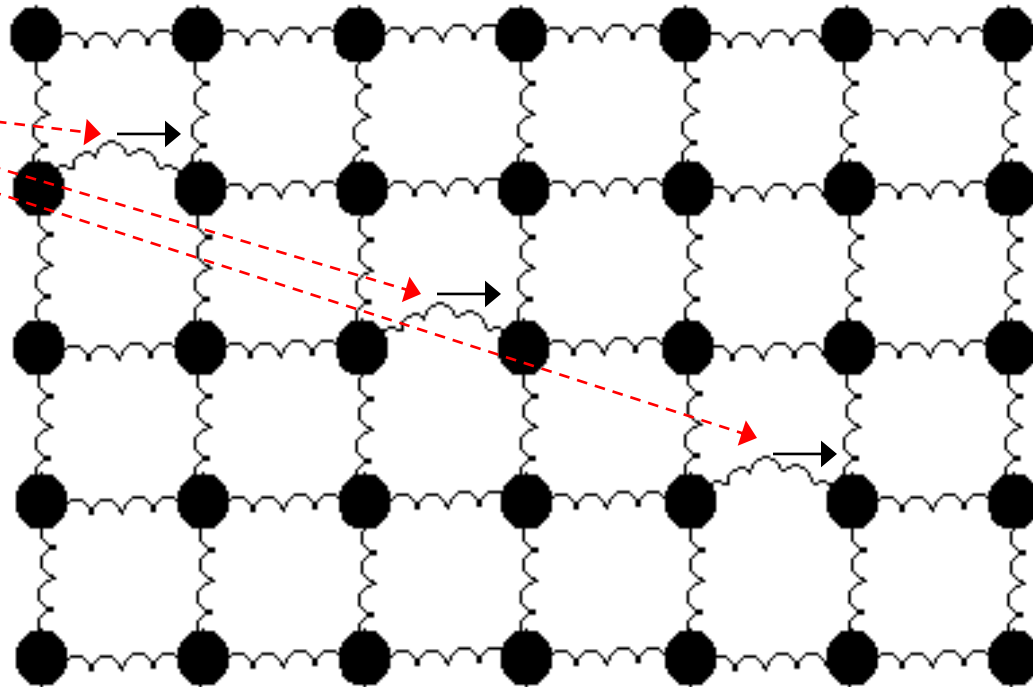
Considering the regular lattice of atoms in a uniform solid material, you would expect there to be energy associated with the vibrations of these atoms. But they are tied together with bonds, so they can't vibrate independently. The vibrations take the form of collective modes which propagate through the material.



Phonon: A Lump of Vibrational Energy

Propagating lattice vibrations can be considered to be sound waves, and their propagation speed is the [speed of sound](#) in the material.

***Phonon:
Sound
Wavepackets***



If N atoms make up the lattice, and the spring constant between the atoms is C, then we can write an equation for the force when the atoms are displaced:

$$F = ma = m \frac{d^2 x}{dt^2} = C \Delta x$$

or

$$m \frac{d^2 x_s}{dt^2} = C(x_{s+1} + x_{s-1} - 2x_s)$$

Using a position/time dependence of $\exp(i\omega t)$ and solving, we get the relationship between wave number k and frequency ω :

$$\omega^2 = \left(2 \frac{C}{m} \right) [1 - \cos(ka)]$$

where

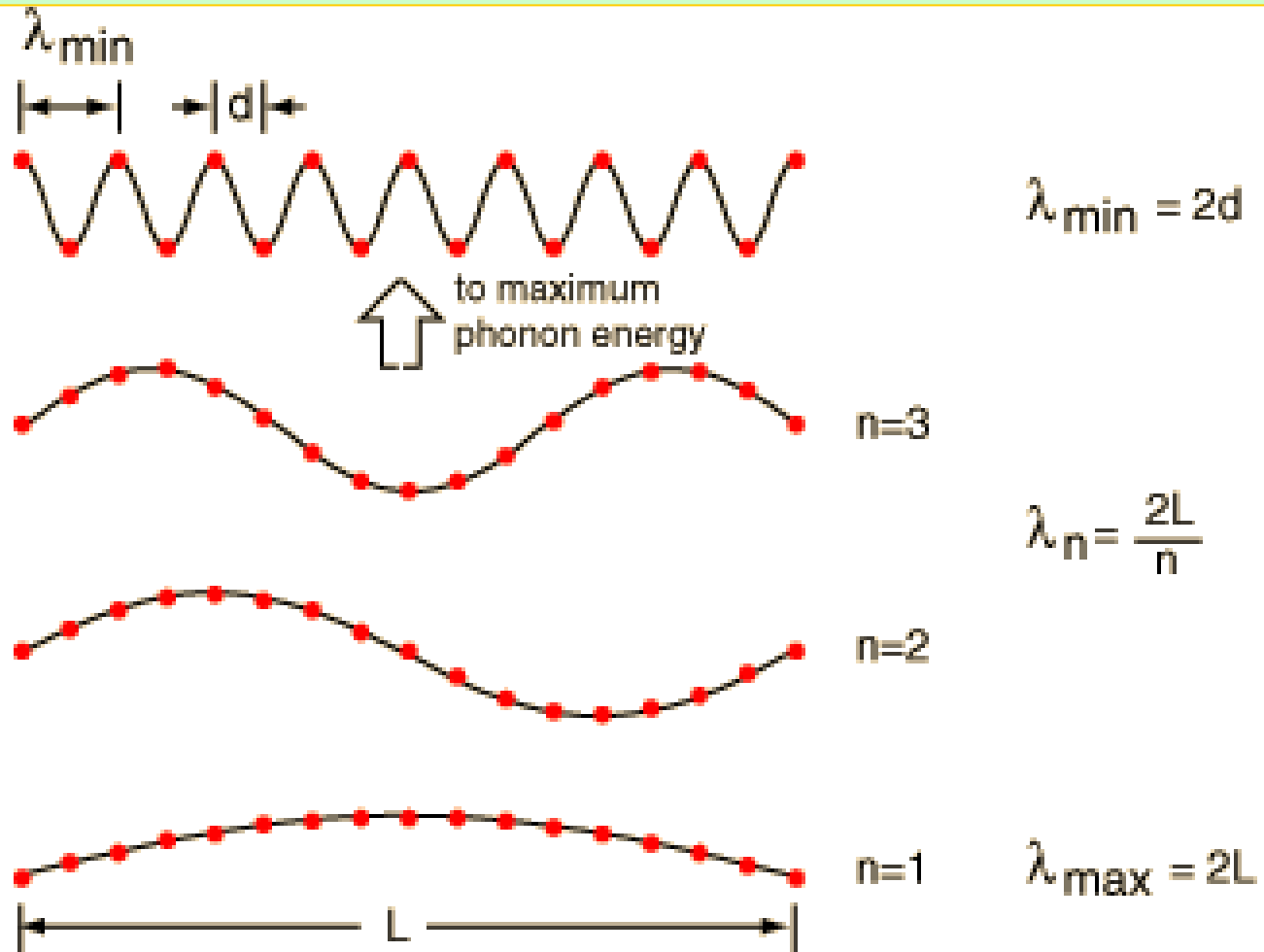
$$k = \frac{n\pi}{Na}, n = 1, 2, \dots, N$$

- It is usually convenient to consider phonon wave vectors \mathbf{k} which have the smallest magnitude ($|\mathbf{k}|$) in their "family". The set of all such wave vectors defines the *first Brillouin zone*. Additional Brillouin zones may be defined as copies of the first zone, shifted by some reciprocal lattice vector.

There are Acoustic and Optical Phonons

- Acoustic phonons occur when wave numbers are small (i.e. long wavelengths) and correspond to sound transmission in crystals. Acoustic phonons vary depending on whether they are longitudinal or transverse
- "Optical phonons," which arise in crystals that have more than one atom in the unit cell. They are called "optical" because in ionic crystals are excited very easily by light (by infrared radiation in NaCl). The positive and negative ions vibrate to create a time-varying dipole moment. Optical phonons that interact in this way with light are called *infrared active*.

Solid is a periodic array of mass points, there are constraints on both the minimum and maximum wavelength associated with a vibrational mode.



Quantization of Elastic Waves

The energy of an elastic mode of angular frequency ω is

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

It is quantized, in the form of phonons, similar to the quantization of light, as both are derived from a discrete harmonic oscillator model.

Elastic waves in crystals are made up of phonons. Thermal vibrations are thermally excited phonons.

Phonon Momentum

A phonon with a wavevector q will interact with particles, like neutrons, photons, electrons, as if it had a momentum (the crystal momentum)

$$\vec{p} = \hbar \vec{q}$$

- **Be careful!** Phonons do not carry momentum like photons do. They can interact with particles as if they have a momentum. For example, a neutron can hit a crystal and start a wave by transferring momentum to the lattice.
- **However,** this momentum is transferred to the lattice as a whole. The atoms themselves are not being translated permanently from their equilibrium positions.
- **The only exception** occurs when $q = 0$, where the whole lattice translates. This, of course, does carry momentum.