Lattice vibrations and Phonons

From the study of the atoms vibrations within the solid (lattice vibrations), the objective of this chapter is to deal with the concept of Phonons (quantization of vibrational modes) and the thermal properties of solids.

<u>1D lattice model</u>

For simplicity we consider, first, a 1D crystal lattice and assume that the forces between the atoms in this lattice are proportional to relative displacements from the equilibrium positions (Hooke's law).
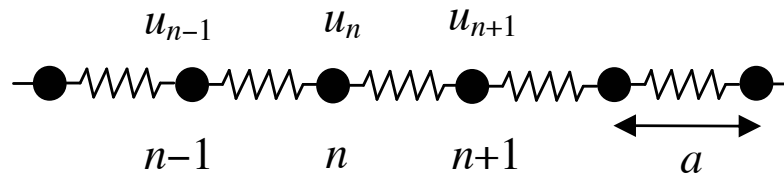
This is known as the harmonic approximation, which holds well provided that the displacements are small. U_n is the displacement of an atom from its equilibrium position $x_n = na$.

$$F_n \quad C(u_n \quad u_n) \quad C(u_n \quad u_n)$$

Lattice vibrations
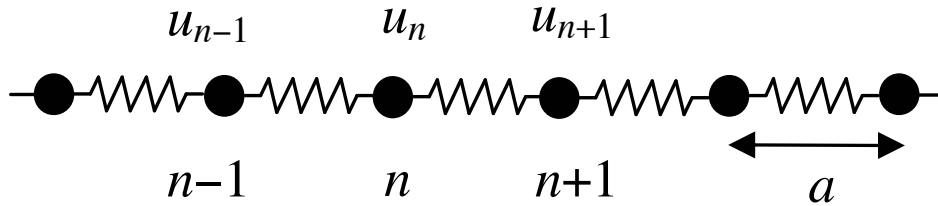
One might think about the atoms in the lattice as interconnected by elastic springs.
Therefore, the force exerted on n-the atom in the lattice is given by:
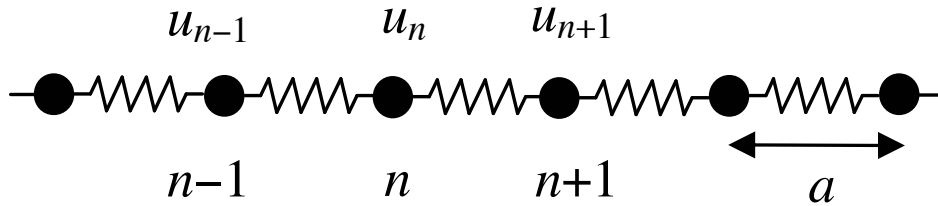
$$F_n = C(u_{n+1} - u_n) + C(u_{n-1} - u_n)$$

where C is the interatomic force (elastic) constant.

Applying Newton's second law to the motion of the n-th atom we obtain:

$$M\frac{d^2 u_n}{dt^2} = F_n = C(u_{n+1} - u_n) + C(u_{n-1} - u_n) = -C(2u_n - u_{n+1} - u_{n-1})$$

M is the mass of the atom. We neglect here the interaction of the n-th atom with all but
its nearest neighbors

$u_{n-1} \quad\quad u_n \quad\quad u_{n+1}$

$n{-}1 \quad\quad n \quad\quad n{+}1 \quad\quad a$

We end with N coupled differential equations, which should be solved simultaneously (N being the total number of atoms in the lattice).
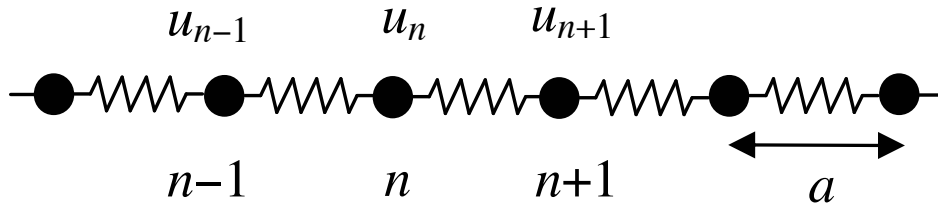
u_n)Now let us attempt a solution of the form:

$$u_n = A e^{i(q x_n - \omega t)}$$

where x_n is the equilibrium position of the n-th atom so that $x_n = na$.
U_n is a traveling wave, in which all the atoms oscillate with the same frequency ω, same amplitude A and same wave-vector q.

) $\quad C(u \quad_1 \quad u) \quad\quad C(2u \quad u \quad_1 \quad u \quad_1)$
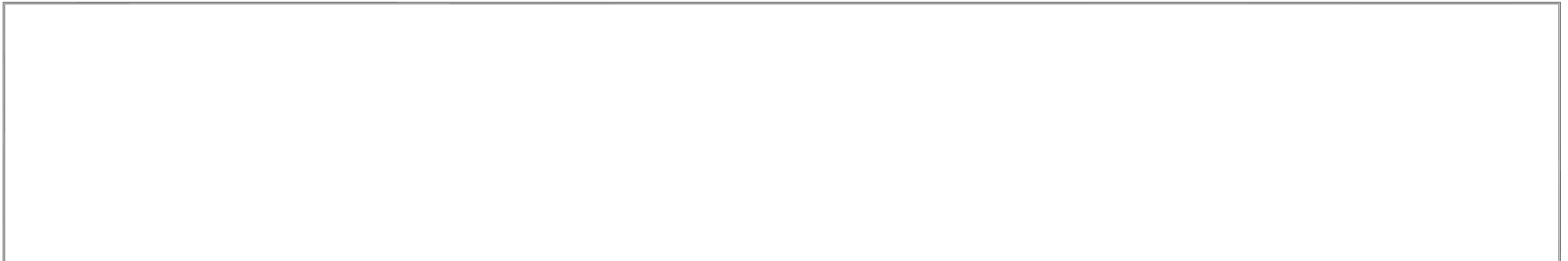
Lattice vibrations

$$u_{n-1} \quad u_n \quad u_{n+1}$$

$$n-1 \quad n \quad n+1 \quad a$$
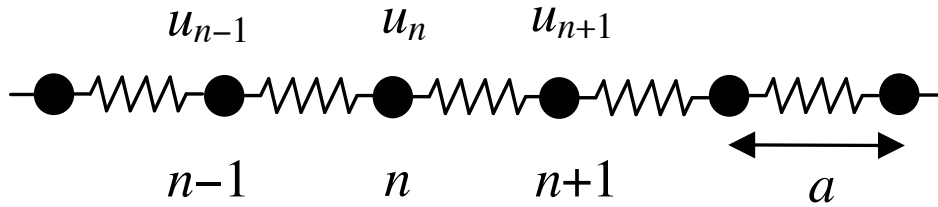
$$u_n = Ae^{i(qx_n - \omega t)}$$

$$M(-\omega^2)Ae^{iqna}e^{-i\omega t} = -C\{2Ae^{iqna}e^{-i\omega t} - Ae^{iq(n+1)a}e^{-i\omega t} - Ae^{iq(n-1)a}e^{-i\omega t}\}$$

$$M\omega^2 = C\{2 - e^{iqa} - e^{-iqa}\}$$

$$M\omega^2 = 2C\{1 - \cos qa\}$$

After some maths, Newton's second law becomes: $\quad M\omega^2 = 4C \sin \dfrac{qa}{2}$
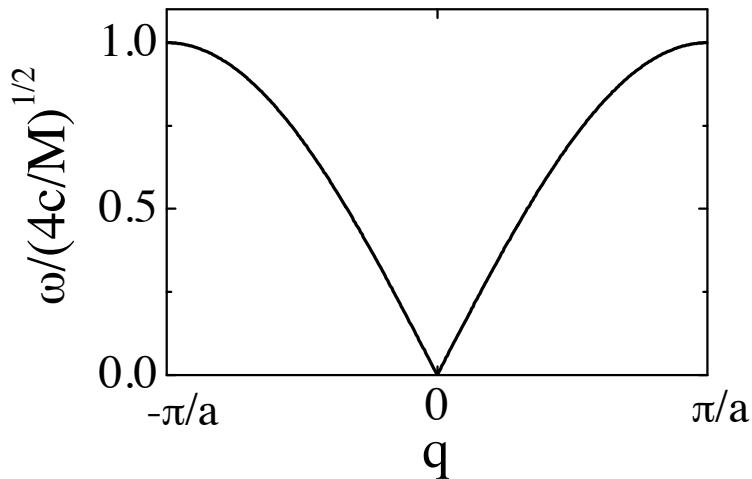
$$\frac{qa}{2}$$

$$u_{n-1} \qquad u_n \qquad u_{n+1}$$

$$n-1 \qquad n \qquad n+1 \qquad a$$

We find therefore the **dispersion relation** for the frequency:

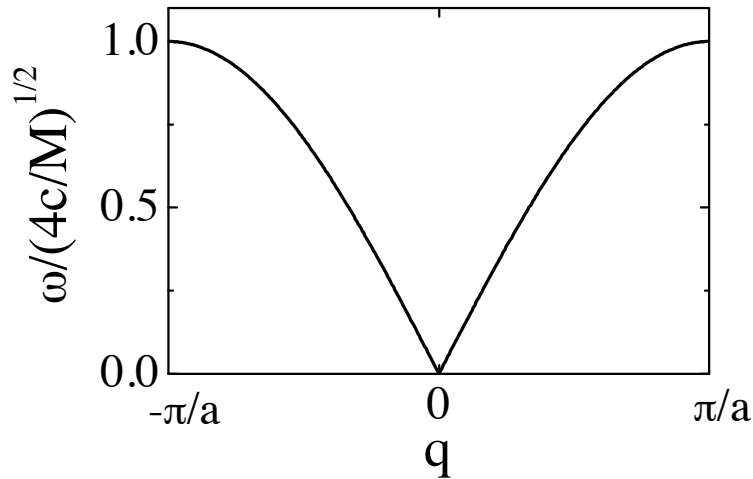$$\omega = \sqrt{\frac{4C}{M}} \left| \sin \frac{qa}{2} \right|$$

u_n) *Reducing to the first Brillouin zone.*

$$U_n\left(q + \frac{2\pi}{a}\right) = A e^{i(qna-\omega t)} e^{i2\pi n} = A e^{i(qna-\omega t)}$$

$$C(u \quad u \quad 0.5 \qquad C(2u \quad u_1 \quad u_1)$$

$$U_n\left(q + \frac{2\pi}{a}\right) = U_n(q)$$
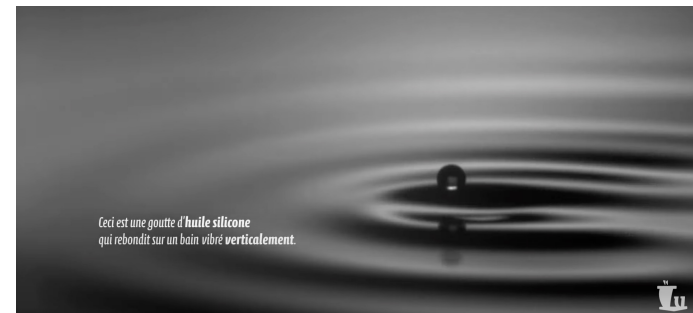
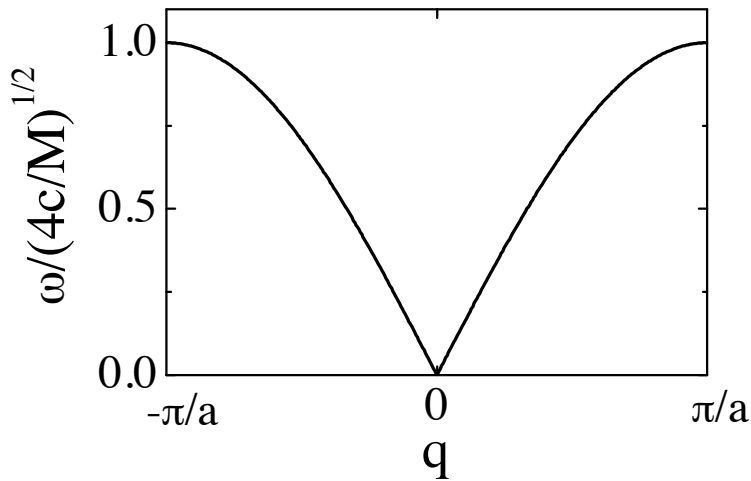$$-\frac{\pi}{a} \leq \quad \leq \frac{\pi}{a}$$

The frequency is symmetric with respect to the sign change in q.

$4C/M$ A mode with positive q corresponds to the wave traveling in the lattice from the left to right and a mode with a negative q corresponds to the wave traveling from the right to the left.

$4C/M$

At the boundaries of the Brillouin zone $q=\pm\pi/a$ the solution represents a standing wave: $u_n = A(-1)^n e^{-i\omega t}$ atoms oscillate in the opposite phases depending on whether n is even or odd.

$$= \frac{\omega}{q}$$

https://www.youtube.com/watch?v=QCiTD_9lE_0

Ceci est une goutte d'**huile silicone** qui rebondit sur un bain vibré **verticalement**.

$$Ca \cos \frac{qa}{2}$$

$$Ca \cos \frac{qa}{2}$$

Long wave-lenght limit: frequency of vibration is proportional to the wavevector = velocity is independent of frequency.
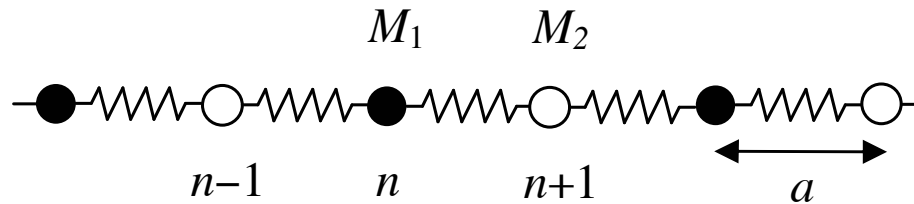
$$\omega = \sqrt{\frac{C}{M}} qa$$

$4C / M$

$$v_p = \frac{\omega}{q} = \sqrt{\frac{C}{M}} a$$ This is the velocity of sound for the one dimensional lattice

$$q \qquad \frac{C}{M} a$$

Diatomic 1D lattice model

Now we consider a one-dimensional lattice with two non-equivalent atoms in a unit cell.

1

M_1 M_2

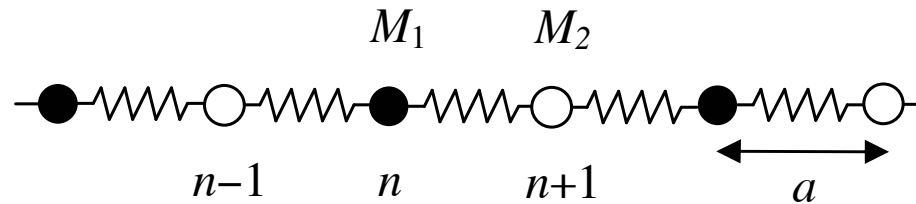
$n-1$ n $n+1$ a

In the present case because we have two different kinds of atoms, we should write two equations of motion:

(2   ) $M_1 \dfrac{d^2 u_n}{dt^2} = -C(2u_n - u_{n+1} - u_{n-1})$

dt $C(2u_n \quad u_n \quad u_n)$ $M_2 \dfrac{d^2 u_{n+1}}{dt^2} = -C(2u_{n+1} - u_{n+2} - u_n)$

Diatomic 1D lattice model

Now we consider a one-dimensional lattice with two non-equivalent atoms in a unit cell.

M_1 M_2

$n{-}1$ n $n{+}1$ a

Solution in the form of traveling mode for the two atoms:

$$(2 \qquad \qquad) \begin{bmatrix} u_n \\ u_{n+1} \end{bmatrix} = \begin{bmatrix} A_1 e^{iqna} \\ A_2 e^{iq(n+1)a} \end{bmatrix} e^{-i\omega t}$$

dt $C(2u_n \quad u_n \quad u_n)$

M_1 M_2

n–1 n n+1 a

$e^{i\omega t}$
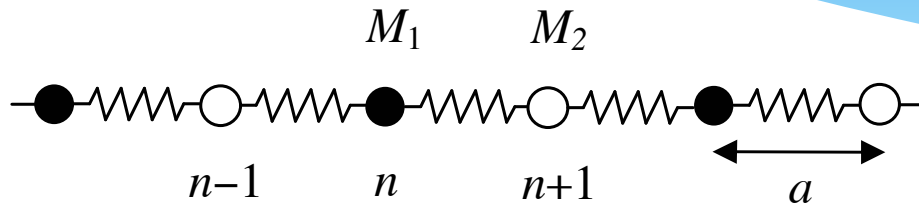
$$\begin{cases} M_1 A_1 \omega^2 = C\{2A_1 - A_2 e^{iqa} - A_2 e^{-iqa}\} \\ M_2 A_2 \omega^2 = C\{2A_2 - A_1 e^{iqa} - A_1 e^{-iqa}\} \\ \end{cases}$$

Sous forme matricielle :

$$\begin{pmatrix} 2C - M_1 \omega^2 & -2C \cos qa \\ -2C \cos qa & 2C - M_2 \omega^2 \end{pmatrix} \begin{pmatrix} A_1 \\ A_1 \end{pmatrix} = 0$$
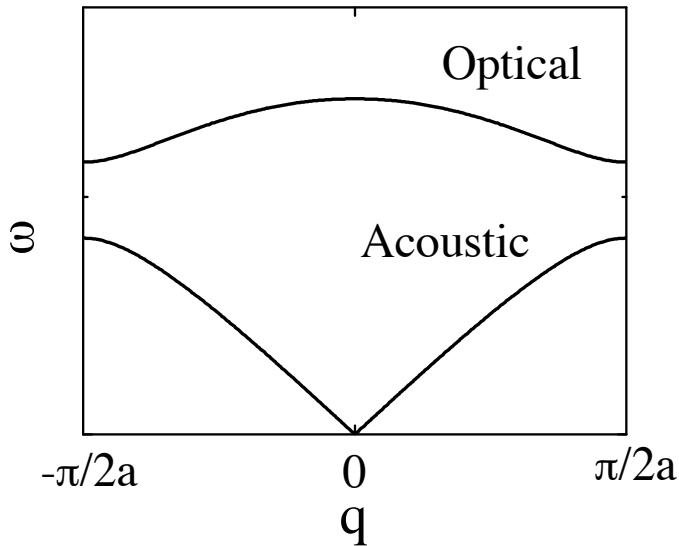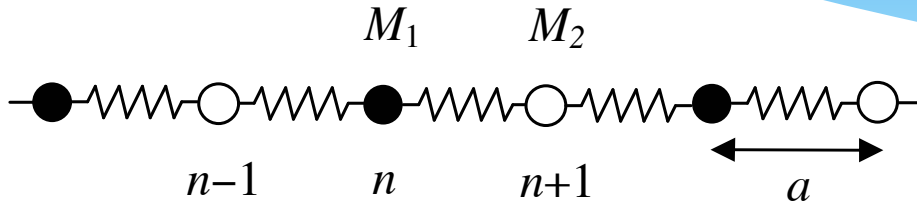
u_n u_n)

Then secular determinant to be solved :

$$\begin{vmatrix} 2C - M_1 \omega^2 & -2C \cos qa \\ -2C \cos qa & 2C - M_2 \omega^2 \end{vmatrix} = 0$$

$$(2 \quad - \quad)(2 \quad - \quad) - 4 \quad \cos \quad = 0$$

2 different solutions corresponding to **2 different dispersion curves**:

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

Lattice vibrations

qa

M_1 M_2

$n-1$ n $n+1$ a

Optical

ω

Acoustic

u_n $u_n)$
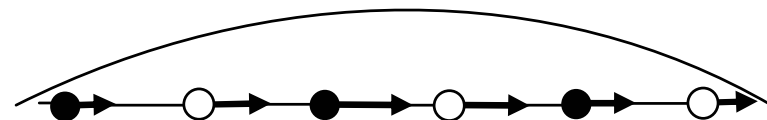
-π/2a   0   π/2a

q

The distinction between the acoustic and optical branches of lattice vibrations can be seen most clearly by comparing them at $q=0$ (infinite wavelength).

$$\begin{pmatrix} 2C & -2C \\ -2C & 2C \end{pmatrix} \begin{pmatrix} A_1 \\ A_1 \end{pmatrix} = 0$$
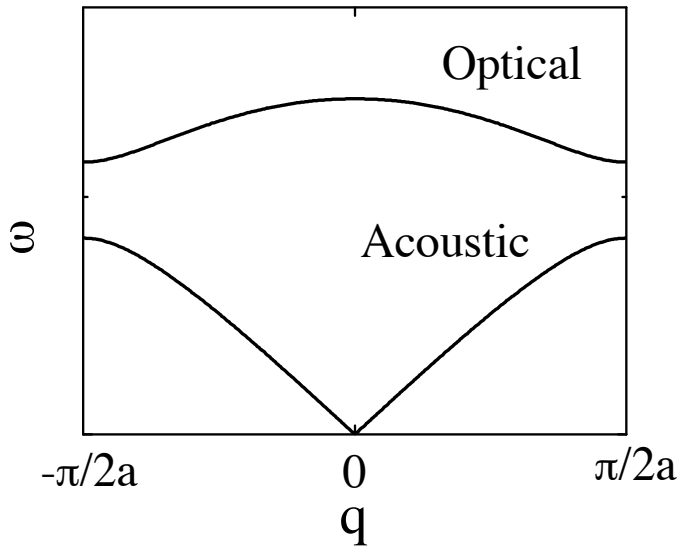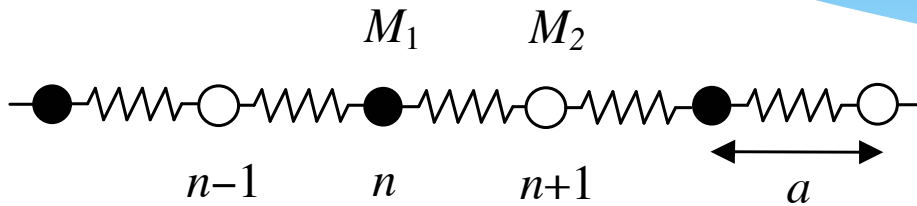
Then $A_1 = A_2$

For the acoustic branch $q=0$, $\omega=0$ and $A_1=A_2$. So in this limit the two atoms in the cell have the same amplitude and the phase.
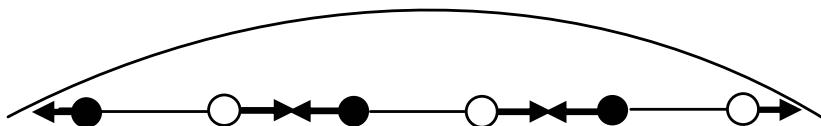
Acoustic

Lattice vibrations

qa

M_1 M_2

$n-1$ n $n+1$ a

-π/2a   0   π/2a

q

Optical

Acoustic

ω

u_n u_n)

For the optical branch, the two atoms move in out of phase. The frequency of these vibrations lies in infrared region which is the reason for referring to this branch as optical.

$$\begin{pmatrix} 2C(1 - M_1(\frac{1}{M_1} - \frac{1}{M_2})) & -2C \\ -2C & 2C(1 - M_1(\frac{1}{M_1} - \frac{1}{M_2})) \end{pmatrix} \begin{pmatrix} A_1 \\ A_1 \end{pmatrix} = 0$$

$$A_2 = -\frac{M_1}{M_2} A_1$$

Optical

Extension to 3D lattice

To avoid mathematical details we shall present only a qualitative discussion. First, the solution of this equation in three dimensions can be represented in terms of normal modes:

$$\mathbf{u} = \mathbf{A}e^{i(\mathbf{q}\mathbf{r}-\omega t)}$$

✓ wave vector $\mathbf{q}$ = wavelength and direction of propagation
✓ vector $\mathbf{A}$ = amplitude as well as direction of vibration of the atoms

The wave is defined as longitudinal if $\mathbf{A}$ is parallel to $\mathbf{q}$
And transverse when $\mathbf{A}$ is perpendicular to $\mathbf{q}$.

If there are s atoms per cell, there are 3s dispersion curves = 3 branches are acoustic, and the remaining (3s −3) are optical.

$= (\quad +\frac{1}{2})\hbar\omega$

$\hbar\omega \qquad \hbar\omega$
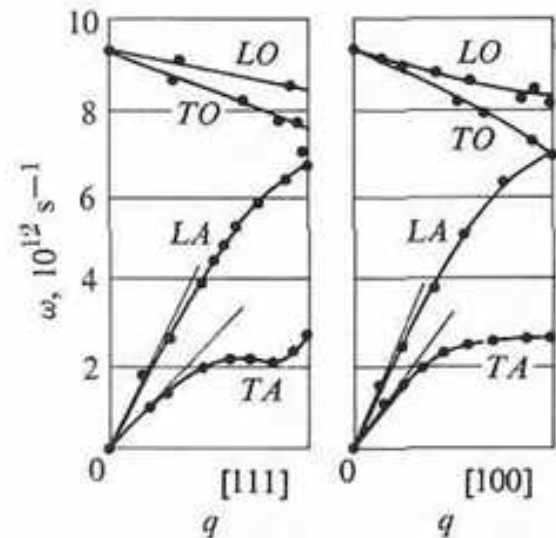
So far we discussed a classical approach to the lattice vibrations, but as we know from quantum mechanics the energy levels of the harmonic oscillator are quantized.
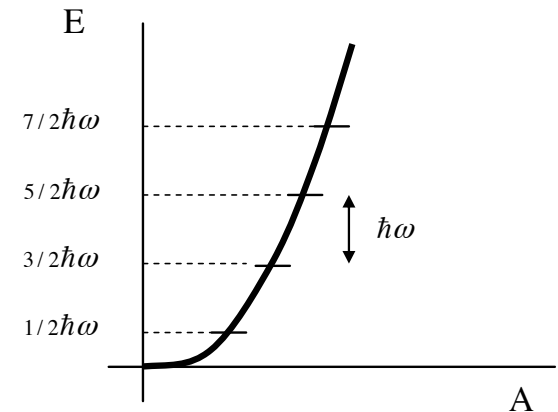
Energy levels of lattice vibrations are quantized.

Phonon = quantum of lattice vibration

Energy of normal mode of vibration: $\quad E = (n + \frac{1}{2})\hbar\omega$

Total energy = sum over all phonons modes

$$E = \sum_{\mathbf{q}p} E_{\mathbf{q}p} = \sum_{\mathbf{q}p} (n_{\mathbf{q}p} + \frac{1}{2})\hbar\omega_p(\mathbf{q})$$

where $n_{\mathbf{q}p}$ is the « occupation number » (number of phonons of energy $\hbar\omega$) of the normal mode of vibration p characterized by the wave vector $\mathbf{q}$.