Soln. The number of atoms in primitive unit cell of $BaTiO_3$ is

$$p = 8\times\frac{1}{8} + 6\times\frac{1}{2} + 1 = 5$$

Therefore, the total number of branches $= 3p = 3\times 5 = 15$.

The number of acoustical branches = 3.

The number of optical branches $= 3p - 3 = 15 - 3 = 12$.

Correct option is (a)

Phonons:

We know that the energy of an electromagnetic wave is quantized and the quanta of this energy is known as photon. In a similar way, the energy of lattice vibration or an elastic wave is also quantized and the quanta of lattice vibration is called as phonon. All types of lattice vibrations in crytals comprise of phonons. Thermal vibrations are thermally excited phonons, sound waves are acoustical phonons and excitations of the branch generate optical phonons.

The energy of phonon is given by $\hbar\omega$, where ω is the angular frequency of a mode of vibration.

If n is the number of phonons in a particular mode of vibration, the total energy of that mode is $n\hbar\omega$, where n can be zero or a positive integer.

Characteristic of Phonons:

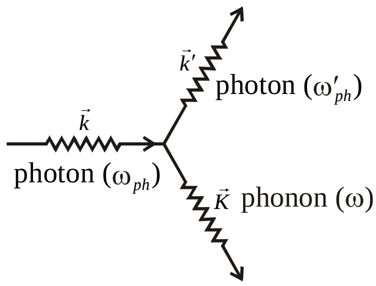
1. Phonons, like photons, have wave-particle duality.
2. Phonons are indistinguishable particles and have integral spin and hence, obey Bose Einstein statistics like photons.
3. The energy of a phonon is taken as $h\nu$, where h is the Planck's constant and ν is the frequency of lattice vibration.
4. The momentum of a phonon, like that of photon, is given by de-Broglie relation $p = \hbar k = \frac{h}{\lambda}$, where k is the wave vector of the phonon. $\hbar k$ is sometimes called crystal momentum. A phonon on a lattice does not really possess any momentum, but for most practical cases it behaves as it carries a momentum $\hbar k$.
5. Phonons travel with velocity of sound in a solid medium, whereas photons travel with the velocity of light in vacuum.
6. A crystal may be regarded as a phonon gas. The number of phonons in crystal can be increased or decreased by raising or lowering the temperature respectively.
7. The thermal energy of a solid is due to the energy of the phonons in it.
8. The interaction between two phonons or between one phonon and one electron can be considered as a scattering collision between two particles.

Momentum of phonons: Physically, a lattice phonon does not carry any momentum, but it interacts with other particles and fields as if it has a momentum $\hbar\vec{K}$, where $\vec{K}$ represents the wavevector of the phonon. Also from the de-Broglie relation $p = \frac{h}{\lambda} = \hbar\left|\vec{K}\right|$.

Thus, it is apparent that a phonon of wavelength λ carries a momentum $\hbar\vec{K}$. This momentum is also known as crystal momentum.

The wavevector conservation law for elastic scattering or the Bragg's diffraction of X-ray photons from crystal is given by $\vec{k}' = \vec{k} + \vec{G}$, where $\vec{k}'$ and $\vec{k}$ represent the wavevectors for the scattered and incident photons respectively and $\vec{G}$ is the reciprocal lattice vector. The conservation of momentum and energy gives

$\hbar\vec{k}' = \hbar\vec{k} + \hbar\vec{G}$ and $\hbar\omega_{ph} = \hbar\omega'_{ph}$. Such a process in which the frequency of the incident photon is the same as that of the scattered photon is called **normal or *N*-process**.



Inelastic scattering of incident photon to produce scattered photon alongwith the emission of a phonon.

In case of inelastic scattering, the wavevector conservation law is given by $\vec{k}' + \vec{K} = \vec{k} + \vec{G}$.

Accordingly, the conservation of momentum and conservation of energy gives

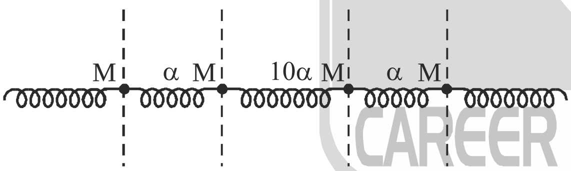
$\hbar\vec{k}' + \hbar\vec{K} = \hbar\vec{k} + \vec{G}$ and $\hbar\omega'_{ph} + \hbar\omega = \hbar\omega_{ph}$, (where ω is the frequency of the phonon).

Such a process is called **umklapp or U-process**.

SOLVED PROBLEMS

1. Consider a linear chain in which the force constants between nearest neighbour atoms are α and 10α alternately. Let the masses be equal and the nearest neighbour separation be $\frac{a}{2}$. For the normal modes, calculate $\omega(k)$ at $k = 0$ and $\frac{\pi}{a}$ and sketch the dispersion relation. **[JNU 2016]**

Soln.



Equations of motion are given by

$$M\frac{d^2\mu_s}{dt^2} = 10\alpha(v_s - u_s) - \alpha(u_s - v_s)$$

where, v_s and u_s are the displacement of adjacent planes.

$$M\frac{d^2v_s}{dt^2} = 10\alpha(u_s - v_s) - \alpha(v_s - u_{s+1}) = \alpha(10u_s + u_{s+1} - 11v_s)$$

Plane wave solution will be

$$u_s = u_0 e^{-i(\omega t - sk_a)};\ v_s = v_0\, e^{-i(\omega t - sk_a)}$$

$$\Rightarrow \quad -M\omega^2 u = \alpha\left(10v_0 + v_0\, e^{-ika} - 11u_0\right)$$

$$-M\omega^2 v = \alpha\left(10u_0 + u_0\, e^{ika} - 11v_0\right)$$

Solving, we get

$$M^2\omega^4 - 22M\omega^2\alpha + 20\alpha^2(1 - \cos ka) = 0$$