PHONONS: Quantization of Lattice Vibrations

According to the quantum theory, electromagnetic energy (light) comes in packets of energy we call **photons**. Since there is energy in lattice vibrations as well, this energy will also be quantized, and we will call these packets of vibrational energy: **phonons**.

1. Energy of phonons:

From the **quantum theory**, the energy of a harmonic oscillator ($PE = \frac{1}{2}kx^2$ put into Schrodinger's Equation) is calculated to be:

$\mathbf{E_{HO} = (n+\frac{1}{2})\hbar\omega}$ (recall that $\hbar = h/2\pi$; ω is the angular frequency).

As in the previous sections we will use **Ω for the frequency of vibration in the solid** to distinguish it from the **ω for the frequency of vibration of an E&M wave**.

Note that even with n=0 there is still a non-zero energy!

From the equipartition of energy theorem, the energy should be equally divided (on average) between each way of having energy (between each degree of freedom). For a harmonic oscillator (mass on a spring), we can have both kinetic energy ($\frac{1}{2}mv^2$) and potential energy ($\frac{1}{2}kx^2$). Thus, the time average (denoted by < >) of the energy is:

$$\langle E_{total}\rangle = (n+\tfrac{1}{2})\hbar\omega = \langle KE + PE\rangle = \langle KE\rangle + \langle PE\rangle ,$$

and from equipartition of energy: $\langle KE\rangle = \langle PE\rangle$, we have

$$\langle E_{total}\rangle = 2\langle KE\rangle , \quad \text{or} \quad \mathbf{\langle KE\rangle} = \tfrac{1}{2}\langle E_{total}\rangle = \mathbf{\tfrac{1}{2}(n+\tfrac{1}{2})\hbar\Omega} .$$

For one wave, the kinetic energy (on average) = $N \frac{1}{2} m v^2$ where N = number of atoms in the crystal, m is the mass of one atom, and $v = du_s/dt$ is the speed where $u_s = u_o e^{iKsa} e^{i\Omega t}$. Note that this v in the KE is the speed of the vibrating atoms, not the phase speed of the wave.

Now Nm = total mass of crystal = $M = \rho V$ (where ρ is the density = M/V, and V is the volume). We can also write the oscillatory parts in terms of sines or cosines instead of exponentials. Therefore, we can write velocity as:

$$v = du_s/dt = d[u_o \cos(Ksa)\cos(\Omega t)]/dt = -\Omega u_o \cos(Ksa)\sin(\Omega t) ,$$

and so the time average of the kinetic energy becomes:

$$\langle KE\rangle = \tfrac{1}{2}\rho V \Omega^2 u_o^2 \cos^2(Ksa)\langle\sin^2(\Omega t)\rangle .$$

The time average of $\sin^2(\Omega t)$ is ½, and the average over the length of $\cos^2(Ksa)$ is also ½. [We can easily see this since the average of $\langle 1\rangle$ is 1, and $\langle 1\rangle = \langle\sin^2\theta + \cos^2\theta\rangle$, and on average $\langle\sin^2\theta\rangle = \langle\cos^2\theta\rangle$; therefore $\langle\cos^2\theta\rangle = \frac{1}{2}$!]

Therefore we get:

$$\langle KE\rangle = (1/8)\rho V \Omega^2 u_o^2 ; \quad \text{and from above:} \quad \langle KE\rangle = \tfrac{1}{2}(n+\tfrac{1}{2})\hbar\Omega ;$$

putting these two equations together and solving for u_o gives:

$$\mathbf{u_o^2 = [4(n+\tfrac{1}{2})\hbar] / [\rho V \Omega]} \quad \text{(amplitude and energy are quantized!).}$$

This relates the square of the amplitude of the oscillation to the quantum number of the energy. The more the energy, the higher the quantum number and the higher the u_o. Note also that the **square** of the amplitude (and the square of the frequency) is related to the energy as is the case for all waves (E&M, sound, etc.), $\langle E_{total}\rangle = 2\langle KE\rangle = \frac{1}{4}\rho V \Omega^2 u_o^2$.

The fact that energy is quantized means that **energy is not continuous** – it comes in **discrete units**, and it is these discrete units that we call **phonons**, with $\langle E_{total} \rangle = \mathbf{(n+½)\hbar\Omega}$, where n is the number of these phonons. The vibrational wave is spread out throughout the solid with $\langle E_{total} \rangle = ¼\rho V\Omega^2 u_o^2$, (note that $u_o^2 \propto 1/\Omega$) but the wave/particle duality comes into play here in that the phonon is localized (as a particle). The wave gives the probability of finding the particle (phonon) at a particular position at a particular time.

We saw this with the diffraction of light – when light goes through an opening, the wave spreads out into a diffraction pattern. However, if we have just one photon going through the opening, that photon will hit at one particular place. If we send a lot of photons through, either one by one or all together, they will hit in such a way as to produce the diffraction pattern as indicated by the wave idea. The same thing happens with the vibrational wave/phonon situation here. The integer n in the above formulas can be interpreted as the number of phonons which is related to the square of the amplitude of the vibrational wave. The wave/particle duality is WEIRD, but IT WORKS!

2. Momentum of phonons:

From the DeBroglie relation, $|\mathbf{p}| = h/\lambda = \hbar|\mathbf{K}|$ ($\mathbf{p}$ is momentum, $|\mathbf{K}| = 2\pi/\lambda$)

3. Scattering of light and phonons:

a) As we saw before, for **elastic** scattering of x-rays:

$$\mathbf{k'} = \mathbf{k} + \mathbf{G}, \quad \omega'=\omega, \quad \text{and} \quad \lambda'=\lambda \quad \text{so} \quad |\mathbf{k'}|=|\mathbf{k}| \quad ;$$

the energy of the x-ray does not change (this is what we mean by elastic) so the frequency of the x-ray does not change, and hence the wavelength of the x-ray does not change, and hence the magnitude of k doesn't change - but the direction does! This seems to violate the conservation of momentum since momentum is a vector. But consider the momentum associated with $\hbar\mathbf{K}$ when $\mathbf{K}=\mathbf{G}$: the group velocity of an oscillation of wavevector $\mathbf{K}=\mathbf{G}$ is zero! [See notes on Monatomic Lattice Vibrations, step 6 on Group velocity.] We interpret this as there being no momentum in the wave of wavevector $\mathbf{K}$ but instead there being a momentum of the whole crystal. Since the photon has such a small momentum compared to the crystal, any change in momentum due to its interaction with the whole crystal will be negligible as far as the crystal as a whole is concerned. [If we hit a crystal with enough photons, we could get the crystal to move. That is, we could have a rocket pushing out photons instead of gas molecules. The engineering aspects of this are not sufficiently advanced as to make this an everyday occurrence yet although theoretically this would be the most efficient use of fuel for a rocket.] Thus by adding $\mathbf{G}$ vectors to our conservation of momentum equation we are not introducing any phonon momentums, only introducing slight changes in the momentum of the entire crystal.

b) For **inelastic** scattering of x-rays we must take into account not only conservation of energy (energy of E&M wave and also energy of lattice vibrations) but also conservation of momentum (momentum of E&M wave and momentum of lattice vibration):

$$\mathbf{k'} \pm \mathbf{K} = \mathbf{k} + \mathbf{G} \qquad [\text{conservation of momentum with } \mathbf{p}_{E\&M} = \hbar\mathbf{k} \text{ and } \mathbf{p}_{lattice} = \hbar\mathbf{K}\,]$$

$$\omega' \pm \Omega = \omega \qquad [\text{conservation of energy with } E_{E\&M} = \hbar\omega \text{ and } E_{lattice} = \hbar\Omega\,]\,;$$

(here $\omega' \neq \omega$ and the magnitude of k does change: $|\mathbf{k'}| \neq |\mathbf{k}|$).

Homework problem 15 *is about the momenta and energies of photons and phonons.*