FYS3410 - Module II

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We are presented with the situation of a one-dimensional system of atoms. We would like to know the density of states while using periodic boundary conditions. Let N be the number of atoms in such that atom number 0 and N is the same with the periodic boundary conditions. The distance between each atom is a so the total length of the chain of atoms becomes $L = Na$.

a)

We describe the phonons by letting the atoms vibrate similarly to a plane wave. The displacement of atom s is described as

$$U_s = U_0 e^{ikas - i\omega t}$$

Using now the periodic boundary conditions we can get a quantization of the wavenumber

$$\begin{aligned} U_s &= U_{s+N} \\ U_0 e^{ikas} e^{-i\omega t} &= U_0 e^{ika(s+N)} e^{-i\omega t} \\ e^{ikas} &= e^{ikas} e^{ikaN} \\ e^{ikaN} &= 1 \end{aligned}$$

This is only true when

$$\begin{aligned} kaN = 2\pi n, &\qquad n \in \mathbb{Z} \\ k &= \frac{2\pi n}{Na} \end{aligned}$$

There is a physical restriction on the n's. From the relation between wavelength and wavenumber we have

$$\begin{aligned} \lambda &= \frac{2\pi}{k} \\ \lambda &= \frac{aN}{n} \end{aligned}$$

For the first mode $n = 1$ the wavelength is L, then there are N number of modes until $n = N$ and the wavelength becomes a. These are the only physically distinct modes we can have as wavelengths outside this region can not be described distinctly without more atoms (in a similar fashion as with Umklapp scattering). Since the k's are uniformly distributed with a distance $\frac{2\pi}{Na}$ the DENSITY (number of states pr. distance) becomes

$$D(k) = \frac{Na}{2\pi} = \frac{L}{2\pi}$$