3.6 Quantum mechanical description of lattice vibrations

Phonons are the quantum mechanical quasi particles which describe lattice vibrations. The Hamiltonian for an Eigenstate of the lattice vibration is

$$H = \hbar\omega(k,\lambda)\left(N + \frac{1}{2}\right) \qquad . \tag{3.31}$$

Here $\omega(k,\lambda)$ is the frequency of one Eigenvalue of the oscillation. N is the number of phonons which occupy this state; since phonons are Bosons, each state can be occupied with an arbitrary number of particles. The factor $1/2$ is the zero point energy of the vibration; this will be neglected in the further considerations. k is the momentum and λ the polarization. λ indicates the different vibration modes (orientation in space , longitudinal, transverse, acoustic, optic). The vibrational Eigenstates we get by diagonalization of the Hamiltonian as described in the last section for the 1D example.

As usual we apply periodic boundary conditions; so each state occupies a k space volume of $\left(\frac{2\pi}{L}\right)^3$. With the often used approximation we find for the complete number of states with momentum values smaller than $|\vec{k}| = k$

$$N(k) = \left(\frac{L}{2\pi}\right)^3 \frac{4}{3}\pi k^3 \qquad . \tag{3.32}$$

Therefor the density of states is

$$D(\omega) = \left(\frac{Vk^2}{2\pi^2}\right)\frac{dk}{d\omega} \qquad . \tag{3.33}$$

In order to apply the Eq. (3.4) to (3.9) we must calculate the density of states or the dispersion relation

$$\omega = \omega(k) \qquad . \tag{3.34}$$

For this we can take the exact solutions or the approximation of section 3.5, i.e. the Einstein- and Debye-model.