VIBRATIONS AND PHONONS
FYS3410: PROBLEM SHEET 2

CANDIDATE 33

2. Density of States (DOS) for Phonons

The phonon density of states in a one-dimensional array of N atoms is derived in the following.

2.a. **DOS as a function of wave-vector.** One can view the one-dimensional array of atoms as a ring where the first and the last atom is connected to each other. Such a boundary condition is known as a Born-von Karman boundary contition. This boundary implies that atom number n is the same atom as atom number $n+N$. The displacement of this atom is

$$\delta x_n = \delta x_{n+N}.$$

Applying Bloch's theorem[1] to this relation gives

$$\delta x_1 e^{ikan} = \delta x_1 e^{ika(n+N)},$$

where k is the wave-vector and a is the lattice parameter. To satisfy this condition we must have

$$1 = e^{ikaN} = \cos(kaN) + i\sin(kaN),$$

which only is satisfied if

$$2\pi\nu = kaN, \quad \nu = 1, 2, \ldots, N$$

which gives

$$k = \frac{2\pi}{Na}\nu.$$

The separation between allowed solution (k-values) is therefore

$$\Delta k = \frac{2\pi}{Na}. \tag{1}$$

Thus, in one dimension the density of states is

$$D(k) = \frac{1}{\Delta k} = \frac{Na}{2\pi} = \frac{L}{2\pi}. \tag{2}$$

One can easily see that the density of states (DOS) is independent of k, so the density of modes in k-space is uniformly distributed.

[1] $\psi(\mathbf{r}+\mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\psi(\mathbf{r})$

2.b. **DOS as a function of angular frequency.** A one-dimensional lattice with one atom in the basis can be modelled as a harmonic chain, where one imagines a spring connecting all the atoms. The dipsersion relation then becomes

$$\omega = \omega_0 \sin\frac{ka}{2}, \quad \omega_0 = 2\sqrt{\frac{g}{m}} \tag{3}$$

where ω is the angular frequency, g is the spring constant and m is the mass of each atom.

One can change between one density of states to the other by way of the following formula

$$D(\omega)d\omega = D(k)dk = \frac{Na}{2\pi}dk. \tag{4}$$

which can be rewritten to include the group velocity

$$D(\omega)d\omega = \frac{Na}{2\pi}\frac{dk}{d\omega}d\omega = \frac{Na}{2\pi}\frac{d\omega}{v_g}. \tag{5}$$

The group velocity is

$$v_g = \frac{dw}{dk} = \omega_0\frac{a}{2}\cos\frac{ka}{2}. \tag{6}$$

This equation is to be inserted in equation 5, but first we also need a function of ω instead of k which is found by inverting equation 3

$$\begin{aligned}
\omega &= \omega_0 \sin\frac{ka}{2} \\
\frac{\omega}{\omega_0} &= \sin\frac{ka}{2} \\
\frac{ka}{2} &= \arcsin\frac{\omega}{\omega_0} \\
k &= \frac{2}{a}\arcsin\frac{\omega}{\omega_0}.
\end{aligned}$$

This can now be inserted into the group velocity

$$\begin{aligned}
v_g &= \omega_0\frac{a}{2}\cos\left(\frac{a}{2}\frac{2}{a}\arcsin\frac{\omega}{\omega_0}\right) \\
&= \omega_0\frac{a}{2}\sqrt{1-\left(\frac{\omega}{\omega_0}\right)^2}.
\end{aligned}$$

inserting this expression into 5 yields

$$D(\omega) = \frac{N}{\pi\omega_0}\frac{1}{\sqrt{1-\left(\frac{\omega}{\omega_0}\right)^2}} \tag{7}$$

which is the density of states as a function of angular frequency.

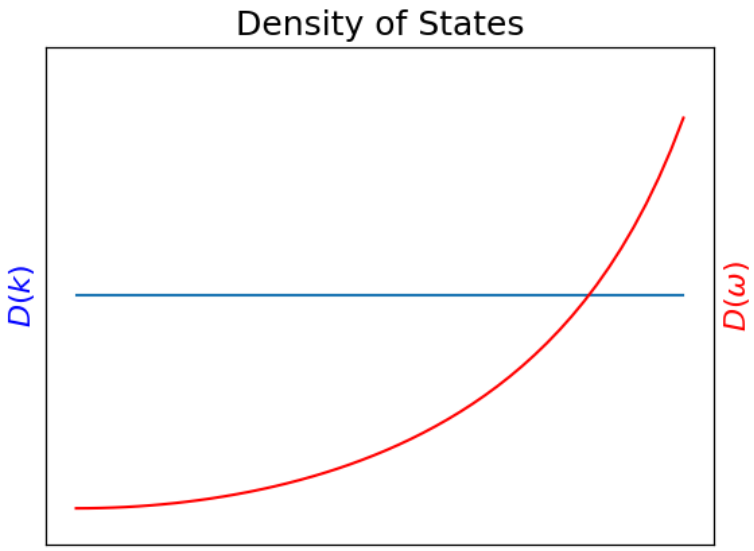

FIGURE 1. Comparison of density of states. $D(k)$ on the left axis and $D(\omega)$ on the right.

2.c. **Comparison of DOS measures.** A comparison of the two DOS measures that has been derived is shown in figure 1. The first y-axis is used for $D(k)$, and the second for $D(\omega)$. Because the density of states for k, $D(\omega)$ is constant for all k, this is much easier to deal with than the ever changing $D(\omega)$. The much more stable density of states i k-space is reason enough to use $D(\omega)$, but this one also has a closer connection with reciprocal space and diffraction patterns.