

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 condition. 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 theorem¹ 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

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

which gives

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

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

$$(1) \quad \Delta k = \frac{2\pi}{Na}.$$

Thus, in one dimension the density of states is

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

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 dispersion relation then becomes

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

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

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

which can be rewritten to include the group velocity

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

The group velocity is

$$(6) \quad v_g = \frac{d\omega}{dk} = \omega_0 \frac{a}{2} \cos \frac{ka}{2}.$$

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

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

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

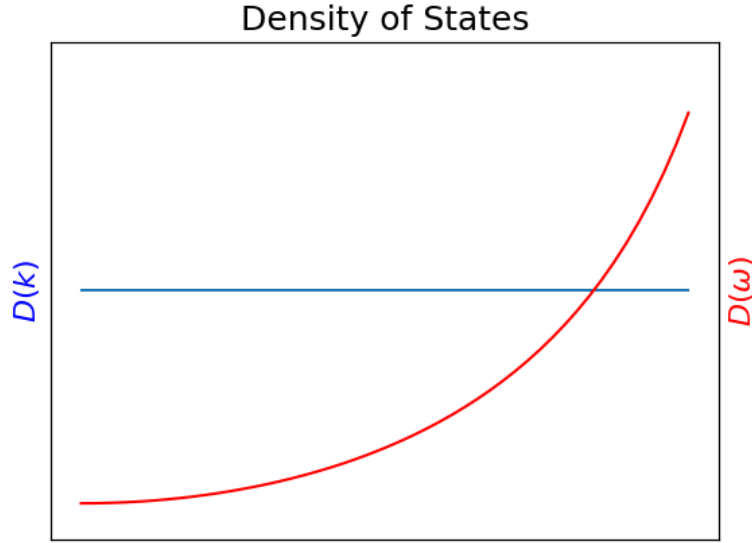


FIGURE 1. Comparison of density of states. $D(k)$ on the left axis and $D(\omega)$ on the right.

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 in k -space is reason enough to use $D(\omega)$, but this one also has a closer connection with reciprocal space and diffraction patterns.

3. DIFFERENT MODELS FOR TEMPERATURE-HEAT CAPACITY DEPENDENCE

3.a. Dulong-Petit. The Dulong-Petit law is a thermodynamic rule proposed in 1819 by French physicists Pierre Louis Dulong and Alexis Thirse Petit. They assume that every mode oscillates according to a classical harmonic oscillator, with continuous energy. In such a classical treatment, the thermal energy density is

$$(8) \quad u = \frac{1}{V} \frac{\int dV e^{-\beta H} H}{\int dV e^{-\beta H}} = -\frac{1}{V} \frac{\partial}{\partial \beta} \ln \int dV e^{-\beta H}$$

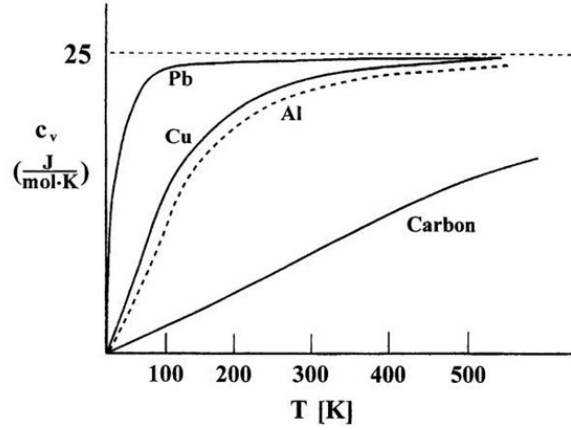


FIGURE 2. Measured heat capacities for lead, copper, aluminum and carbon. The horizontal line is the classical Dulong and Petit value.

where $\beta = 1/k_B T$ and H is the enthalpy. By making a change of variables, one finds that the integral equates to²

$$(9) \quad u = u_{eq} + 3nk_B T,$$

which yields the heat capacity

$$(10) \quad C_v = \frac{\partial u}{\partial T} = 3nk.$$

The heat capacity is a straight line, and measured heat capacities come quite close to the Dulong and Petit value. However, when temperature drops, the heat capacity falls well below the Dulong and Petit value. Moreover, when the temperature gets large, it seems fairly clear that the curve never quite reaches the precise value, as can be seen in figure 2. In conclusion, the law of Dulong and Petit is a reasonable approximating for higher temperatures.

3.b. Einstein.

3.c. Debye.

²I will not make the full calculation here, but rather stick to a brief description.