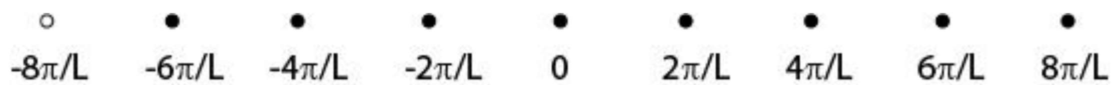
Summary Chapter 5 part 2.

As shown in Fig. 13, Debye's density of state approximation which assumes a constant phonon speed is only valid for low w value. For 3d crystals large differences are expected towards the cut-off frequency, ω_D. Kittel provides more general expressions for the density of states on pages 117-119 that can be used to calculate the density of states for arbitrary dispersion relations. To get appreciation for those expressions, let us revisit the 1D density of states calculation that we did earlier in the chapter. We focus here on the case with the periodic boundary conditions. K-space for a system with 8 atoms is shown in the figure below. You can see that the mode density in K-space is constant, i.e. for each $2\pi/L$ length of K-space there is one mode. So we have $L/2\pi$ modes per unit length of K-space.

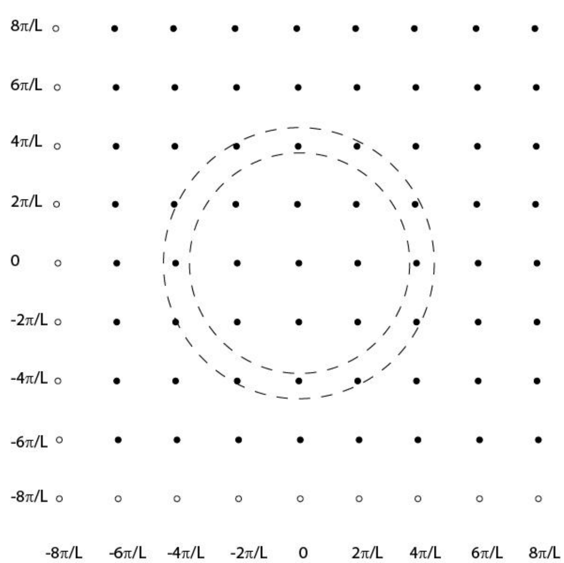


In order to convert this to a density of state as a function of ω we have to make assumptions about the dispersion relation, i.e. the relation between ω and K. Debye assumed a constant phonon velocity, i.e.

$$v|K| = \omega \qquad [1]$$

Note that there are two phonon modes at each frequency. One moving clockwise (positive K) and one moving counter clockwise (negative K) through the circular 1D system of Fig. 4.

Now let us look at a 2D system with the same dispersion. K-space for a 2D system consisting of 8x8 unit cells is plotted in the figure below. The mode density seems to be again constant through K-space. For every $(2\pi/L)^2$ surface area in K-space we have basically one mode. So the mode density is $(L/2\pi)^2$. Note that there are now much more than just two modes with approximately the same frequency. All the phonon modes situated between the two circles have approximately the same frequency.



So I expect the number of modes for large frequency or large |K|-value to be larger than the number of modes for small |K| value. From the figure above one can see that the number of modes between |K| and |K|+d|K| is expected to be proportional to the circumference of the circle, i.e. proportional to |K|. Note that both circles are constant ω contours because of the linear relation between ω and K. Since for our simplified dispersion relation w and K are linear proportional we expect the D(ω) will be linear with ω as well.

For the 3D case we expect that there are many more phonon modes with approximately the same ω value. Constant ω contours are now surfaces, i.e. spheres. The number of states between them will be proportional to the volume between a sphere of |K| and a sphere of |K|+d|K|. This volume will be proportional to the surface of a sphere, i.e. to $|K|^2$. With our simplified dispersion relation this suggests that D(ω) for the 3D case is linear proportional to ω^2.

Kittel found for the density of states:

$$D_{1D}(\omega) = \frac{L}{\pi} \frac{1}{d\omega / dK} \qquad [2]$$

$$D_{3D}(\omega) = \frac{VK^2}{2\pi^2} \frac{1}{d\omega / dK} \qquad [3]$$

Note that dω/dK is the group velocity. So the density of states depends on the phonon speed, or the dispersion relation, i.e. ω(K). Those areas of K-space that have a smaller slope will contribute stronger to the density of states. The figure below shows the dispersion relation for the 1D case we calculated in chapter 4. For higher K-vectors, the slope is smaller, so much more modes have approximately the same ω. In chapter 4 we calculated the dispersion relation for a simple 1D case, i.e. equation (7) of chapter 4. We could use that to find a more specific expression for $D_{1D}(\omega)$.

For 2D and 3D systems the analysis will be more complicated as the constant w contours are no longer circles and spheres but weird shaped surfaces in K-space. To find D(ω) we would need to determine the volume between the constant ω contours in K-space and divide by the K-gradient of w, i.e.

$$D(\omega) = \frac{V}{(2\pi)^3} \int \frac{dS_\omega}{|\nabla_K(\omega)|}$$

Where dS_ω is a small segment on a constant ω contour in K-space. More details are provided on page 117-119 in Kittel.