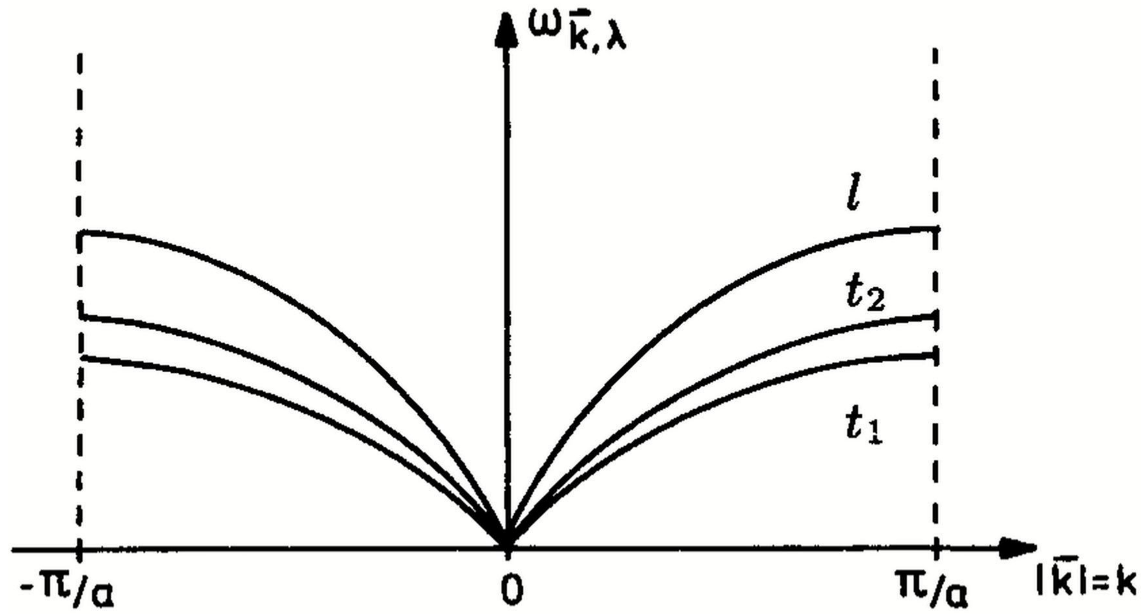
Chapter 3.9: The Debye Model

Debye (1911): Consider (known) vibrational eigenmodes in a solid, but use Einstein quantization
Then: Approximate dispersion for small energies.

Classical vibrational eigenmodes of a 3D monoatomic solid:

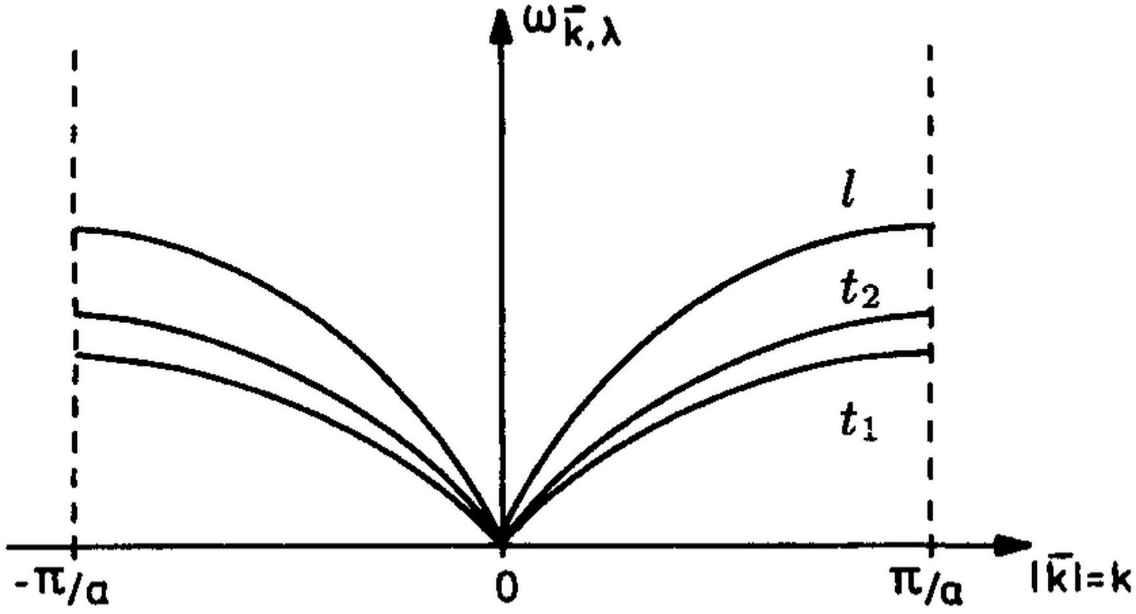
2 transverse and one longitudinal modes



Independent distinguishable modes: $\varepsilon = \sum_{\alpha} \sum_{\vec{k}} \varepsilon_{\vec{k},\alpha} = \sum_{\alpha} \sum_{\vec{k}} \hbar \omega_{\vec{k},\alpha} (n_{\vec{k},\alpha} + \frac{1}{2})$

$$Z_{\vec{k},\alpha} = \frac{1}{2\sinh(\beta\hbar\omega_{\vec{k},\alpha})} \qquad \ln Z = \sum_{\alpha} \sum_{\vec{k}} \ln Z_{\vec{k},\alpha}$$

$$c_V = \sum_{\alpha} \sum_{\vec{k}} k_B (\beta\hbar\omega_{\vec{k},\alpha})^2 \frac{e^{\beta\hbar\omega_{\vec{k},\alpha}}}{(e^{\beta\hbar\omega_{\vec{k},\alpha}} - 1)^2}$$



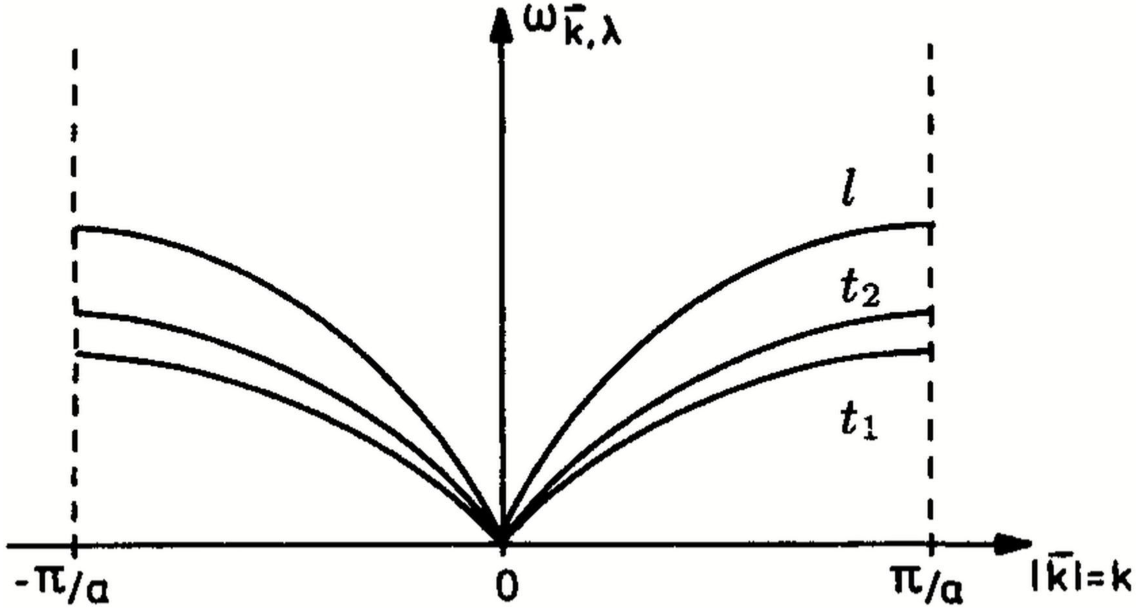
Debye approximation:

1.) The dispersion is linear and isotropic for all modes with an average velocity v

2.) The total number of modes is limited to $3N$. This determines a cutoff wavevector k_D.

3.) There is only one parameter for both the average velocity and the cutoff: $\omega_D = v k_D$

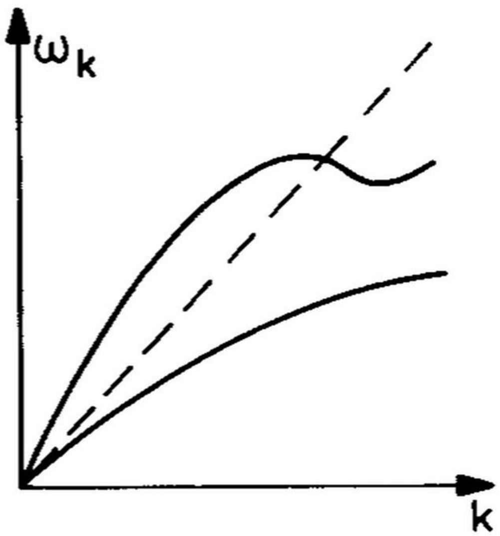
$$c_V = \sum_{\alpha} \sum_{\vec{k}} k_B (\beta\hbar\omega_{\vec{k},\alpha})^2 \frac{e^{\beta\hbar\omega_{\vec{k},\alpha}}}{(e^{\beta\hbar\omega_{\vec{k},\alpha}} - 1)^2}$$

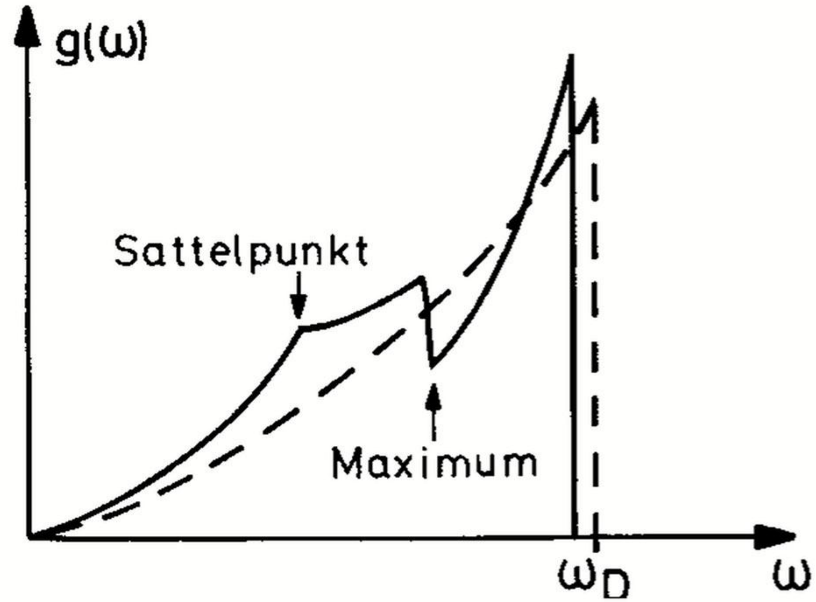


Debye density of (frequency) states:

$$\omega_{\vec{k},\alpha} \approx v\left|\vec{k}\right|$$

$$g(\omega) = \sum_{\vec{k},\alpha} \delta(\omega_{\vec{k},\alpha} - \omega)$$



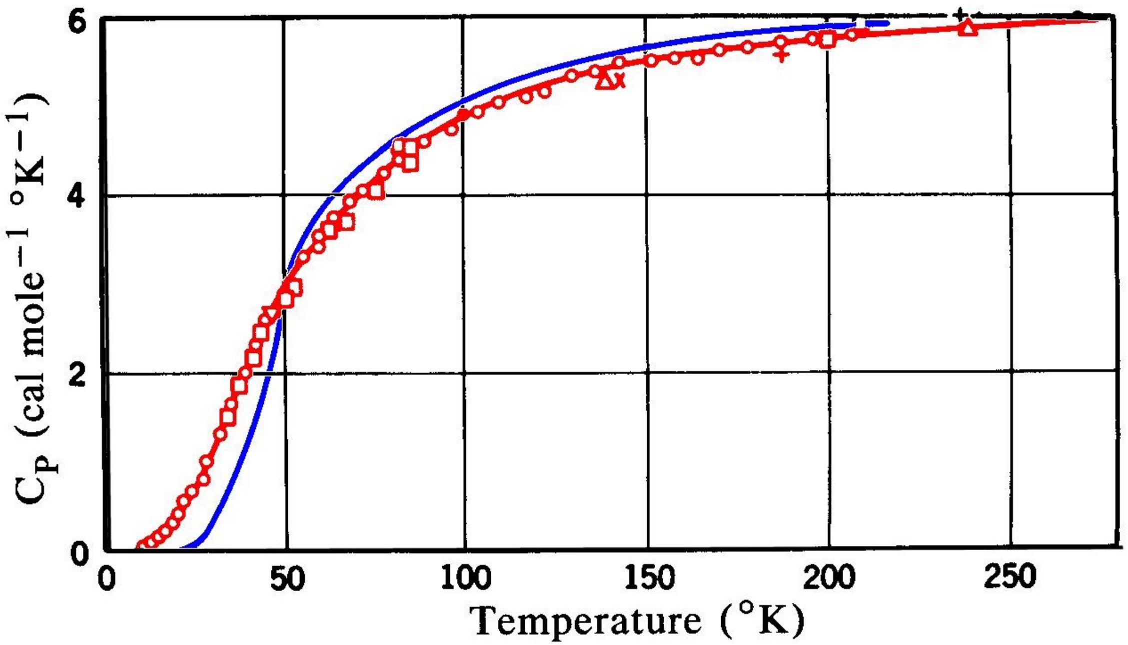


Debye energy and specific heat

$$\langle \varepsilon(\omega) \rangle = \frac{\hbar\omega}{2} \frac{\cosh \beta\hbar\omega}{\sinh \beta\hbar\omega}$$

$$E = \int d\varepsilon \; g(\varepsilon) \langle \varepsilon(\omega) \rangle$$

$$c_V = \frac{\partial E}{\partial T}$$



Specific heat data (points) for silver. The lines are the fits from the Einstein and Debye results. The Debye curve goes through the data points.