Chapter 5: Phonon properties

The heat capacity is in general

$$C_v = \left(\frac{\partial U}{\partial T}\right)_v$$

The proportionaly of heat capacity in different materials

- Metal: $C_v \propto I + QT^3$
- Insulator: $C_v \propto T^3$

The Energy of an N particle system is $E = Nk_BT$. and the heat capacity is

$$C_v = \frac{\partial E}{\partial T} = \omega k_B$$

The total energy is

$$U_{tot} = \sum k, p\hbar\omega_{k,p}\langle n_{k,p}\rangle$$

where $\langle n_{k,p}\rangle$ is the Bose-Einstein distribution

$$\langle n_\omega\rangle = \frac{1}{\exp\left(\frac{\hbar\omega}{k_BT}\right) - 1}$$

where there is no chemical potential. At low temperatures the constant goes to

$$\exp\left(\frac{\hbar\omega}{k_BT}\right)$$

or a boltzmann distribution.

$$U_{tot}\sum_{k,p}\frac{\hbar\omega_{k,p}}{\exp\left(\frac{\hbar\omega_{k,p}}{k_BT}\right) - 1}$$

or into an integral

$$\int \mathrm{d}k\, f(\omega) \rightarrow \int \mathrm{d}\omega\, f(\omega)\frac{1}{\frac{\mathrm{d}\omega}{\mathrm{d}k}}$$

We can compute this numerically from the phonon dispersion relation. For the Heat capacity of a solid, this T^3 term is in the order of 3 meV. We only need to take the acoustic modes into account for finding $\frac{\mathrm{d}\omega}{\mathrm{d}k}$ which approximately a constant C, so

$$\int_0^a \mathrm{d}\omega\,\frac{\hbar\omega^2}{\exp\left(\frac{\hbar\omega}{k_BT}\right) - 1}$$

where we can simplify using the substitution

$$x = \frac{\hbar\omega}{k_BT}$$

to change the integral from k space to ω space and the integral becomes

$$T^2\int_0^\infty \mathrm{d}x\,\frac{x}{\exp(x) - 1}$$

where the T^2 term comes from substituting for ω twice. So the total energy is

$$U_{tot} = \sum_p \int \mathrm{d}\omega\, D_p(\omega) \frac{\hbar\omega}{\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1}$$

where $D_p(\omega)$ is the density of states. Using the substition for x we get

$$U_{tot} = \sum_p \int \omega\, \mathrm{d}\omega\, D_p(\omega) \frac{x}{e^x - 1}$$

and the heat capacity is

$$C_v = \frac{\partial U_{tot}}{\partial T} = k_B \sum_p \int \mathrm{d}\omega\, D_p(\omega) \frac{x^2 e^x}{(e^x - 1)^2}$$

The density of states (DOS) is given by

$$D(\omega) = \frac{\mathrm{d}N}{\mathrm{d}\omega}$$

where N is the number of states. For a 3D phonon gas, the total allowed states is

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

Which is equivalent to the volume of a sphere for each unit volume. So the DOS is

$$D(\omega) = \frac{\mathrm{d}N}{\mathrm{d}\omega} = \frac{\mathrm{d}N}{\mathrm{d}k}\frac{\mathrm{d}k}{\mathrm{d}\omega} = \frac{V}{2\pi^2}\frac{k^2}{1}$$

and the heat capacity is

$$C_v \propto k_B \sum_p \in \mathrm{d}\omega\, \frac{k^2 V}{2\pi^2} \frac{1}{\frac{\mathrm{d}\omega}{\mathrm{d}k}} \frac{x^2 e^x}{(e^x - 1)^2}$$

and since $\omega = vk$ and $\frac{\mathrm{d}\omega}{\mathrm{d}k} = v$ we get

$$C_v \propto \sum_p \int_0^{\omega_D} \mathrm{d}\omega\, \frac{V}{1} \frac{\omega^2}{v^3} \frac{x^2 e^x}{(e^x - 1)^2}$$

so we get the number of states

$$N = \int_0^{\omega_D} \mathrm{d}\omega\, D(\omega)$$

where

$$\omega_D^2 = \frac{6\pi^2 N}{V}$$

the total energy is

$$U_{tot} = \int_0^{\omega_D} \mathrm{d}\omega\, \frac{V\omega^2}{2T^2 v^3} \frac{\hbar\omega}{\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1}$$

and substituting for x we get

$$\propto T^4 \int_0^{x_D} \mathrm{d}x\, x^2 \frac{x}{e^x - 1}$$

where we have four x terms that are substituted thus the T^4 term. We get Debye's law for the heat capacity

$$U_{tot} \propto T^4 f(x_D) \qquad C_v = \frac{\partial U}{\partial T} \propto T^3$$

for low temperature $T \to 0$, $x_D \to \infty$ so the $f(x_D) \to 1$ which will give us Debye's law. Some constants: ω_D is the Debye frequency and the Debye temperature is

$$\theta_D = \frac{\hbar \omega_D}{k_B}$$

Einstein Model

$$D(\omega) = N\delta(\omega - \omega_0)$$

so we get a simple expression for the total energy

$$U_{tot} \propto \frac{\hbar\omega_o}{\exp\left(\frac{\hbar\omega_o}{k_B T}\right) - 1}$$

and the heat capacity is

$$C_v = \frac{\partial U}{\partial T}\bigg|_{T\to 0} \propto \frac{1}{T} \frac{\exp\left(\frac{\hbar\omega_o}{k_B T}\right)}{\left(\exp\left(\frac{\hbar\omega_o}{k_B T}\right) - 1\right)^2} \to T\exp\left(\frac{\hbar\omega}{k_B T}\right)$$

For the einstein model we get a wrong number because we assumed the density of states is a delta functions ,but it reality it is a constant.