Debye model

Review

1) Solve wave equation for elastic waves
2) Solid is a cube / cubical lattice
3) Boundary Conditions on the 6 faces of the cube $k_i = \frac{n_i \pi}{L}$
4) For every combination of n_1 n_2 n_3 with $n_i = 1, 2, 3, 4, \ldots$ there is a normal mode
5) In k space, the normal modes on the lattice sites of cubical lattice each corner is a unit cell of allowed $\vec{k}$ vector having a side lenght π/L and Volume $= (\pi/L)^3$ in k space
6) Each corner is shared by 8 cubes, one atom per cube

$$dn(k) \quad \begin{matrix}\#\text{ of allowed} \\ k\text{-vectors}\end{matrix} = \frac{\text{Volume of Spherical Shell}}{\text{Volume of 1 cell}} = \frac{\frac{1}{8} 4\pi k^2 dk}{(\pi/L)^3} = \frac{L^3 k^2 dk}{2\pi^2} = \frac{V}{2\pi^2}\left(\frac{\omega}{v}\right)^2 \frac{dk}{d\omega} d\omega$$

$$dn(k) = \frac{V}{2\pi^2} \frac{\omega^2}{v^3} d\omega \quad \text{(no dispersion)}$$

$$dn(k) = \frac{V}{(2\pi)^2} \omega^2 d\omega \frac{3}{\bar{v}^3} \quad \text{average of transverse \& longitudinal waves}$$

In a cubical cavity only the v_T is electromagnetic $v_T = c$ the phase velocity of elastic waves. The v_L don't exist

$$dn = \frac{\cancel{3}V \omega^2 d\omega}{2\pi^2 \bar{v}^3} \quad \text{the number of standing elastic waves}$$

For low ω can consider as a continuous structure
The total number of degrees of freedom N

$$3N = \int_0^{\omega_{max}} dn = \int_0^{\omega_D} \frac{V\omega^2 d\omega}{2\pi^2 \bar{v}^3} \quad \text{assume some maximum frequency}$$

$$\cancel{dn = \frac{9N\omega^2 d\omega}{\omega_D^3}} \qquad 3N = \frac{V}{2\pi^2 \bar{v}^3} \frac{\omega_D^3}{3}$$

$$\frac{V}{2\pi^2 \bar{v}^3} = \frac{9N}{\omega_D^3}$$

$$\therefore \boxed{dn = \frac{9N\omega^2 d\omega}{\omega_D^3}} \quad \text{dimensionless}$$

Take this as the number of normal modes / motions of the atoms

$$dn = \frac{9N\omega^2}{\omega_D^3} d\omega = f(\omega)\, d\omega$$

Previously showed that the <energy> of one SHO mode is:

$$\bar{E} = \frac{\hbar\omega}{e^{\hbar\omega/kT} - 1} + \frac{\hbar\omega}{2}$$

$\hbar\omega/2$: can ignore the zero point energy

The average energy of the solid can be written in terms of the density of states

$$\bar{E} = \sum_{\alpha=1}^{3N} \frac{\hbar\omega_\alpha}{(e^{\hbar\omega_\alpha/kT} - 1)} = \int_0^{\omega_D} \left(\frac{\hbar\omega}{e^{\hbar\omega/kT} - 1}\right) f(\omega)\, d\omega$$

we don't know what the ω_α's are - assume they are infinitely close together

$$\bar{E} = \frac{9N}{\omega_D^3} \int_0^{\omega_D} \frac{\hbar\omega^3 d\omega}{(e^{\hbar\omega/kT} - 1)}$$

make the integral deminsionless $x = \frac{\hbar\omega}{kT}$ $x_D = \frac{\hbar\omega_D}{kT}$ $d\omega = \frac{kT}{\hbar}dx$

$$\boxed{\bar{E} = \frac{9N\hbar}{\omega_D^3}\left(\frac{kT}{\hbar}\right)^4 \int_0^{x_D} \frac{x^3 dx}{(e^x - 1)}}$$

exact expression of the deBye model

even in the high temperature limit $x_D \ll 1$ so all $x \ll 1$

$$\frac{x^3}{e^x - 1} \sim \frac{x^3}{1 - x - 1} \sim x^2$$

as $T \to \infty$

$$\lim_{T\to\infty} \bar{E} = \frac{9N\hbar}{\omega_D^3}\left(\frac{kT}{\hbar}\right)^4 \frac{x_D^3}{3} = \frac{9N\hbar}{\omega_D^3}\left(\frac{kT}{\hbar}\right)^4 \frac{1}{3}\left(\frac{\hbar\omega_D}{kT}\right)^3 = 3NkT$$

$$\lim_{T\to\infty} C_V = \left(\frac{\partial E}{\partial T}\right)_V = 3Nk$$ Dulong - Petit rule

In the low temperature limit, define $\Theta_D = \frac{\hbar\omega_D}{k}$ the debye temperature

as $T \to 0$ $x_D \gg 1$ $x^3 e^{-x}$ goes to $\emptyset$ as $x_D \to \infty$

$$\lim_{T\to 0} \bar{E} = \frac{9N\hbar}{\omega_D^3}\left(\frac{kT}{\hbar}\right) \underbrace{\int_0^\infty \frac{x^3 dx}{e^x - 1}}_{\pi^4/15} = \frac{9Nk^4T^4}{\hbar^3\omega_D^3}\frac{\pi^4}{15} = \frac{3}{5}\frac{\pi^4 k^4 N T^4}{\hbar^3\omega_D^3}$$

$$\lim_{T\to 0} C_V = \lim_{T\to 0}\left(\frac{\partial E}{\partial T}\right)_V = \frac{12}{5}\frac{\pi^4 k^4}{\hbar^3\omega_D^3} N T^3$$

all normal mode $\omega \simeq$ constant

$C_V \propto T^3$ is an experimental fact

$\Theta_D = \frac{\hbar\omega_D}{k}$ $\quad C_V = \frac{12}{5}\pi^4 Nk\left(\frac{T}{\Theta_D}\right)^3$ Low temperature limit

ω_D fits to data

Experimental facts give a way to estimate ω_D for different solids.

$$\int_0^{\omega_D} f(\omega)\,d\omega = 3N$$

$$f(\omega)\,d\omega = \frac{9N\,\omega^2 d\omega}{\omega_D^3} = 3\left(\frac{3N}{\omega_D^3}\right)\omega^2 d\omega = 3\left(\frac{V}{2\pi^2 \bar{v}^3}\right)\omega^2 d\omega$$

$$\frac{3V}{2\pi^2 \bar{v}^3}\int_0^{\omega_D} \omega^2 d\omega = 3N$$

$$\frac{3V}{2\pi^2 \bar{v}^3}\,\frac{\omega_D^3}{3} = 3N$$

$$\omega_D^3 = \frac{3N}{V}\,2\pi^2 \bar{v}^3$$

$$\omega_D = (6\pi^2)^{1/3}\left(\frac{N}{V}\right)^{1/3}\bar{v}$$

frequency related to the elastic constant

$\frac{V}{N}$ = average volume of of an atom ~~# of atoms~~

phase velocity of elastic waves.

$\frac{V}{N} = a^3 \quad \frac{N}{V} = \frac{1}{a^3}$ $\quad a$ = interatomic spacing

$$\omega_D = (6\pi^2)^{1/3}\,\frac{\bar{v}}{a}$$ related to elastic constants

Table 6.4 in Mandl shows why deBye is considered successful gets the energies within 10%

Element	$\bar{v}/10^5$ cm/s	a (Å)	$\omega_D/10^{12}\ s^{-1}$	Θ_D (K)	Thermal (K)
Al	3.4	2.5	5.2	399	380
Cu	2.6	2.3	4.4	335	310
Pb	0.8	3.1	9.8	75	86

Lecture 15 continued... Blackbody Radiation

Once we know the deBye model, can study blackbody radiation. Consider electromagnetic radiation confined to a cavity. While the cavity could be spherical, it is easier to solve a cubical cavity and the results are the same. As long as the dimensions of the box are larger than the wavelength of the vibrations, the number of modes is the same

$$f(\omega)d\omega = \frac{V\omega^2 d\omega}{2\pi^2}\left(\cancel{\frac{1}{V_L^3}}^{\,0} + \frac{2}{c^3}\right) = \frac{V}{\pi^2 c^3}\,\omega^2 d\omega$$

Even though we applied it to a cavity in the case of elastic waves, this will work at all temperatures and give exact results for the number of modes between ω and $\omega + d\omega$. Infinite degrees of freedom.

$$\bar{E} = \sum_{\alpha=1}^{\infty} \frac{\hbar\omega_\alpha}{e^{\hbar\omega_\alpha/kT}-1} = \int_0^\infty \underbrace{\left(\frac{\hbar\omega}{e^{\hbar\omega/kT}-1}\right)}_{\substack{\text{average energy}\\ \text{per oscillator}\\ \text{(or per normal}\\ \text{mode)}}} \underbrace{\left(\frac{V\omega^2 d\omega}{\pi^2 c^3}\right)}_{\substack{\text{number of modes}\\ \text{in interval}}}$$

$$\bar{E} = \frac{V\hbar}{\pi^2 c^3}\int_0^\infty \frac{\omega^3 d\omega}{e^{\hbar\omega/kT}-1}$$

Things to Know:

1) Thermal equilibrium is when the same amount absorbed is emitted.
2) The inability to explain blackbody radiation was a first clue that something was wrong with classical physics. Planck's results showed that quantization was crucial.