Review: $U = \int_0^\infty \hbar\omega \, D(\omega) \frac{1}{e^{\hbar\omega/kT}-1} \, d\omega$

$$D(\omega)\,d\omega = \frac{1}{\left(\frac{2\pi}{L}\right)^3} \, 4\pi k^2 \, dk$$

Debye model: $\omega = vk$

$$D(\omega) = \frac{Vol}{8\pi^3} \cdot 4\pi \left(\frac{\omega}{v}\right)^2 \frac{1}{v}$$

ω_D given by $N = \int_0^{\omega_D} D(\omega)\,d\omega$

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

Done with first 2 steps on handout

Now: $U = \int \hbar\omega \, D(\omega) \frac{1}{e^{\hbar\omega/kT}-1} \, d\omega \quad \leftarrow \times 3$ (# of acoustic phonon branches in 3D; assume v = same for all three)

$$= 3\int_0^{\omega_D} \left(\frac{V}{2\pi^2 v^3}\omega^2\right) \frac{1}{e^{\hbar\omega/kT}-1} (\hbar\omega) \, d\omega$$

As in handout, let $x = \frac{\hbar\omega}{kT} \rightarrow \omega = \frac{kT}{\hbar} x$

$$\left(x_D = \frac{\hbar}{kT}\omega_D\right) \qquad d\omega = \frac{kT}{\hbar} dx$$

$$U = 3\int_0^{x_D} \left(\frac{V}{2\pi^2 v^3}\left(\frac{kT}{\hbar}x\right)^2\right) \frac{1}{e^x-1} \hbar\left(\frac{kT}{\hbar}x\right)\left(\frac{kT}{\hbar}dx\right)$$

$$\boxed{U = \frac{3\,Vol}{2\pi^2 v^3} \frac{k^4 T^4}{\hbar^3} \int_0^{x_D} \frac{x^3}{e^x-1} \, dx}$$

end of step (c) on handout

Pause. Note integral sometimes uses "Debye temperature" given by

$$\hbar\omega_D = kT_D$$

T_D also called Θ_D

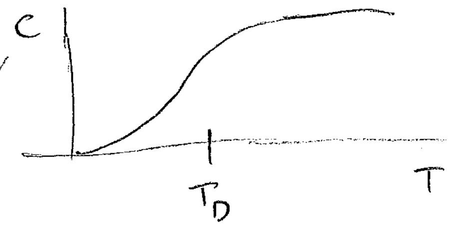
or just Θ

We now have $U(T)$

But note $U(T)$ does <u>not</u> go as T^4 because x_D is a function of T.

However, we could now presumably program that into a computer, take derivative $\frac{\partial U}{\partial T}$.

Result:



really $\bar{C}$ molar heat capacity

marks a boundary between two types of behavior

Fig 7 pg 113

(could be exam problem: have Mathematica make this graph)

Compare to Fig 8

More details:

(1) Low T approximation. Notice $x_D \to \infty$ as $T \to 0$

$$U = \frac{3}{2\pi^2}\frac{V}{v^3}\frac{k^4T^4}{\hbar^3}\underbrace{\int_0^\infty \frac{x^3}{e^x-1}\,dx}_{=\pi^4/15}$$

$$U = \frac{\pi^2}{10}\frac{V}{v^3}\frac{k^4}{\hbar^3}T^4$$

$$C = \frac{\partial U}{\partial T} = \frac{\pi^2}{10}\frac{V}{v^3}\frac{k^4}{\hbar^3}(4T^3)$$

$$\boxed{C = \frac{2\pi^2}{5v^3}\frac{k^4}{\hbar^3}T^3 \cdot \mathrm{Vol}}$$

"Debye T^3 law"
end of step (d)

book puts in terms of N and T_D to eliminate Vol and v

Recall $N = \int_0^{w_D} D(w)\, dw$

(gave us) $\longrightarrow$ $w_D = \left(\frac{N}{V} 6\pi^2 v^3 \right)^{1/3}$

$$w_D^3 = \frac{N}{V} 6\pi^2 v^3$$

$$\frac{Vol}{v^3} = N \cdot \frac{6\pi^2}{w_D^3}$$

Recall $T_D = \frac{\hbar w_D}{k} \rightarrow w_D = \frac{k T_D}{\hbar}$

So $\frac{Vol}{v^3} = \underline{N \cdot 6\pi^2 \cdot \frac{\hbar^3}{k^3 T_D^3}}$

plug into C: $C = \frac{2\pi^2}{5} \frac{k^4}{\hbar^3} \; N \cdot \frac{6\pi^2 \hbar^3}{k^3 T_D^3} \cdot T^3$

$$\boxed{C = \frac{12\pi^4}{5} N k \left(\frac{T}{T_D}\right)^3} \approx 234\, N k \left(\frac{T}{T_D}\right)^3$$

(2) high T approximation, When T = big, x = small

$$e^x - 1 \approx (1+x) - x = x$$

$$U = \frac{3}{2} \frac{V}{\pi^2 v^3} \frac{k^4 T^4}{\hbar^3} \underbrace{\int_0^{x_D} \frac{x^{\cancel{3}\,2}}{\cancel{x}}\, dx}_{}$$

$$\frac{1}{3} x_D^3$$

$$= \frac{1}{3} \frac{\hbar^3 w_D^3}{k^3 T^3}$$

$$= \frac{1}{3} \frac{\hbar^3}{k^3 T^3} \left(6\pi^2 v^3 \frac{N}{V} \right)$$

"then a miracle occurs"

$$U = \frac{3}{2} \frac{\cancel{V}}{\cancel{\pi^2 v^3}} \frac{k^4 T^4}{\cancel{\hbar^3}} \cdot \frac{1}{3} \frac{\cancel{\hbar^3}}{\cancel{k^3 T^3}} 6\pi^2 \cancel{v^3} \frac{N}{\cancel{V}}$$

$$U = 3 k T N$$

$C = \frac{\partial U}{\partial T} \longrightarrow \boxed{C = 3kN}$

end of step (2)

matches "Dulong Petit Law",

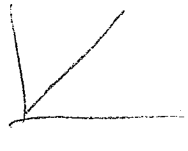
equipartition theorem

w/ 6 d.o.f $\left\langle \begin{array}{l} 3 \text{ vibrational KE} \\ 3 \text{ vibrational PE} \end{array} \right.$

Each d.o.f. has $\frac{kT}{2}$ energy

Day 19 pg 4.

Review: Debye model used $\omega = vk$



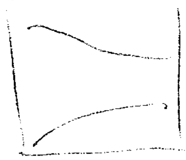
mention $\times 3$ for 3 acoustic branches

OK for acoustic branch.

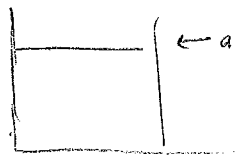
horrible for optical branch.

New model: Einstein model (for optical branch(es))

diatomic lattice again



$\longrightarrow$ model as



$\leftarrow$ all at freq. ω_0

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

$\searrow$ Dirac delta

$$U = \int D(\omega)\, \frac{\hbar\omega}{e^{\hbar\omega/kT}-1}\, d\omega$$

Trivial!

$$\boxed{U = \frac{N\hbar\omega_0}{e^{\hbar\omega_0/kT}-1}}$$

ω_0 = characteristic (optical phonon) frequency

define Θ_E: $\hbar\omega_0 = k_B\Theta_E$

(can use as fit parameter)

$$C_V = \frac{dU}{dT} = N k_B \left(\frac{\hbar\omega_0}{kT}\right)^2 \frac{e^{\hbar\omega_0/kT}}{\left(e^{\hbar\omega_0/kT}-1\right)^2}$$

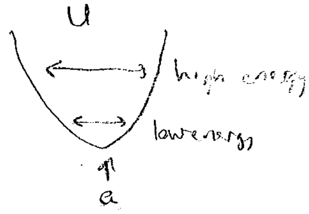
Fig 11 pg 117

$\leftarrow$ also goes to $3Nk_B$

$e^{-\text{const}/T}$ not good at all (Debye better)

Beyond the Harmonic Approximation

some big problems 1)



No change in lattice constant as energy is added!

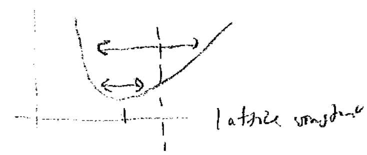
2). No way for phonons to interact.
(like light – if not nonlinear crystal, can't get 800 nm → 400 nm conversion in pulsed Ti sapph)

$\omega_3 = \omega_1 + \omega_2$ → present w/ phonons like in photons

Actuality: if phonon present, produces some strain, which modulates in space + time the elastic constants

Full nonlinear ("anharmonic") theory very complicated.

For us.

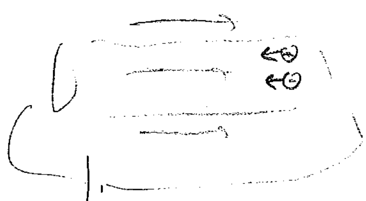


increases when more energy!

Kittel: $x_{ave} = \frac{3}{4} kT \cdot \frac{g}{c^2}$ → g: cubic coefficient; c^2: quadratic coefficient

Thermal Conductivity

first: electrical conductivity (really in Ch 6, pg 147–148)



Do electrons accelerate all the way down the wire?

$F = qE$, $E = \frac{V}{\ell}$

No! Why not? → scattering