If not linear dispersion, than eg

$$1D: \quad D(\omega) = \frac{L}{2\pi} \cdot 2 \cdot \frac{1}{(d\omega/dk)}$$

$$3D: \quad D(\omega) = \frac{Vol}{(2\pi)^3} \times (4\pi k^2) \times \frac{1}{d\omega/dk}$$

or if not even spherical approximation

$$\frac{Vol}{(2\pi)^3} \times \int_{\substack{\text{surface} \\ \text{constant } \omega}} \frac{dA}{|\nabla_k \omega|}$$

$\nabla_k \omega$ ↳ $\frac{\partial\omega}{\partial k_x} + \frac{\partial\omega}{\partial k_y} + \frac{\partial\omega}{\partial k_z}$

↓

pg 118, we won't ever use

Back to main problem

from before

$$U_{tot} = \sum_{\text{all pts}} (n_{ave} + \tfrac{1}{2}) \hbar\omega_n = \sum \left(\frac{1}{e^{\hbar\omega_n/kT} - 1} + \frac{1}{2} \right) \hbar\omega_n$$

↳ drop $\frac{1}{2}$ (textbook never includes)

since we'll be taking derivative

Translate to integral

$$U = \int D(\omega)\, d\omega \cdot \underbrace{\frac{1}{e^{\hbar\omega/kT} - 1}}_{\text{prob of mode}} \times \hbar\omega$$

↓

---

day 18 pg 1

Linear Dispersion now

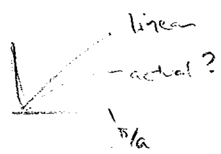
Another problem!

Limits of integration = ?

<u>Debye model</u>

use $\boxed{\omega = vk}$ approximation

(only acoustic branch, 1 atom/unit cell)



we knew that $\int D(\omega)\, d\omega = N$ (# atoms),

so cut off integral early to force that to be true

$$\int_0^{W_{cutoff}} \mathcal{D}(\omega)\, d\omega = N$$

← called ω_{Debye}, or ω_D

$$\int_0^{\omega_D} \frac{Vol}{(2\pi)^3} 4\pi \left(\frac{\omega}{v}\right)^2 \frac{1}{v}\, d\omega = N$$

$$\frac{1}{2\pi^2} \frac{Vol}{v^3} \underbrace{\int_0^{\omega_D} \omega^2\, d\omega}_{\frac{1}{3}\omega_D^3} = N$$

$$\boxed{\omega_D = \left[\frac{6\pi^2 v^3 N}{V}\right]^{1/3}}$$

$\frac{N}{V} = n$, atomic density (in Ch 1 Table)

then

$$U = 3\int_0^{\omega_D} \frac{V}{(2\pi)^3} 4\pi \left(\frac{\omega}{v}\right)^2 \frac{1}{v}\, d\omega \frac{\hbar\omega}{e^{\hbar\omega/kT}-1}$$

3 → polarizations, another assumption: that velocity the same for all 3.

Warning! k_B, not wavevector!

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

=

"simplification": define DeBye temperature

$$\hbar\omega_D = k_B T_D$$

T_D → symbol "Θ"

$$\Theta = \frac{\hbar}{k_B}\left[\frac{6\pi^2 v^3 N}{V}\right]^{1/3}$$

→ solve for V, plug into eqn for U

$$C_V = \frac{\partial U}{\partial T}$$

note: "heat capacity", not "molar heat capacity", same symbol in 123

... more algebra ...

$$\boxed{C_V = 9Nk_B\left(\frac{T}{\Theta}\right)^3 \int_0^{\Theta/T} \frac{x^4 e^x}{(e^x-1)^2}\, dx}$$

→ can use Mathematica to do numerical integral as needed!

Limit $T \to 0$ then integral $\int_0^\infty \frac{x^4 e^x}{(e^x-1)^2}\,dx$ = constant

$$C_v \sim T^3 \qquad \left(= \frac{12\pi^4}{5} N k_B \left(\frac{T}{\Theta}\right)^3 \text{ to be precise} \right)$$

Limit $T \to \infty$ then x is always small!,

$$\frac{x^4 (1+\cancel{x}^{\,0})}{(1+x-1)^2} = x^2$$

$$\int_0^{\Theta/T} x^2\,dx = \frac{1}{3}\left(\frac{\Theta}{T}\right)^3$$

$$C_v = 9 N k_B \cancel{\left(\frac{T}{\Theta}\right)^3} \frac{1}{3} \cancel{\left(\frac{\Theta}{T}\right)^3}$$

$$\boxed{C_v = 3 N k_B}$$

Dulong Petit law!

Equipartition theorem: 6 d.o.f.

3 vibrational KE
3 " PE

each d.o.f. has $\frac{k_B T}{2}$ energy.

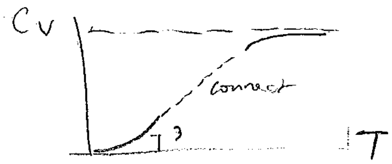


Fig 7 → Fig 8 pg 113

possible HW: use Mathematica to make Fig 7 pg 113
(numerical integral)

Nah.

But can discuss how you'd do that to find Θ_0

rescale so x-axis is T, not T/Θ
for Silicon

rescale y-axis to cal/mol

use Θ from Table 1 pg 116

Compare to Fig 8.