

Solutions Problem Set #1

Prob 1.1

Problem 1

Simon 2.1

$$(a) \quad Z = \int \frac{d\vec{p}}{(2\pi\hbar)^3} \int d\vec{x} e^{-\beta(\frac{p^2}{2m} + \frac{kx^2}{2})}$$

$$= \frac{1}{(2\pi\hbar)^3} \int d\vec{p} e^{-\beta \frac{p^2}{2m}} \int d\vec{x} e^{-\beta \frac{kx^2}{2}}$$

assume space is isotropic so $d\vec{p} = dp_x dp_y dp_z = 4\pi p^2 dp$

same for $d\vec{x}$

$$Z = \frac{1}{(2\pi\hbar)^3} (4\pi)^2 \int_0^\infty p^2 e^{-\beta \frac{p^2}{2m}} dp \int_0^\infty x^2 e^{-\beta \frac{kx^2}{2}} dx$$

$$\int_0^\infty x^2 e^{-ax^2} dx = \frac{\sqrt{\pi}}{4a^{3/2}}$$

$$\therefore Z = \frac{1}{(2\pi\hbar)^3} (4\pi)^2 \left(\frac{2m}{\beta}\right)^{3/2} \left(\frac{2}{\beta k}\right)^{3/2} \frac{\pi}{16}$$

$$Z = \left(\frac{m}{\beta^2 k \hbar^2}\right)^{3/2}$$

↑ spring constant

$$\langle E \rangle = -\frac{1}{Z} \frac{\partial Z}{\partial \beta} = -\left(\frac{\beta^2 k \hbar^2}{m}\right)^{3/2} \left(\frac{m}{k \hbar^2}\right)^{3/2} \frac{-3}{\beta^4}$$

$$= +\frac{3}{\beta} = 3 k_B T$$

$$C = \frac{\partial \langle E \rangle}{\partial T} = 3 k_B$$

This is per atom

N_A atoms per mole

$$C_{mole} = 3 N_A k_B = 3 R!$$

②

Problem 1.2

(B) $Z = \sum_j e^{-\beta E_j}$

now like Simon page 8 (This is just like in picture)

$Z = \sum_{n=0}^{\infty} e^{-\hbar\omega(n+1/2)\beta}$ for 1 oscillator in 1D

$= e^{-\beta\hbar\omega/2} \sum_{n=0}^{\infty} e^{-\hbar\omega n\beta} = e^{-\beta\hbar\omega/2} \left(1 + \sum_{n=1}^{\infty} e^{-\beta\hbar\omega n}\right)$

recall that $\sum_{n=1}^{\infty} e^{-xn} = \frac{1}{e^x - 1}$

so $Z = e^{\beta\hbar\omega/2} \left(1 + \frac{1}{e^{\beta\hbar\omega} - 1}\right) = e^{\beta\hbar\omega/2} \left[\frac{1 + e^{\beta\hbar\omega} - 1}{e^{\beta\hbar\omega} - 1}\right]$

$Z = \frac{e^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega}}$ for a 1D oscillator

for 3D $Z_{3D} = Z_{1D}^3$

$\langle E \rangle_{3D} = \frac{-1}{Z_{3D}} \frac{\partial Z_{3D}}{\partial \beta} = \frac{-1}{(Z_{1D})^3} 3 (Z_{1D})^2 \left[-\frac{\hbar\omega}{2} \frac{e^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega}} \right]$

$= \frac{-1}{(Z_{1D})^3} 3 (Z_{1D})^2 \left[\frac{e^{-\beta\hbar\omega/2}}{(1 - e^{-\beta\hbar\omega})^2} (-1)(-1)e^{-\beta\hbar\omega} \hbar\omega (-1) \right]$

$\langle E \rangle_{3D} = 3 \left[\frac{\hbar\omega}{2} + \frac{\hbar\omega e^{-\beta\hbar\omega}}{1 - e^{-\beta\hbar\omega}} \right]$

$\langle E \rangle_{3D} = 3 \left[\frac{\hbar\omega}{2} + \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1} \right]$

$C = \frac{\partial}{\partial \beta} \langle E \rangle = \frac{(-1)}{(k_B T)^2} \left(3 \hbar\omega (-1) e^{\beta\hbar\omega} \hbar\omega \right)$
 $= 3 k_B \left[\frac{\hbar\omega}{k_B T} \right]^2 \frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega} - 1)^2}$

Prbl. 3 (3)

The Connection with Bose Statistics is

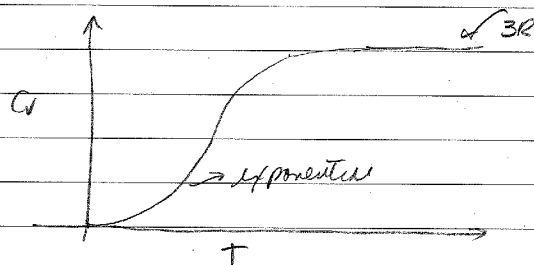
The factor $\frac{1}{e^{\beta h\nu} - 1} = n$

which for $\beta = 0$ ($KT \rightarrow \infty$) where $e^x \approx 1+x$
 Bose $\rightarrow \frac{1}{(1+\beta h\nu - 1)} = \frac{KT}{h\nu}$ increases

but for $\beta \rightarrow \infty$ ($T \rightarrow 0$) $n \rightarrow 0$ for any
 state other than $h\nu = 0$ state

at high temp $C = \frac{3KB}{T} \left[\frac{h\nu}{KT} \right]^2 \frac{(1)}{(1+\beta h\nu - 1)^2}$
 $= 3KB \left[\frac{h\nu}{KT} \right]^2 \frac{1}{(KT)^2} = 3KB$ per oscillator

for a mole of oscillators $C = 3k_B N = 3R!$
 ulong Dulong result as expected



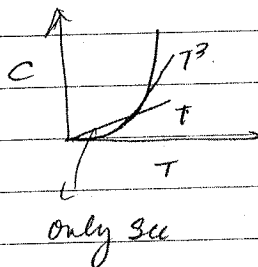
(Taken from lecture notes)

Actual density $C \sim T^3$

How can you tell. Plot C vs $T^3 \rightarrow$ get a straight line

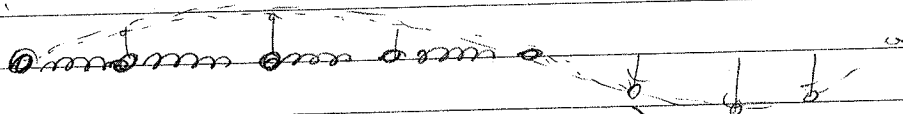
START HERE

\rightarrow What about electrons?



\rightarrow Debye for further refinement (put in knowledge of waves)

(A) \rightarrow treat independent oscillators



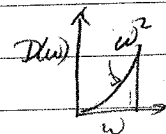
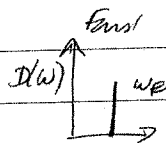
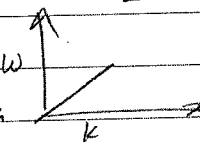
cyclical boundary conditions (periodic)

new use 2 things

$$K = \frac{2\pi}{\lambda_{\text{max}}} = \frac{2\pi}{L}$$

$$K = n \frac{2\pi}{L}$$

\swarrow phase velocity
 $\omega = vK$ energy \rightarrow wavelength



(Important for problem set)

$$\sum_n \rightarrow \sum_K \rightarrow \frac{L}{2\pi} \int_{-\infty}^{\infty} dk$$

but in 3D $\sum_K \rightarrow \frac{L^3}{(2\pi)^3} \int d\vec{k} \rightarrow 4\pi \int_0^{\infty} k^2 dk$ (isotropic)

(B) so $\langle E \rangle = \frac{3L^3}{(2\pi)^3} 4\pi \int K^2 dk (\hbar\omega) \left(\frac{1}{2} + \frac{1}{e^{\hbar\omega\beta} - 1} \right)$

switch to ω

$$\langle E \rangle = \frac{3L^3}{(2\pi)^3} 4\pi \int \frac{\omega^2}{v^3} d\omega \hbar\omega \left(\frac{1}{2} + \frac{1}{e^{\hbar\omega\beta} - 1} \right)$$

2.2

$$\langle E \rangle = \frac{12 \pi L^3}{(2\pi)^3} \int_0^\infty \frac{\hbar \omega^2 d\omega}{v^3} \left(\frac{1}{2} + \frac{1}{e^{\beta \hbar \omega} - 1} \right)$$

$$NL^3 = N$$

atoms
unit vol

$$\langle E \rangle = \frac{12 \pi L^3}{(2\pi)^3 v^3} \int_0^\infty \hbar \omega^2 d\omega \left[\frac{1}{2} + \frac{1}{e^{\beta \hbar \omega} - 1} \right]$$

$$\langle E \rangle = \int_0^\infty g(\omega) \hbar \omega \left[\frac{1}{2} + \frac{1}{e^{\beta \hbar \omega} - 1} \right]$$

Density of states \rightarrow

$$g(\omega) = \frac{12 \pi L^3 \omega^2}{(2\pi)^3 v^3} = N \left[\frac{12 \pi \omega^2}{(2\pi)^3 n v^3} \right] = N \frac{9 \omega^2}{\omega_D^3}$$

of levels
AE

$$\omega_D^3 = 6 \pi^2 n v^3$$

sound velocity

$$\omega_D = \sqrt[3]{6 \pi^2 n v}$$

Debye frequency

$$\langle E \rangle = \frac{9 N \hbar}{\omega_D^3} \int_0^\omega d\omega \frac{\omega^3}{e^{\beta \hbar \omega} - 1} + \text{temp independent}$$

let $x = \beta \hbar \omega$ $d\omega = \frac{dx}{\beta \hbar}$ $\omega^3 = \frac{x^3}{(\beta \hbar)^3}$

$$\langle E \rangle = \frac{9 N \hbar}{\omega_D^3} \frac{1}{(\beta \hbar)^4} \int_0^\omega \frac{dx x^3}{e^x - 1} \rightarrow \pi^4/15$$

$$\langle E \rangle = 9 N \frac{(k_B T)^4}{(\hbar \omega_D)^3} \frac{\pi^4}{15}$$

LOW T
LIMIT

$$C = \frac{\partial E}{\partial T} = 9 N \frac{4 k_B^4 T^3}{(\hbar \omega_D)^3} \frac{\pi^4}{15} \quad +^3 \checkmark$$

can scale $\omega / \omega_D \rightarrow \hbar \omega_D = k_B T_D$

but can't have T^3 freud

so $3N = \int_0^{\omega_{cut-off}} d\omega g(\omega)$ ← the phonon is it?

$$3N = \int_0^{\omega_{cut-off}} d\omega \cdot \frac{N \cdot 9\omega^2}{\omega_D^3}$$

$$= \left[\frac{N \cdot 9}{\omega_D^3} \cdot \frac{\omega^3}{3} \right]_0^{\omega_{cut-off}}$$

$$3N = 3N \left[\frac{\omega_{cut-off}}{\omega_D} \right]^3 \quad \omega_{cut-off} = \omega_D \checkmark$$

limitations

$\omega_{cut-off}$

$\omega = v_k$ (linear)

still need to explain $C \sim T$

Put it all together

$$\langle E \rangle = \int_0^{w_{\max}} g(w) k w \left[\frac{1}{2} + \frac{1}{e^{\beta k w} - 1} \right] dw$$

when $T \rightarrow 0$ then $\frac{k w_{\max}}{k_B T} \rightarrow \infty$

\Rightarrow may as well have $w_{\max} = \infty$

LOW T
LIMIT AGAIN then $\langle E \rangle \propto T^4$ and $C = \frac{d\langle E \rangle}{dT} \propto T^3$

but when T is high then keep $w_{\max} = w_D$

HIGH
T
LIMIT
HERE

$$\langle E \rangle = \int_0^{w_D} g(w) k w \left[\frac{1}{2} + \frac{1}{e^{\beta k w} - 1} \right] dw$$

only T dependence is in $\frac{1}{e^{\beta k w} - 1}$ so keep only 2nd term
for C

$$\langle E \rangle_{\text{temp dep}} = \int_0^{w_D} g(w) \frac{k w}{e^{\beta k w} - 1} dw$$

$e^x \approx 1 + x$ for x small so $\frac{1}{e^{\beta k w} - 1} \rightarrow \frac{1}{\beta k w}$

$$\langle E \rangle_{\text{temp dep}} = \int_0^{w_D} g(w) \frac{k w}{k w \beta} dw$$

$$= K_B T \int_0^{w_D} (g(w) dw) \leftarrow 3N$$

$$\langle E \rangle = 3N K_B T$$

$C_{\text{vib}} = 3N K_B$ Dulong-Petit

Problem 2.2 (B) and (C)

(2.5)

Here is the Potassium^{isotope} data. plotted

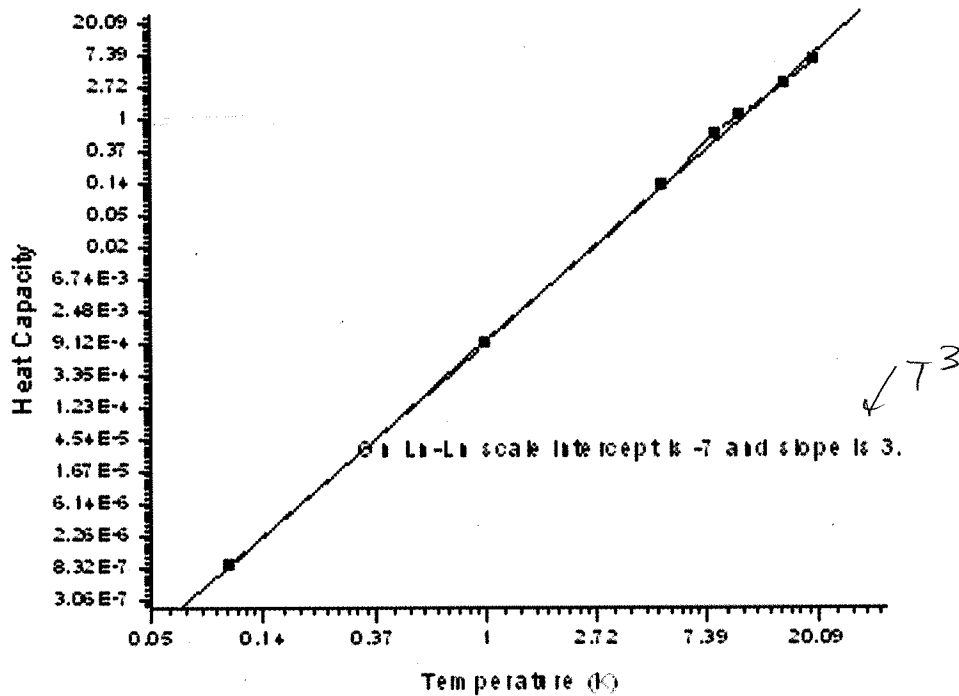
$\ln C$ vs $\ln T$

$$\text{If } C = Nk_B \frac{T^3}{T_D^3} \frac{12\pi^4}{5}$$

$$\text{then } \ln C = \ln \frac{Nk_B 12\pi^4}{T_D^3} + 3 \ln T$$

1

(B)



(C) Since slope is 3 this confirms the expected slope.

$$\text{At } 1K = T \quad C = 8.6 \times 10^{-4} \text{ J/K mole}$$

$$\therefore T_D^3 = Nk_B (1K)^3 \frac{12\pi^4}{5} = (6 \times 10^{23}) (1.4 \times 10^{-23} \frac{J}{K}) (12) \frac{(\pi^4)}{5} (K^3)$$

Good agreement w/ internet

$$T_D = 131 K$$

$$\text{at } 129 K!$$

C at 1K

$$8.6 \times 10^{-4} \text{ J/K mole}$$

$$\leftarrow T_D^3 = 2.28 \times 10^6 K$$

Problem 3 Simon 2.3

Assumptions

 Periodic boundary conditions $K = 2\pi n$

$$K = \frac{2\pi}{L} (n_1, n_2) \quad \text{allowed } L$$

$$\sum_K \rightarrow \frac{L^2}{(2\pi)^2} \int_{\Gamma_{2D}} d\vec{K}$$

So we will have a 2D solid that has
 motion in 3D (2 in plane modes, 1 out of plane)
 Assume all modes are linear $\therefore \omega = vK$
 Assume all v are the same (probably a bad
 assumption in that out of plane mode
 will be different than in plane but lets leave it)

$$\langle E \rangle = 3 \sum_{\vec{K}(2D)} \hbar \omega(\vec{K}) \left[n(\beta \hbar \omega) + \frac{1}{2} \right]$$

3 modes (or polarization = 2 transverse + 1 longitudinal)

$$= 3 \int \frac{L^2}{(2\pi)^2} d\vec{K}_{2D} \hbar \omega(K) \left[n_B(\beta \hbar \omega) + \frac{1}{2} \right]$$

Circular symmetry $\rightarrow \int d\vec{K} \rightarrow \int_0^{K_{max}} 2\pi K dK$ and $K = \frac{\omega}{v}$
 $dK = \frac{d\omega}{v}$

$$\langle E \rangle = 3 \frac{L^2}{(2\pi)^2} 2\pi \int_0^{\omega_{max}} \hbar \omega \frac{\omega}{v} \frac{d\omega}{v} \left[n(\beta \hbar \omega) + \frac{1}{2} \right]$$

$$\langle E \rangle = \frac{3}{(2\pi)} \frac{L^2}{v^2} \hbar \int_0^{\omega_{max}} \omega^2 d\omega \left[n(\beta \hbar \omega) + \frac{1}{2} \right]$$

For $C = \frac{\partial E}{\partial T} = \frac{\partial}{\partial T} \frac{\partial E}{\partial \beta}$ only this term counts

Problem 3.2

$$\langle E \rangle_{\text{avg}} = \frac{3}{(2\pi)} \frac{L^2 \hbar}{v^2} \int_0^{w_{\text{max}}} \frac{w^2 dw}{e^{\beta \hbar w} - 1}$$

$$\frac{\partial \langle E \rangle}{\partial \beta} = \frac{3}{(2\pi)} \frac{L^2 \hbar}{v^2} \int_0^{w_{\text{max}}} \frac{w^2 dw}{(e^{\beta \hbar w} - 1)^2} (-1) e^{\beta \hbar w} \hbar w$$

$$\therefore C = \left(-\frac{1}{k_B T^2} \right) \left(-\frac{3}{(2\pi)} \frac{L^2 \hbar^2}{v^2} \int_0^{w_{\text{max}}} \frac{w^3 dw}{(e^{\beta \hbar w} - 1)^2} e^{\beta \hbar w} \right)$$

$$\downarrow$$

$$-\frac{\partial \beta}{\partial T}$$

In the high Temp limit $T \rightarrow \infty$ so $\beta \rightarrow 0$

$$e^x \underset{x \rightarrow 0}{=} 1 + x$$

$$\therefore C = \frac{3}{k_B T^2} \frac{L^2 \hbar^2}{(2\pi) v^2} \int_0^{w_{\text{max}}} \frac{w^3 dw}{(\beta \hbar w)^2} (1)$$

$$= \frac{3}{(2\pi)} \frac{k_B L^2}{v^2} \frac{w^2}{2} \Big|_0^{w_{\text{max}}}$$

How to get w_{max} in 2D

$$N = \left(\frac{1}{2} 2\pi \right)^2 (\pi k^2) \quad \text{area of 2D circle}$$

\uparrow # of modes of 1 polarization

$$g(w) = \frac{dN}{dw} = \left(\frac{L}{2\pi} \right)^2 \pi^2 k^2 \frac{dk}{dw}$$

$$\text{but } w = vk \quad \therefore \frac{dk}{dw} = \frac{1}{v} \quad k = \frac{w}{v}$$

$$\text{so } g(w) = \left(\frac{L}{2\pi} \right)^2 \pi^2 2 \left[\frac{w}{v^2} \right] = \frac{L^2}{2\pi} \frac{w}{v^2}$$

Problem 3.3

$$\text{So } N = \int_0^{\omega_{\max}} g(\omega) d\omega$$

$$N = \int_0^{\omega_{\max}} \frac{L^2 \omega}{2\pi v^2} d\omega = \frac{L^2 \omega_{\max}^2}{4\pi v^2}$$

$$\omega_{\max}^2 = \frac{N}{L^2} \frac{4\pi}{v^2} \rightarrow \omega_{\max} = \sqrt{\frac{N 4\pi v^2}{L^2}}$$

$$\text{So going back to } C = \frac{3}{2\pi} \frac{k_B L^2}{v^2} \frac{\omega^2}{2} \Big|_0^{\omega_{\max}}$$

$$= \frac{3}{2\pi} \frac{k_B L^2}{v^2} \frac{N 4\pi v^2}{L^2} \frac{1}{2} = 3k_B N$$

So we get the same high temp result as in 3D because we assumed the oscillators could move in 3D. If the rest of plane motion were restricted then we would have only 2 polarizations (transverse and longitudinal) and the $3k_B N \rightarrow 2k_B N$

Now for the low Temp limit

$$C = \frac{3}{k_B T^2} \frac{1}{2\pi} \frac{L^2}{v^2} \frac{k_B^2}{v^2} \int_0^{\omega_{\max}} \frac{\omega^3 d\omega e^{\beta \hbar \omega}}{(e^{\beta \hbar \omega} - 1)^2}$$

$$\text{let } x = \beta \hbar \omega$$

$$C = \frac{3}{k_B T^2} \frac{1}{2\pi} \frac{L^2}{v^2} \frac{k_B^2}{v^2} \int_0^{x_{\max}} \frac{x^3 dx e^x}{(e^x - 1)^2} \frac{1}{(\beta \hbar)^4}$$

$$\text{as } T \rightarrow 0 \quad \beta \rightarrow \infty \quad \omega_{\max} \rightarrow \infty$$

Problem 8.4

$$C = \frac{3}{k_B T^2} \frac{1}{2\pi} \frac{L^2 \hbar^2}{v^2} \frac{1}{(\beta \hbar)^4} \int_0^\infty \frac{x^3 dx e^x}{(e^x - 1)^2}$$

$$\int_0^\infty \frac{x^3 e^x dx}{(e^x - 1)^2} = 6 \zeta(3) \approx 7.2$$

↑ zeta function

$$C = \frac{(3)(7.2)}{k_B T^2} \frac{1}{2\pi} \frac{L^2 \hbar^2}{v^2} k_B \left(\frac{k_B T}{\hbar}\right)^{\frac{n}{2}}$$

$$\boxed{C = \frac{(3)(7.2)}{2\pi} \frac{L^2}{\hbar^2 v^2} k_B^3 T^2} \quad n=2$$

check units = $\frac{\text{length}^2}{\text{energy}^2 \cdot \text{sec}^2} \frac{\text{length}^2}{\text{sec}^2} \frac{\text{energy}^3}{\text{OK}^3}$

= $\frac{\text{energy}}{\text{OK}} \checkmark$

Problem 4.1

Problem 4

Highest + and lowest Debye Temp

$$\Theta_D = \frac{h \omega_D}{k_B} = \frac{h}{k_B} \underbrace{[6\pi^2]^{1/3} n^{1/3} v}_{\text{constants}}$$

$n^{1/3} \rightarrow$ [material density]^{1/3}
 $v \rightarrow$ velocity of sound

so Θ_D high when number density is high
 close atomic bonds
 and when speed of sound is high (so when
 the material is hard.)

See attachments from Kittel Intro to Solid State Physics

Elements w/ highest atomic density	C	$17.6 \times 10^{22} / \text{cm}^3$
	B	12.1 "
	Ni	9.4 "
	Co	8.7 "

Elements w/ lowest atomic density	K	$1.4 \times 10^{22} / \text{cm}^3$
	Rb	1.15 "
	Cs	0.905 "
	Ba	1.6 "

See attachment from book Understanding the Properties
 of Matter by de Podesta

Problem 4.2

Elements w/ large speeds of sound

Carbon 18350 m/s

Be 12890 "

Cr 6600

Ti 6130

" w/ low speeds of sound

Pb 2160

Cd 2780

Au 3240

Pt 3260

so we would anticipate that ϕ_D is high
for C (diamond) and maybe Be or B
and should be low for Cs and maybe Pb
or Rb.

lets look them up (see attachment from Kettel)

highest Carbon $\phi_D = 2230$

Be = 1460

lowest Cs $\phi_D = 38$

Rb = 56

so our predictions were pretty good.

Problem 5.1

Problem 5 (Simon 2.5)

Estimate Θ_D for diamond

$$\Theta_D = \frac{\hbar \omega_D}{k_B} \quad \text{where } \omega_D = \left[6\pi^2 n \right]^{1/3} v$$

from previous problem $n = 17.6 \times 10^{22} / \text{cm}^3$
 $v = 18350 \text{ m/s}$

$$\omega_D = \left[6\pi^2 17.6 \times 10^{22} / \text{cm}^3 \right]^{1/3} 1.835 \times 10^6 \text{ cm/s}$$

$$\omega_D = 3.93 \times 10^{14} / \text{s}$$

$$\Theta_D = \frac{(6.58 \times 10^{-16} \text{ eV} \cdot \text{s}) \left(3.93 \times 10^{14} / \text{s} \right)}{(8.6 \times 10^{-5} \text{ eV} / \text{K})}$$

$$\Theta_D = 3.02 \times 10^3 \text{ } ^\circ\text{K}$$

From previous problem value is about 2280°K
 so we have overestimated.

Probably the speed of sound goes down as the material gets hotter as it starts to soften
 so we don't have as high a Θ_D also it
 might expand so $n \downarrow$ as $T \uparrow$

Grad Students only.

Problem 6 - Simon 2.6

(A) If $v_t \neq v_l$ then

$$\begin{aligned} \langle E \rangle &= 2 \sum_{\vec{k} \text{ transverse}} k w_k [n(\beta k w) + 1/2] + \sum_{\vec{k} \text{ longitudinal}} k w_k [n(\beta k w) + 1/2] \\ &= \frac{2 L^3}{(2\pi)^3} \int d\vec{k} k w [n(\beta k w) + 1/2]_{\text{transverse}} \\ &\quad + \frac{L^3}{(2\pi)^3} \int d\vec{k} k w [n(\beta k w) + 1/2]_{\text{longitudinal}} \end{aligned}$$

let $w_{\text{transverse}} = v_t k$ and
 $w_{\text{longitudinal}} = v_l k$

$$\begin{aligned} \text{then } \langle E \rangle &= \frac{2 L^3}{(2\pi)^3} \int 4\pi \frac{w^2 dw}{v_t^3} (n(\beta k w) + 1/2) \\ &\quad + \frac{L^3}{(2\pi)^3} \int 4\pi \frac{w^2 dw}{v_l^3} n(\beta k w + 1/2) \\ &= \left[\frac{2}{v_t^3} + \frac{1}{v_l^3} \right] \frac{L^3}{(2\pi)^3} \int 4\pi w^2 dw (n(\beta k w) + 1/2) \end{aligned}$$

So this modifies $g(w)$

$$\text{from } \frac{L^3 (4)(3) \pi w^2}{(2\pi)^3 v^3} \rightarrow \frac{L^3 4 \pi w^2}{(2\pi)^3} \left[\frac{2}{v_t^3} + \frac{1}{v_l^3} \right]$$

So that w_0^3 now is equal to

$$w_0^3 = 6\pi^2 n \left[\frac{2}{v_t^3} + \frac{1}{v_l^3} \right]^{-1} \quad \begin{array}{l} \text{need this} \\ \text{to get} \\ \text{right behav} \\ \text{when} \\ v_t = v_l \end{array}$$

Temp dependence of C remains the same
 but slope of $C = \alpha T^3$ ← slope is different.

Problem 6.2

- (5) If instead $v_x \neq v_y \neq v_z$
then lets backtrack to page 9

$$E = \hbar\omega \left[n_x + \frac{1}{2} \right] + \left[n_y + \frac{1}{2} \right] + \left[n_z + \frac{1}{2} \right]$$

but lets keep them separate for a while

Such that

$$\langle E \rangle = \sum_{k_x} \sum_{k_y} \sum_{k_z} \hbar\omega(k_x, k_y, k_z) \quad n(\beta\hbar\omega(k_x, k_y, k_z) + \frac{1}{2})$$

$$\sum_{k_x} \rightarrow \int_{-\infty}^{\infty} \frac{L}{2\pi} dk_x$$

$$\text{so } \omega = \alpha |k| \quad \text{where } |k| = \sqrt{k_x^2 + k_y^2 + k_z^2}$$

$$\text{so } \omega^2 = v_x^2 k_x^2 + v_y^2 k_y^2 + v_z^2 k_z^2$$

$$\text{so } \alpha = \frac{|k|}{\omega} = \frac{\sqrt{k_x^2 + k_y^2 + k_z^2}}{\sqrt{v_x^2 k_x^2 + v_y^2 k_y^2 + v_z^2 k_z^2}}$$

$$\text{then } \langle E \rangle = 3 \frac{L^3}{(2\pi)^3} \int d\vec{k} \hbar|\omega| \left(n(\beta\hbar\omega) + \frac{1}{2} \right)$$

$$\text{where } d\vec{k} = dk_x dk_y dk_z$$

So we need to solve the integral (see attached)

Assume $w = \sqrt{v_x^2 k_x^2 + v_y^2 k_y^2 + v_z^2 k_z^2}$

let $v_x = a, v_y = b, v_z = c$ and $k_x = x, k_y = y, k_z = z$

In[1]:= Integrate[$\sqrt{a^2 x^2 + b^2 y^2 + c^2 z^2} / (\text{Exp}[d \times \sqrt{a^2 x^2 + b^2 y^2 + c^2 z^2}] - 1)$,
 $\{x, -\infty, \infty\}, \{y, -\infty, \infty\}, \{z, -\infty, \infty\}$]

$d = \beta \hbar$

Out[1]= ConditionalExpression[$\frac{4 \pi^5}{15 \sqrt{a^2 b^2} d^4 \text{Abs}[c]}$, Re[d] > 0]

In[3]:= (* Lets say that one of the velocities was huge
 (i.e. $v_x \gg v_y$ and v_z , then the energy associated with any k_x
 0 would be enormous and for most values of T except very high,
 the mode would be unoccupied. That would be the same as if we didn't integrate
 over k_x (it would be held at $k_x=0$). Then our integral changes as below. *)

Integrate[$\sqrt{b^2 y^2 + c^2 z^2} / (\text{Exp}[d \times \sqrt{b^2 y^2 + c^2 z^2}] - 1)$, $\{y, -\infty, \infty\}, \{z, -\infty, \infty\}$]

Out[3]= ConditionalExpression[$\frac{4 \pi \text{Zeta}[3]}{\sqrt{b^2 c^2} d^3}$, Re[d] > 0]

Low Temperature limit:

→ If $v_x \neq v_y \neq v_z$ but all are within a reasonable range of one another then

$\langle E \rangle = \frac{3L^3}{(2\pi)^3} \frac{\hbar 4\pi^5}{15 v_x v_y v_z (\beta \hbar)^4} \propto T^4$

So $C = \frac{\partial E}{\partial T} \sim T^3$

→ If $v_x \gg v_y$ and $v_x \gg v_z$

then

$\langle E \rangle \sim \frac{1}{d^3}$ and $\sim \frac{1}{v_y v_z} T^3$

So $C = \frac{\partial \langle E \rangle}{\partial T} \sim T^2$