HW#3 solutions

(1.) O Ch. 3, Q. 3

In the Debye model, the atoms interact to produce sound waves by collective lattice vibrations. These waves are assumed to be independent. As a result the waves do not decay or change with time. In the Einstein model, atoms vibrate independently at a fixed frequency ω_E.

(2.) O Ch. 3, Q. 14

The phonon mean-free path is determined by phonon-phonon scattering, scattering of phonons by impurities and by sample boundaries.

Recall that $\underset{\text{thermal conductivity}}{K} = \frac{1}{3} \overset{\text{specific heat}}{C_v} v_s \overset{\text{phonon mfp}}{\ell}$

(a) One can measure $K(T)$ and $C_v(T)$ to extract $\ell(T)$.

(b) One can measure ultrasound attenuation to find ℓ (decay of the "phonon beam")

3. θ Ch. 3, Pr. 6

a) $E_{cl} = 3RT = 3R\theta_D =$

$= 3\left(8.31 \frac{J}{K\cdot mole}\right)\times 340\,K = 8.48\times 10^3\ J/mol,$

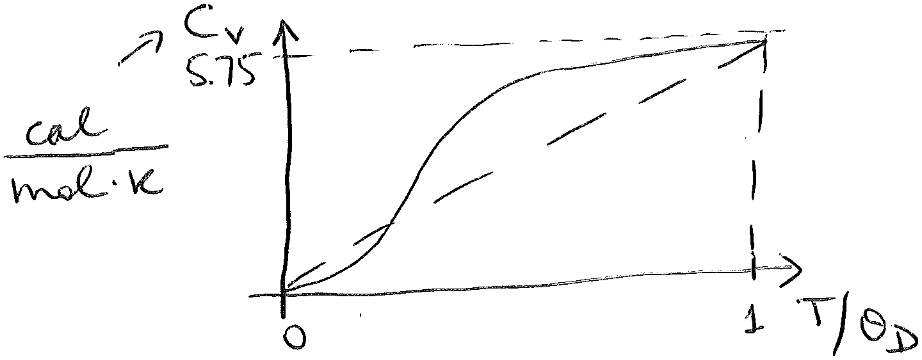
for 1 mole of Cu.

b) Convert to calories/mol:

$E_{cl} = 3\left(2 \frac{cal}{K\cdot mol}\right)\times 340\,K = 2040 \frac{cal}{mol}.$

Fig. 3.13 shows C_V vs. T/Θ_D for Cu + 3 other substances.

For a rough estimate, replace the actual curve with a triangle:



$E_D = \int_0^{\theta_D} dT\, C_V(T) \simeq \frac{1}{2}\times 5.75\times 340 \frac{cal}{mol} \simeq$

$\simeq 977 \frac{cal}{mol}.$

Thus $E_D \simeq \frac{1}{2} E_{cl}$.

c) $E_D \sim \langle T \rangle + \langle V \rangle \sim 2 \langle V \rangle$,

$$E_D \sim 2\left(\frac{1}{2} m \omega_D^2 \langle x^2 \rangle\right),$$

$$\langle x^2 \rangle \sim \frac{E_D}{m \omega_D^2}, \text{ or}$$

$$\boxed{\sqrt{\langle x^2 \rangle} \sim \frac{1}{\omega_D} \sqrt{\frac{E_D}{m}}}.$$

$$E_D \sim k_B \Theta_D = 1.38 \times 10^{-23} \times 340$$

$$m \sim Z m_p = \overset{Cu}{29} \times 1.6 \times 10^{-27}$$

proton

Θ_D

$$\omega_D \sim \frac{k_B \Theta_D}{\hbar} = \frac{1.38 \times 10^{-23} \times 340}{1.05 \times 10^{-34}} \simeq$$

$$\simeq 4.5 \times 10^{13}$$

$$\sqrt{\langle x^2 \rangle} \sim \frac{1}{4.5 \times 10^{13}} \sqrt{\frac{340 \times 1.38 \times 10^{-23}}{29 \times 1.6 \times 10^{-27}}} \sim$$

$$\sim 7 \times 10^{-10}\ \text{m} = 7\ \text{Å}.$$

So, at $T = \Theta_D$ the maximum displacement is several lattice spacings (typically 2-3 Å).

(4.) $\omega = C_s k^2, \quad k = \sqrt{\frac{\omega}{C_s}}$

a) $N(k) \Rightarrow N(\omega) \Rightarrow \frac{dN(\omega)}{d\omega}$.

$$N(k) = \frac{\frac{4}{3}\pi k^3}{(2\pi)^3/V} = \frac{V}{6\pi^2} k^3.$$

$V = L^3$

Then $N(\omega) = \frac{V}{6\pi^2}\left(\frac{\omega}{C_s}\right)^{3/2}$, and

$$\underset{\substack{\uparrow \\ \text{per mode}}}{D(\omega)} = \frac{dN(\omega)}{d\omega} = \frac{3}{2}\left(\frac{V}{6\pi^2 C_s}\right)\left(\frac{\omega}{C_s}\right)^{1/2}.$$

So, $D(\omega) = \frac{V}{4\pi^2 C_s}\sqrt{\frac{\omega}{C_s}}$.

There is only a single mode b/c of 1 atom/unit cell.

b) $N = \int_0^{\omega_{max}} D(\omega)d\omega$ defines ω_{max}

$$N = \left(\frac{V}{4\pi^2}\right)\frac{1}{C_s^{3/2}}\frac{\omega_{max}^{3/2}}{3/2} =$$

$$= \left(\frac{V}{6\pi^2}\right)\left(\frac{\omega_{max}}{C_s}\right)^{3/2}.$$

Then
$$\omega_{max} = c_s \left(6\pi^2 \frac{N}{V} \right)^{2/3} .$$

c)
$$U(T) = \int_0^{\omega_{max}} \frac{D(\omega)\hbar\omega\, d\omega}{e^{\hbar\omega/k_B T} - 1} =$$

$$= \left(\frac{V}{4\pi^2 c_s^{3/2}} \right) \int_0^{\omega_{max}} d\omega \, \frac{\hbar \omega^{3/2}}{e^{\hbar\omega/k_B T} - 1} .$$

Since
$$\frac{\partial}{\partial T} \left(e^{\frac{\hbar\omega}{k_B T}} - 1 \right)^{-1} = \frac{\hbar\omega}{k_B T^2} \frac{e^{\hbar\omega/k_B T}}{\left(e^{\hbar\omega/k_B T} - 1\right)^2},$$

$$C_V = \frac{\partial U}{\partial T} = \frac{V}{4\pi^2 c_s^{3/2}} \frac{\hbar^2}{k_B T^2} \int_0^{\omega_{max}} d\omega \; \times$$
$$\times \; \frac{\omega^{5/2} e^{\hbar\omega/k_B T}}{\left(e^{\hbar\omega/k_B T} - 1\right)^2} .$$

Using $x = \hbar\omega / k_B T$,
$$C_V = \underset{\text{const}}{A} \frac{1}{T^2} T^{7/2} \underbrace{\int_0^{\infty} dx \, \frac{x^{5/2} e^{x}}{(e^{x} - 1)^2}}_{I(5/2)} .$$

Thus $C_V \sim T^{3/2}$. Note that the upper limit is ∞ in $\int_0^\infty dx$ b/c $k_B T \ll \hbar\omega_{max}$.

(5.) $\omega = c k$ for photons

$\uparrow$ speed of light

Similar to the Debye model, but w/no upper limit:

$$U(T) = \int_0^\infty \frac{D(\omega)\hbar\omega\, d\omega}{\left(e^{\frac{\hbar\omega}{k_B T}} - 1\right)} = \frac{V}{2\pi^2 c^3}\int_0^\infty d\omega \frac{\hbar\omega^3}{e^{\frac{\hbar\omega}{k_B T}} - 1} =$$

$$= \frac{V}{2\pi^2 c^3}\frac{(k_B T)^4}{\hbar^3}\underbrace{\int_0^\infty dx \frac{x^3}{e^x - 1}}_{\pi^4/15}.$$

$x = \frac{\hbar\omega}{k_B T}$

So, $$U(T) = \frac{V}{2\pi^2}\frac{\pi^4}{15}\frac{(k_B T)^4}{(\hbar c)^3}.$$

$$C_V = \frac{\partial U}{\partial T} = 4 k_B \frac{V}{2}\frac{\pi^2}{15}\frac{(k_B T)^3}{(\hbar c)^3} =$$

$$= \frac{2\pi^2}{15} V k_B \left(\frac{k_B T}{\hbar c}\right)^3.$$

So, $$\underline{\underline{\frac{C_V}{V} = \frac{2\pi^2}{15} k_B \left(\frac{k_B T}{\hbar c}\right)^3}}.$$

Note that $\frac{C_V^{\text{phonon}}}{C_V^{\text{photon}}} \sim \left(\frac{c}{v_s}\right)^3 \gg 1.$

⑥ θ Ch. 3, Pr. 4

As shown in class,

$$\int_0^\infty dp\, e^{-\alpha p^2} = \frac{1}{2}\sqrt{\frac{\pi}{\alpha}},$$

$$\int_0^\infty dp\, p^2 e^{-\alpha p^2} = \frac{\sqrt{\pi}}{4\alpha^{3/2}}.$$

For a SHO in 1D,

$$\bar{\epsilon} = \bar{T} + \bar{V} =$$

$$= \frac{1}{2m} \frac{\int_0^\infty dp\, p^2 e^{-p^2/2mk_BT}}{\int_0^\infty dp\, e^{-p^2/2mk_BT}} +$$

$$+ \frac{m\omega^2}{2} \frac{\int_0^\infty dq_0\, q_0^2 e^{-\frac{m\omega^2 q_0^2}{2k_BT}}}{\int_0^\infty dq_0\, e^{-\frac{m\omega^2 q_0^2}{2k_BT}}}, \quad \text{since}$$

$$\epsilon = \frac{p^2}{2m} + \frac{m\omega^2 q_0^2}{2}.$$

For the 1st term on the RHS,

$\alpha = \frac{1}{2mk_BT}$, which gives

$$\frac{\sqrt{\pi}/4\alpha^{3/2}}{\sqrt{\pi/\alpha}\ 1/2} = \frac{1}{2\alpha} = mk_BT.$$

For the 2nd term,

$$\alpha = \frac{m\omega^2}{2k_BT} \Rightarrow \frac{1}{2\alpha} = \frac{k_BT}{m\omega^2}.$$

Then $\bar{\epsilon} = \frac{1}{2m} m k_B T + \frac{m\omega^2}{2} \frac{k_B T}{m\omega^2} =$

$$= k_B T.$$

(7.) θ Ch. 3, Pr. 5

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

$$\bar{\epsilon} = \langle E_n \rangle = \hbar\omega\left(\langle n \rangle + \frac{1}{2}\right)$$, where

$$\langle n \rangle = \frac{\sum_{n=0}^{\infty} n e^{-n\hbar\omega/k_B T}}{\sum_{n=0}^{\infty} e^{-n\hbar\omega/k_B T}}.$$

as shown in class,

$$\begin{cases} \sum_{n=0}^{\infty} x^n = \frac{1}{1-x}, \\ \sum_{n=0}^{\infty} n x^n = \frac{x}{(1-x)^2} \end{cases}$$

Then $\langle n \rangle \underset{x = e^{-\hbar\omega/k_B T}}{=} \frac{1}{e^{\hbar\omega/k_B T} - 1}$, and

$$\bar{\epsilon} = \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1} + \underbrace{U_0}_{\text{zero point energy}}$$