45/45

# HW#3 solutions



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

In the Einstein model the atoms are independent simple harmonic oscillators (SHOs), with a single frequency $\omega_E$.

In the Debye approach the atoms interact to produce collective lattice vibrations. However, there are no interactions between these waves. As a result, lattice vibrations (waves) do not scatter or decay with time, which is not true in general.

(2.) O. Ch. 3, Q. 4

Sound waves are compression waves. You cannot have a sound wave in a single small molecule, but sound waves can be sustained by a gas or liquid of small molecules. Sound waves can propagate in gaseous substances (such as air!), and

$$\underbrace{v_s}_{\text{speed of sound}} \sim \sqrt{p}\ ,$$ where $p$ is the pressure of the gas

③ O. Ch. 3, Q. 13

Diamond has a large thermal conductivity ($\approx$ 3 times better than copper), and thus is used to transport heat away efficiently in electronic devices.

④ O. Ch. 3, Pr. 4

As shown in class,

$$\epsilon = \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2} \quad \Leftarrow \text{energy of a 1D oscillator}$$

Then

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

$$+ \frac{\frac{m\omega^2}{2}\int_0^\infty q^2 e^{-\frac{m\omega^2 q^2}{2k_BT}}\,dq}{\int_0^\infty e^{-\frac{m\omega^2 q^2}{2k_BT}}\,dq} .$$

Using $\begin{cases} \int_0^\infty dx\, e^{-\alpha x^2} = \frac{1}{2}\sqrt{\frac{\pi}{\alpha}}, \\ \int_0^\infty dx\, x^2 e^{-\alpha x^2} = \frac{\sqrt{\pi}}{4}\alpha^{-3/2}, \end{cases}$

we obtain:

$$\bar{T} = \frac{1}{2m} \frac{\sqrt{\frac{\pi}{\alpha}}\frac{1}{4\alpha}}{\frac{1}{2}\sqrt{\frac{\pi}{\alpha}}} = \frac{1}{4m\alpha} = \frac{k_B T}{2},$$

$$\alpha = \frac{1}{2mk_BT}$$

$$\bar{V} = \frac{\cancel{m\omega^2}}{2}\frac{1}{2}\frac{2k_BT}{\cancel{m\omega^2}} = \frac{k_BT}{2}.$$

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

Hence $\bar{\epsilon} = \frac{k_BT}{2} + \frac{k_BT}{2} = k_BT$, as expected

(5.) $\theta$. Ch. 3, Pr. 5

$$\bar{\epsilon} = \frac{\sum_{n=0}^{\infty} \epsilon_n e^{-\epsilon_n/k_BT}}{\sum_{n=0}^{\infty} e^{-\epsilon_n/k_BT}}, \quad \text{where}$$

$\epsilon_n = n\hbar\omega$ (neglecting the zero-point energy)

Then $$\bar{\epsilon} = \frac{\hbar\omega \sum_{n=0}^{\infty} n e^{-\frac{n\hbar\omega}{k_BT}}}{\sum_{n=0}^{\infty} e^{-\frac{n\hbar\omega}{k_BT}}}.$$

Using
$$\begin{cases} \sum_{n=0}^{\infty} x^n = \frac{1}{1-x} & \leftarrow \text{shown in class} \\ \sum_{n=0}^{\infty} n x^n = \frac{x}{(1-x)^2}, \end{cases}$$

we obtain:

$$\bar{\epsilon} = \hbar\omega \, \frac{x/(1-x)^2}{1/(1-x)} = \hbar\omega \, \frac{x}{1-x} = \hbar\omega \, \frac{1}{1/x - 1},$$

where $x \equiv e^{-\frac{\hbar\omega}{k_B T}}$.

Thus $\bar{\epsilon} = \dfrac{\hbar\omega}{e^{\frac{\hbar\omega}{k_B T}} - 1}$, as desired.

**6.** Θ Ch. 3, Pr. 6

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

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

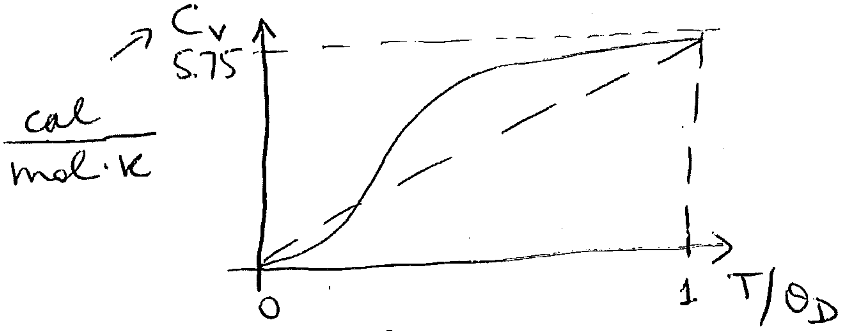
for 1 mole of Cu.

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. $T/\Theta_D$ 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) $E_D \sim \langle T \rangle + \langle V \rangle \sim 2\langle V \rangle$,

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

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

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

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

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

proton

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

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

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

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

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

7. O. Ch. 3, Pr. 8

The internal energy is given by

$$E = \frac{3V}{2\pi^2 v_s^3} \int_0^{\omega_D} d\omega \, \frac{\hbar \omega^3}{e^{\hbar\omega/k_B T} - 1}$$ in

the Debye model.

shown in class

$$C_v = \left(\frac{\partial E}{\partial T}\right)_v = \left(\frac{3V\hbar}{2\pi^2 v_s^3}\right) \int_0^{\omega_D} d\omega \, \omega^3 \frac{\partial}{\partial T}\left(\frac{1}{e^{\frac{\hbar\omega}{k_B T}} - 1}\right).$$

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

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

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

Define $\Theta_D \equiv \dfrac{\hbar\omega_D}{k_B}$,

$x \equiv \dfrac{\hbar\omega}{k_B T}$, $x_D = \dfrac{\hbar\omega_D}{k_B T} = \dfrac{\Theta_D}{T}$ to obtain:

$$C_v = \underbrace{\left(\frac{3V}{2\pi^2 v_s^3}\right) \frac{\hbar^2}{k_B T^2} \left(\frac{k_B T}{\hbar}\right)^5}_{(3k_B)\left(\frac{V}{2\pi^2 v_s^3}\right)\left(\frac{k_B T}{\hbar}\right)^3} \int_0^{x_D} dx \, \frac{x^4 e^x}{(e^x - 1)^2}.$$

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

$$= (3k_B)\left(\frac{V}{2\pi^2 v_s^3}\right)\left(\frac{k_B T \omega_D}{\hbar \omega_D}\right)^3 = (3k_B)\left(\frac{V}{2\pi^2 v_s^3}\right)\left(\frac{T}{\Theta_D}\right)^3 \omega_D^3 \quad (11)$$

$= (9k_B) N \left(\frac{T}{\theta_D}\right)^3$

using $\omega_D^3 = 6\pi^2 v_s^3 \left(\frac{N}{V}\right)$

Therefore,

$$C_V = (9R)\left(\frac{T}{\theta_D}\right)^3 \int_0^{x_D} dx \, \frac{x^4 e^x}{(e^x-1)^2}, \quad \text{as expected.}$$

per mole of substance

8. Einstein considered a solid to be a collection of simple harmonic oscillators (SHOs) whose energies are quantized.

(i) He assumed that all oscillators vibrate independently w/same frequency

(ii) At high-T, $C_v = 3R$ is recovered (the classical limit)

(iii) At low-T, the Einstein specific heat falls below the classical value, and $\lim_{T \to 0} C_v \to 0$.

However, $C_v$ approaches $\emptyset$ exponentially at low Ts, which is faster than what was observed experimentally.

9.

$\omega = ck$ for photons

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

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

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

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

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