Homework 3 Solutions

Physics 406.

1. O chap. 3 Q 3.

In the Einstein model the atoms are treated as independent simple harmonic oscillators (SHOs), with a single frequency w_E.

By contrast in the Debye approach the atoms interact to produce collective lattice motions (eg sound waves) but there is assumed to be no interaction between these waves. As a result a single wave does not decay or transform with time, and this model does not include thermal expansion

2. O chap. 3 Q. 14.

The phonon mean-free path is primarily determined by

(i) phonon-phonon scattering

(ii) scattering of phonons by defects in the solid

(iii) scattering of the phonons by samples boundaries

If we assume the relation

$$K = \frac{1}{3} C_v v l$$

the phonon mean-free path can be determined by

(a) direct comparison of measurements of $\kappa(T)$ and $c_v(T)$

(b) ultrasound attenuation

(measured attenuation of "phonon beam")

(c) Raman and Brillouin (light) scattering

↑ optical phonon   ↑ acoustic phonon

Rayleigh Line - Static impurities

Stokes Lines - Phonon scattering

⋮

3. O chap 3 p. 6.

a) $E = 3RT = 3R\,\Theta_D$

$= (3)(8.31\ \text{J K}^{-1}\text{mole}^{-1})(340\ \text{K})$

$= (3)(8.31)(340)\ \text{J mol}^{-1}$

$\boxed{\text{1 mole of Cu} \Rightarrow 8.48 \times 10^3\ \text{J}}$

For comparison to the value that we'll get from the graph in Fig 3.13 (see b), we want this energy in calories ⇒

then

$$E_{class} = 3RT = 3\,(2\ \text{cal}\ K^{-1}\,\text{mol}^{-1})\,(340$$

$$= 2040\ \text{calories mol}^{-1}$$

$$\Downarrow$$

$$\boxed{1\ \text{mole of Cu} \Rightarrow E_{class} = 2040\ \text{calories}}$$

b)

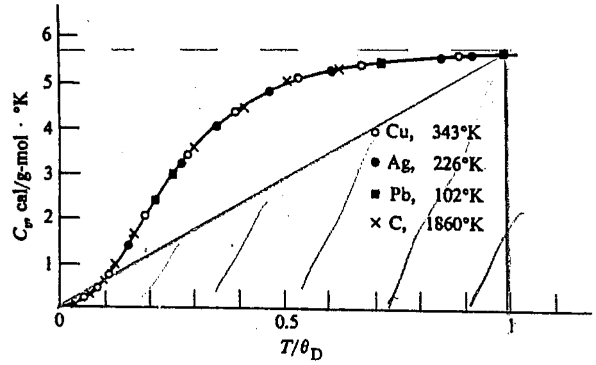

Fig. 3.13 Specific heats versus reduced temperature for four substances. Numbers refer to Debye temperatures. Note the high Debye temperature for diamond.

$$E_{Debye} \sim \int_0^{\Theta_D} dT\ C_V$$

$$\sim \frac{1}{2}\,(5.75)\,(340) \sim 977 \quad \text{calories}$$

Therefore

$$E_{\text{Debye}} < E_{\text{classical}}.$$

c) $$E_{\text{Debye}} \sim \langle T \rangle + \langle V \rangle \sim 2 \langle V \rangle$$

$$\Downarrow$$

$$E_{\text{Debye}} \sim 2 \left(\frac{1}{2} m \omega_D^2 \langle x^2 \rangle \right)$$

$$\Downarrow$$

$$\langle x^2 \rangle \sim \frac{E_{\text{Debye}}}{m \omega_D^2}.$$

$$\Downarrow$$

$$\sqrt{\langle x^2 \rangle} \sim \frac{1}{\omega_D} \sqrt{\frac{E_{\text{Debye}}}{m}}$$

$$[L] \overset{?}{=} [T] \sqrt{\frac{[M]\,[L]^2 / [T]^2}{[M]}}$$

$$\overset{?}{=} [T] \frac{[L]}{[T]} \quad \checkmark$$

$$[L] = [L] \quad \checkmark .$$

$$E_D \sim (340)\, k_B \sim (340)(1.4 \times 10^{-23})$$

$$m \sim Z m_p \sim (29)(1.6 \times 10^{-27}).$$

$$\omega_D \sim \frac{k_B T_D}{\hbar} \sim \frac{(1.4) \times 10^{-3})\ (340)}{1.05 \times 10^{-34}}$$

$$\sim 4.5 \times 10^{13}.$$

$$\sqrt{\langle x^2 \rangle} \sim \frac{1}{4.5 \times 10^{13}} \sqrt{\frac{(340)(1.4 \times 10^{-23})}{(29)(1.6 \times 10^{-27})}}$$

$$\sim \frac{10^2}{4.5 \times 10^{13}} \sqrt{\frac{(340)(1.4)}{(29)(1.6)}}$$

$$\sqrt{\langle x^2 \rangle} \sim 7 \times 10^{-10} \text{ m} = 7 \text{ Å}$$

This is to be compared w/ the lattice spacing of copper, which is 2Å. Therefore at $T \sim \Theta_D$ the maximum displacement of the atoms is about 3.5 lattice spacings

4.

a. In the Einstein model

$$U(T) = \sum_{n} \left(n+\frac{1}{2}\right) \hbar\omega_E$$

$$T=0 \Rightarrow U = \frac{1}{2}\hbar\omega_E \qquad \text{since} \quad n=0$$

For a harmonic oscillator $\langle T \rangle = \langle V \rangle$

$$\Downarrow$$

$$\langle E \rangle = \langle T \rangle + \langle V \rangle = 2\langle V \rangle$$

$$= 2\left(\frac{1}{2} m\omega_E^2 \langle x^2 \rangle\right) = \frac{1}{2}\hbar\omega_E$$

$$\Downarrow$$

$$\langle x^2 \rangle = \frac{\hbar}{2m\omega_E}$$

Typically $\omega_E \sim 10^{13}\ s^{-1}$

Use $m_p \sim 10^9\ eV/c^2$

$$\Downarrow$$

$$\sqrt{\langle x^2 \rangle} = \frac{(hc)\ c}{4\pi\,(mc^2)\,(\omega_E)}$$

→

$$\sqrt{\langle x^2 \rangle} = \frac{(\hbar c)\, c}{4\pi (mc^2)(\omega_E)} = \frac{(12400\ \mathrm{eV\text{-}\AA})(3 \times 10^{18}\ \mathrm{\AA/s})}{(4\pi)(10^9\ \mathrm{eV})(10^{13})}$$

$$\sim \frac{(1.24)(3)}{4\pi} \quad \frac{10^4\ \cancel{10^{18}}}{10^9\ \cancel{10^{13}}}$$

$$\sim .3\ \mathrm{A}$$

$$\boxed{\sqrt{\langle x^2 \rangle} \sim .3\ \mathrm{\AA}}$$

5. For photons $\omega = ck$ => same dispersion as phonons at low temperatures

✓ same as Debye with no upper limit !

$$u(T) = \int_0^\infty \frac{\mathcal{D}(\omega)\, \hbar\omega\, d\omega}{(e^{\hbar\omega/kT} - 1)} = \frac{V}{(2\pi^2 c^3)} \int_0^\infty \frac{\omega^2\, \hbar\omega\, d\omega}{(e^{\hbar\omega/kT} - 1)}$$

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

Therefore

$$U(T) = \left(\frac{V}{2\pi^2}\right)\left(\frac{\pi^4}{15}\right)\frac{(kT)^4}{(\hbar c)^3}.$$

$$\Downarrow$$

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

$$\Downarrow$$

$$\boxed{\frac{c_V}{V} = \left(\frac{2\pi^2}{15}\right)\left(\frac{kT}{\hbar c}\right)^3 k_B}$$

N.B.

$$\frac{c_V^{\text{lattice}}}{c_V^{\text{photon}}} \sim \left(\frac{c}{v}\right)^3 \sim \left(\frac{10^8 \text{ m/s}}{10^3 \text{ m/s}}\right)^3 \sim 10^{15}$$

where v is speed of sound

6.

$\omega = c_s k^2 \quad \Rightarrow \quad k = \left(\frac{\omega}{c_s}\right)^{1/2}$

a) $\mathcal{D}(\omega)$

Strategy: (i) Calculate $N(k)$

(2) Use dispersion relation $\Rightarrow$ $N(\omega)$

(3) $\mathcal{D}(\omega) = \frac{dN(\omega)}{d\omega}$

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

where $V = L^3$

$$\Downarrow$$

$$N(\omega) = \frac{V}{6\pi^2}\left(\frac{\omega}{c_s}\right)^{3/2}$$

$$\Downarrow$$

$$\mathcal{D}(\omega) = \frac{dN(\omega)}{d\omega} = \frac{3}{2}\left(\frac{V}{6\pi^2 c_s}\right)\left(\frac{\omega}{c_s}\right)^{1/2}$$

$$\boxed{\mathcal{D}(\omega) = \left(\frac{V}{4\pi^2}\right)\frac{\omega^{1/2}}{c_s^{3/2}}}$$

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

$$\Downarrow$$

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

$$\Downarrow$$

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

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

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

We note that

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

$$\Downarrow$$

$$c_v = \frac{dU}{dT} = \frac{V}{4\pi^2 c^{3/2}}\,\frac{\hbar^2}{kT^2}\int_0^{\omega_{max}} \frac{\omega^{5/2}\, e^{\hbar\omega/kT}\, d\omega}{\left(e^{\hbar\omega/kT}-1\right)^2}$$

$$\Downarrow$$

$$c_v = A\left(\frac{1}{kT^2}\right)(kT)^{7/2}\underbrace{\int_0^{\infty}\frac{x^{5/2}\, e^{x}\, dx}{\left(e^{x}-1\right)^2}}_{B}$$

$$x = \hbar\omega/kT$$

$$c_v = \underset{\substack{\downarrow \\ \text{constant}}}{\tilde{A}}\; T^{3/2} \Rightarrow \boxed{c_v \propto T^{3/2}}$$

7.

- Einstein considered a solid to be an ensemble of simple harmonic oscillators (SHOs) whose vibrational energies are quantized
- He assumed that they were independent with one frequency
- At high temperatures he was able to recover the expected classical value of the specific heat (c_V).
- At low temperatures the Einstein specific heat was well below the classical value and

$$\lim_{T \to 0} c_V \to 0$$

- However Einstein's specific heat went to zero at low temperatures faster than what was observed experimentally.