1. O chap. 3  Q. 3.

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

By contrast in the Debye approach the atoms interact to produce collective lattice vibrations (e.g. 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 sample boundaries

If we assume the relation

$$\lambda = \frac{1}{3} \rho v \nu l$$
the phonon mean-free path can be determined by:
(a) direct comparison of measurements of $\kappa(T)$ and $c_v(T)$
(b) ultrasonic attenuation
(measured attenuation of "phonon beam")
(c) Raman and Brillouin (light) scattering

\[
\text{Rayleigh line} \quad - \quad \text{Static impurities}
\]
\[
\text{Stokes lines} \quad - \quad \text{Phonon scattering}
\]

3.
8. 6 chap 3 p. 6.

a) \[ E = 3RT = 3R \Theta_D \]

\[ = (3)(8.31 \text{ J K}^{-1} \text{ mol}^{-1})(340 \text{ K}) \]

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

1 mol of Cu $\Rightarrow$ 8.48 $\times$ 10$^3$ 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 →

\[ E_{\text{class}} = 3RT = 3 \left( 2 \text{ cal K}^{-1} \text{ mol}^{-1} \right) \times 1340 \]

\[ = 2040 \text{ calories mol}^{-1} \]

1 mol of H₂ → \( E_{\text{class}} = 2040 \text{ calories} \)

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

\[ E_{\text{Debye}} \sim \int_0^{\Theta_0} dT \cdot c_V \]

\[ \sim \frac{1}{2} \left( 5.75 \right) \left( 340 \right) \sim 977 \text{ calories} \]
Therefore

\[ E_{\text{Debye}} < E_{\text{Classical}} \]

\[ E_{\text{Debye}} \sim \langle T \rangle + \langle V \rangle \sim 2 \langle V \rangle \]

\[ E_{\text{Debye}} \sim 2 \left( \frac{1}{2} m w D^2 \langle x^2 \rangle \right) \]

\[ \langle x^2 \rangle \sim \frac{E_{\text{Debye}}}{m w D^2} \]

\[ \sqrt{\langle x^2 \rangle} \sim \frac{1}{w D} \sqrt{\frac{E_{\text{Debye}}}{m}} \]
\[ [L] = \sqrt{\frac{[M] [L]^2}{[T]^2}} \]
\[ [T] [L] \checkmark \]
\[ [L] = [L] \checkmark . \]

\[ E_\text{D} \sim (340) k_B \sim (340)(1.4 \times 10^{-23}) \]
\[ m \sim \frac{2}{7} m_p \sim (29)(1.6 \times 10^{-27}) . \]
\[ \omega_\text{D} \sim \frac{k_B T_D}{h} \sim \frac{(1.4) \times 10^{-3}}{1.05 \times 10^{-34}} \]
\[ \sim 4.5 \times 10^{13} . \]

\[ \sqrt{\langle x^2 \rangle} \sim \frac{1}{4.5 \times 10^{13}} \]
\[ \sim \frac{10^2}{4.5 \times 10^{13}} \]

\[ \sqrt{\frac{(340)(1.4 \times 10^{-23})}{(29)(1.6 \times 10^{-27})}} \]

\[ \sqrt{\frac{(340)(1.4)}{(29)(16)}} \]
\[ \sqrt{\langle x^2 \rangle} = 7 \times 10^{-10} \text{ m} = 7 \text{ Å} \]

This is to be compared with the lattice spacing of copper, which is 2 Å. Therefore at \( T \approx T_d \), the maximum displacement of the atoms is about 3.5 lattice spacings.
4. In the Einstein model
\[ U(T) = \sum_n \left( n + \frac{1}{2} \right) k_\text{B} \omega_E \]

\[ T = 0 \Rightarrow U = \frac{1}{2} k_\text{B} \omega_E \quad \text{since} \quad n = 0 \]

For a harmonic oscillator \( \langle T \rangle = \langle V \rangle \)

\[ \langle E \rangle = \langle T \rangle + \langle V \rangle = 2 \langle V \rangle \]

\[ = 2 \left( \frac{1}{2} m \omega_E^2 \langle x^2 \rangle \right) = \frac{1}{2} k_\text{B} \omega_E \]

\[ \downarrow \]

\[ \langle x^2 \rangle = \frac{k_\text{B}}{2m\omega_E} \]

Typically \( \omega_E \sim 10^{13} \text{ s}^{-1} \)

\[ \mu_e \sim m_p \sim 10^9 \text{ eV/}c^2 \]

\[ \downarrow \]

\[ \sqrt{\langle x^2 \rangle} = \frac{\hbar c}{4\pi (mc^2)(\omega_E)} \]
\[ \sqrt{\langle x^2 \rangle} = \frac{(hc)c}{4\pi (mc^2)(\omega_E)} = \frac{(12400 \text{ eV} \cdot \text{Å})}{(4\pi) (10^3 \text{ eV}) (10^{13})} \]

\[ \sim \frac{(1.24)(3)}{4\pi} \frac{10^4}{10^{18}} \]

\[ \sim 0.3 \text{ Å} \]

\[ \sqrt{\langle x^2 \rangle} \sim 0.3 \text{ Å} \]

5. For photons \( \omega = c k \nu \) => same dispersion as phonons at low temperatures

\[ \sqrt{\text{same as Debye with no upper limit!}} \]

\[ U(T) = \int_0^{\infty} \frac{\Theta(\omega) \omega^2 \nu_0 \omega \, d\omega}{(e^{\omega/(kT)} - 1)} = \frac{V}{(2\pi c^3)} \int_0^{\infty} \frac{\omega^2 \nu_0 \omega \, d\omega}{(e^{\omega/(kT)} - 1)} \]

\[ = \frac{V}{(2\pi^2 c^3)} \frac{(kT)^4}{h^3} \int_0^{\infty} \frac{x^3}{(e^x - 1)} \, dx \]

\[ = \frac{\pi^4}{15} \]
Therefore

\[ U(T) = \left( \frac{V}{2\pi^2} \right) \left( \frac{\pi^4}{15} \right) \frac{(kT)^4}{(hc)^3} \]

\[ \Downarrow \]

\[ c_v = \frac{\partial U}{\partial T} = 4k_B \left( \frac{V}{2\pi^2} \right) \left( \frac{\pi^4}{15} \right) \frac{(kT)^3}{(hc)^3} \]

\[ \Downarrow \]

\[ \frac{c_v}{V} = \left( \frac{2\pi^2}{15} \right) \left( \frac{kT}{hc} \right)^3 \approx k_B \]

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

a) \( \Theta(\omega) \)

Strategy:

1. Calculate \( N(k) \)
2. Use dispersion relation \( \Rightarrow N(\omega) \)
3. \( \Theta(\omega) = \frac{dN(\omega)}{d\omega} \)

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

where \( V = L^3 \)

\[ \downarrow \]

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

\[ \downarrow \]

\[ \Theta(\omega) = \frac{dN(\omega)}{d\omega} = \frac{3}{2} \left( \frac{V}{6\pi^2 c_s} \right) \left( \frac{\omega}{c_s} \right)^{1/2} \]

\[ \Theta(\omega) = \left( \frac{V}{4\pi^2} \right) \frac{\omega^{1/2}}{c_s^{3/2}} \]
b) \[ N = \int_0^{w_{\text{max}}} \Theta(w) \, dw \] defines \( w_{\text{max}} \)

\[ N = \left( \frac{V}{4\pi^2} \right) \frac{1}{c_s^{3/2}} \frac{w_{\text{max}}^{3/2}}{c_s} \]

(c) \[ U(T) = \int_0^{w_{\text{max}}} \frac{\Theta(w) \, \hbar w \, dw}{\left( e^{\frac{\hbar w}{kT}} - 1 \right)} \]

\[ = \left( \frac{V}{4\pi^2 c_s^{3/2}} \right) \int_0^{w_{\text{max}}} \frac{\hbar w^{3/2} \, dw}{\left( e^{\frac{\hbar w}{kT}} - 1 \right)} \]
He notes that

$$\frac{\partial}{\partial t} \left( e^{\frac{Kw}{kT}} - 1 \right)^{-1} = \frac{Kw}{kT^2} \left( e^{\frac{Kw}{kT}} - 1 \right)^2$$

\[ \downarrow \]

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

\[ \downarrow \]

$$c_v = A \left( \frac{1}{kT^2} \right) (kT)^{3/2} \int_0^{\infty} \frac{x^{5/2} e^x}{\left( e^x - 1 \right)^2} \, dx$$

$$= \frac{B}{x = \frac{Kw}{kT}}$$

$$c_v = \tilde{A} T^{3/2} \quad \Rightarrow \quad c_v \propto T^{3/2}$$

\[ \text{constant} \]
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.