Stat Mech: HW #10: | Allen Murray

#1: a) Show that in Debye theory $E(T)$ can be expressed as,

$$E = 9N \frac{(kT)^4}{(\hbar\omega_D)^3} \int_0^{\beta\hbar\omega_D} \frac{x^3 dx}{e^x - 1}.$$ Ignoring ground state energy.

- b) Show this gives correct answers in high/low temp limits.
- c) Compute integral explicitly, and compare with Einstein formula; $E = \frac{3N\hbar\omega_0}{e^{\beta\hbar\omega_0} - 1}$; ω_0 = characteristic oscillation freq.

Can we relate ω_0 to ω_D? How do heat capacities differ?

- d) Use diamond.dat compare Einstein & Debye formula. Which gives the better fit? Find ω_0 for diamond.
- e) Compute ω_0 as a theoretical value based on material properties of diamond and compare with (d).

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a) Start with, $E = \sum_{\substack{\text{modes} \\ \omega}} \hbar\omega(n_B(\beta) + \frac{1}{2})$ where we change

$$\sum_{\substack{\text{modes} \\ \omega}} \Rightarrow \int \frac{d^3x\, d^3p}{(2\pi\hbar)^3} \quad \text{where} \quad p = \hbar k = \frac{\hbar\omega}{c_s}$$

$$= \frac{3V}{(2\pi\hbar)^3} \left(\frac{\hbar}{c_s}\right)^3 \int 4\pi\omega^2 d\omega = \int g(\omega) d\omega \; ; \quad g(\omega) = \text{density of states.}$$
$$= 9N\frac{\omega^2}{\omega_D^3} ; \quad \omega_D^3 = 6\pi^2 n c_s^3$$

Energy then is,

$$E = 9N \int_0^\infty \frac{\omega^2 d\omega}{\omega_D^3} \hbar\omega(n_B(\beta) + \tfrac{1}{2}) \to \infty \quad \text{let} \quad x = \beta\hbar\omega \quad dx = \beta\hbar d\omega$$

$$E - E_{gs} = 9N \int \frac{\hbar\omega^3 d\omega}{\omega_D^3 (e^{\beta\hbar\omega} - 1)} = \frac{9N}{\omega_D^3} \frac{\hbar}{(\beta\hbar)^4} \int_0^{\beta\hbar\omega_D} \frac{x^3 dx}{e^x - 1}$$ since integrating to $+\infty$ gives catastrophe.

Ignore ground state:

$$\boxed{E = 9N \frac{(kT)^4}{(\hbar\omega_D)^3} \int_0^{\beta\hbar\omega_D} \frac{x^3 dx}{e^x - 1}}$$

b) low temp limit: $T \to 0$, $\beta \to \infty$; $\beta\hbar\omega_0 \gg 1$

$$E = 9N\frac{(kT)^4}{(\hbar\omega_D)^3}\int_0^{\beta\hbar\omega_0}\frac{x^3dx}{e^x-1}$$ this time we can let $x \to \infty$

$$E = 9N\frac{(kT)^4}{(\hbar\omega_D)^3}\underbrace{\int_0^{\infty}\frac{x^3dx}{e^x-1}}_{\frac{\pi^4}{15}} = \boxed{\frac{3N\pi^4}{5(\hbar\omega_D)^3}(kT)^4}$$

high temp limit: $\beta\hbar\omega_D \ll 1$ $n_B(\beta) \approx \frac{1}{\beta\hbar\omega}$

$$E = \frac{9NkT}{\omega_D^3}\int_0^{\omega_D}\omega^2 d\omega = \boxed{3NkT}$$ Usual ideal gas result.

c)

$$E = 9N\frac{(kT)^4}{(\hbar\omega_D)^3}\int_0^{\beta\hbar\omega_D}\frac{x^3dx}{e^x-1} = 9N\frac{(kT)^4}{(\hbar\omega_D)^3}\left[6Li_4(e^{\beta\hbar\omega_D}) - \beta\hbar\omega_D(24Li_3(e^{\beta\hbar\omega_D})\right.$$ Too long continued below.

$$\boxed{E = 9N\frac{(kT)^4}{(\hbar\omega_D)^3}\left[6Li_4(e^{\beta\hbar\omega_D}) - \frac{\beta\hbar\omega_D(24Li_3(e^{\beta\hbar\omega_D}) - \beta\hbar\omega_D 12Li_2(e^{\beta\hbar\omega_D}) + \beta\hbar\omega_D(4\ln(1-e^{\beta\hbar\omega_D}) - \beta\hbar\omega_D)))}{4} - \frac{\pi^4}{15}\right]}$$

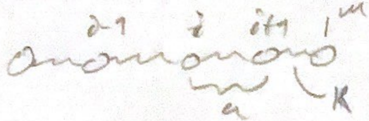
But, thats very uncool looking so instead I'll do it numerically and include a plot. I find that $\boxed{\omega_D \simeq \frac{4}{3}\omega_0}$ gives a decent fit.

d) Debye gives a better fit for the data when we let $\boxed{\omega_D = 2.6 \times 10^{15}\frac{1}{s}}$

e) use $c_s = \omega_D a$ so, $\omega_D = \frac{c_s}{a}$ where a = atomic spacing, c_s = sound speed in Diamond.

$$\omega_D = \frac{(1.2 \times 10^4 m/s)}{(0.15 \times 10^{-9} m)} = \boxed{8 \times 10^{13}\frac{1}{s}} \simeq 10^{14}$$ which is an order of magnitude off.

#2: Estimate a formula for sound speed in a material assuming set of masses on springs with mass m, spring constant K, and atomic spacing a.



so $\omega = \sqrt{\frac{K}{m}}$

$$F = m\ddot{x} \Rightarrow \delta\ddot{x} = \frac{F}{m} = -\frac{K}{m}(\delta x_i - \delta x_{i+1}) - \frac{K}{m}(\delta x_i - \delta x_{i-1})$$

$$= -\omega_0^2 (2\delta x_i - \delta x_{i+1} - \delta x_{i-1})$$

let $\delta x_i \propto e^{ikx - i\omega t}$

so, $\delta\ddot{x} = -\omega^2 \delta x_i$

$$\cancel{+}\omega^2 \cancel{\delta x_i} = \cancel{+}\omega_0^2 (2\cancel{\delta x_i} - e^{+ika}\cancel{\delta x_i} - e^{-ika}\cancel{\delta x_i})$$

$$\omega^2 = \omega_0^2 (2 - 2\cos(ka) = \underline{4\omega_0^2 \sin^2(\tfrac{ka}{2})})$$

$\omega = 2\omega_0 |\sin(\frac{ka}{2})|$

let $ka \ll 1$ so, $\omega = \cancel{2}\omega_0 \frac{ka}{\cancel{2}} = \omega_0 ka = c_s k$

then, $c_s = \frac{\omega}{k} = \boxed{\sqrt{\frac{K}{m}}\, a = c_s}$

let $\omega = \omega_D$ then $\frac{\omega_D}{k} = \omega_0 a \Rightarrow \omega_D = \omega_0 ka$

If wave # is inverse order of a then $\boxed{\omega_D \simeq \omega_0.}$

since $k = \frac{2\pi}{\lambda}$ and $\lambda \sim a$

then $k \approx a$.