PHY 481 & 581 HOMEWORK I

Northern Arizona University

Solutions

Due Date: 09/14/18

1 Einstein Solid

(1.1) Classical Einstein (or "Boltzmann") Solid: Consider a three dimensional *classical* simple harmonic oscillator with mass m and spring constant κ, which is the same for all three directions. The Hamiltonian is given by

$$H = \frac{1}{2m}|\vec{p}|^2 + \frac{\kappa}{2}|\vec{x}|^2. \tag{1}$$

(a) Calculate the classical partition function

$$Z = \int \frac{d\vec{p}}{(2\pi\hbar)^3} \int d\vec{x} e^{-\beta H(\vec{p},\vec{x})} \tag{2}$$

(b) Using the partition function, calculate the heat capacity, which gives $3k_B$.

(c) Conclude that if a solid consists of N atoms, all of which are in harmonic wells, then the heat capacity should be $3Nk_B = 3R$, where R is the "gas constant," in agreement with the law of Dulong and Petit.

(1.2) Quantum Einstein Solid: Now consider the harmonic oscillators having quantized energy values

$$E_n = \hbar\omega(\tfrac{1}{2} + n), \tag{3}$$

where $n \geq 0$ is an integer.

(a) Calculate the quantum partition function

$$Z = \sum_n e^{-\beta E_n} \tag{4}$$

where the sum over n is for all eigenstates.

(b) Find an expression for the heat capacity.

(c) Show that the high temperature limit agrees with the Dulong-Petit law.

(d) Sketch the heat capacity as a function of temperature.

1.1

(a) Calculate the classical partition function for the Boltzmann Solid

$$H = \frac{1}{2m}|\vec{p}|^2 + \frac{K}{2}|\vec{x}|^2 \quad ; \quad \vec{p} = (p_x, p_y, p_z)$$
$$\vec{x} = (x, y, z)$$

$$Z = \int \frac{d\vec{p}}{(2\pi\hbar)^3} \int d\vec{x}\, e^{-\beta H(\vec{p},\vec{x})}$$

- Use $\int_{-\infty}^{+\infty} dy\, e^{-ay^2} = \sqrt{\frac{\pi}{a}}$

- Solve one integral first, then use symmetry

$$|\vec{x}|^2 = x^2 + y^2 + z^2$$

$$\int_{-\infty}^{+\infty} dx \exp\left(\frac{-\beta K}{2}x^2\right) \quad , \quad a \equiv \frac{\beta K}{2} \Rightarrow \sqrt{\frac{\pi}{a}} = \sqrt{\frac{\pi 2}{\beta K}}$$

- multiply by y + z integrals $\left(\sqrt{\frac{\pi 2}{\beta K}}\right)^3$

- $\int_{-\infty}^{+\infty} dp_x \exp\left(\frac{-\beta}{2m}p_x^2\right) \quad , \quad a \equiv \frac{\beta}{2m} \Rightarrow \sqrt{\frac{\pi}{a}} = \sqrt{\frac{2\pi m}{\beta}}$

- mult. by y + z integrals $\left(\sqrt{\frac{2\pi m}{\beta}}\right)^3$

1.1 continued

$$Z = \frac{1}{(2\pi\hbar)^3}\left(\sqrt{\frac{2\pi}{\beta K}}\right)^3\left(\sqrt{\frac{2\pi m}{\beta}}\right)^3$$

- recall $\omega \equiv \sqrt{\frac{K}{m}}$ or $K = \omega^2 m$

$$Z = \frac{1}{\hbar^3}\left[\frac{1}{(2\pi)^3}(2\pi)^{3/2}(2\pi)^{3/2}\right]\left(\sqrt{\frac{1}{\beta K}}\right)^3\left(\sqrt{\frac{m}{\beta}}\right)^3$$

$$= \frac{1}{\hbar^3}\left(\sqrt{\frac{1}{\beta\omega^2 m}}\right)^3\left(\sqrt{\frac{m}{\beta}}\right)^3 = \frac{1}{(\hbar\beta\omega)^3}$$

or $\boxed{Z = (\hbar\omega\beta)^{-3}}$

(b) $U = \left(\frac{-1}{Z}\right)\frac{\partial Z}{\partial\beta} = -(\hbar\omega\beta)^3 \cdot -3(\hbar\omega)^{-3}\beta^{-4}$

$$= \frac{3}{\beta} = 3k_B T$$

$$\frac{\partial u}{\partial T} = 3k_B$$

(c) each oscillator holds $3k_B T$ in 3D,

so heat capacity for N atoms $3Nk_B$

$= 3R$

1.2 Quantum harmonic oscillator

$$E_n = \hbar\omega\left(\tfrac{1}{2} + n\right) \quad , n \geq 0$$

(a) $$Z = \sum_j e^{-\beta E_j}$$

$$Z_{1D} = \sum_{n \geq 0} e^{-\beta\hbar\omega(n + 1/2)}$$

$$= \frac{e^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega}} = \left(2\sinh\left(\frac{\beta\hbar\omega}{2}\right)\right)$$

- the expectation value

$$\langle E \rangle = -\frac{1}{Z}\frac{\partial Z}{\partial \beta} = \frac{\hbar\omega}{2}\coth\left(\frac{\beta\hbar\omega}{2}\right)$$

(b) $$c = \frac{\partial \langle E \rangle}{\partial T} = \frac{\partial}{\partial T}\left[\hbar\omega\left(\frac{1}{e^{\hbar\omega/kT} - 1}\right) - \frac{1}{2}\right]$$

1.2 continued

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

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

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

$$= \frac{(\hbar\omega)^2}{kT^2}\frac{e^{\hbar\omega/kT}}{e^{\hbar\omega/kT}-1}$$

$$\boxed{C = k_B(\beta\hbar\omega)^2\frac{e^{\beta\hbar\omega}}{\left(e^{\beta\hbar\omega}-1\right)^2}}$$

(c) let $x = \beta\hbar\omega$

$$C = \frac{k_B(x^2)e^x}{(e^x-1)^2}, \quad \text{high } T, \; x \to 0$$

1.2 continued

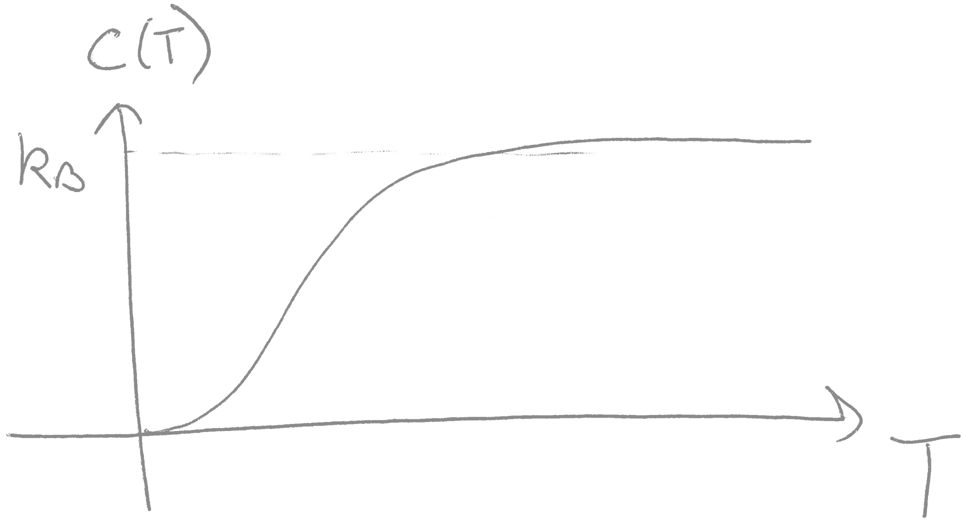
- in the denominator, $e^x \approx 1 + x + \ldots$

$$C \approx \frac{k_B (x^2) e^x}{(1 + x + \ldots - 1)^2}$$

$$e^x \to 1$$

$$C \approx \frac{k_B x^2}{x^2} = k_B$$

(d)



(2.1) in 1D, we have the density of states

$$g(\omega) = \frac{L}{\pi}\frac{1}{v}, \quad v \equiv \text{speed of sound}$$

- in 3D, each point in k-space (k_x, k_y, k_z) occupies a volume of $\left(\frac{2\pi}{L}\right)^3$

- the number of modes in a sphere of radius k

$$\left(\frac{L}{2\pi}\right)^3 \frac{4\pi}{3} k^3$$

$$= \frac{V}{(2\pi)^3}\frac{4\pi}{3}k^3, \quad V \equiv \text{volume of solid}$$

- \# of modes in a shell of thickness dk

$$= \frac{d}{dk}\left(\frac{V}{(2\pi)^3}\frac{4\pi}{3}k^3\right) = \frac{V}{(2\pi)^3} 4\pi k^2 dk$$

- use the dispersion relation, $\omega = vk$ or $k = \frac{\omega}{v}$

$$g(\omega)d\omega = \frac{V}{(2\pi)^3} 4\pi \left(\frac{\omega}{v}\right)^2 \frac{d\omega}{v}$$

$$\Rightarrow g(\omega) = \frac{V}{2\pi^2}\frac{\omega^2}{v^3}$$

(2.2) total energy of solid

$$E = \frac{3V}{2\pi^2 v^3} \int \frac{\hbar\omega^3}{e^{\beta\hbar\omega}-1}\, d\omega$$

$$\int_0^{\omega_d} g(\omega)\, d\omega = 3N$$

$$= \int_0^{\omega_d} \frac{3V}{2\pi^2} \frac{\omega^2}{v^3}\, d\omega = 3N$$

$$= \frac{V}{2\pi^2} \frac{\omega_d^3}{v} = 3N$$

$$\Rightarrow \omega_d^3 = \frac{3N\, 2\pi^2 v^3}{V}$$

$$\boxed{\omega_d = (6n\pi^2 v^3)^{1/3}}, \quad n \equiv N/V$$

(2.3) $$E = \frac{3V}{2\pi^2 v^3} \int_0^{\omega_d} \frac{\hbar\omega^3}{e^{\beta\hbar\omega}-1}\, d\omega$$

$$\frac{\partial E}{\partial T} = \frac{3V}{2\pi^2 v^3} \int_0^{\omega_d} \frac{\hbar\omega^3}{(e^{\beta\hbar\omega}-1)^2}\, d\omega \, \frac{1}{T^2} \frac{\hbar\omega}{k_B}$$

$$\boxed{C_v = \frac{3V}{2\pi^2 v^3} \frac{\hbar^2}{k_B T^2} \int_0^{\omega_d} \frac{\omega^4 e^{\hbar\omega/k_B T}}{(e^{\hbar\omega/k_B T}-1)^2}\, d\omega}$$

(2.4) using $\displaystyle\int_0^{\infty} \frac{x^4 e^x}{(e^x-1)^2}\, dx = \frac{4\pi^4}{15}$

$$\left.\begin{aligned} x &= \beta\hbar\omega \\ dx &= \beta\hbar\, d\omega \end{aligned}\right\} \quad \omega^4 = \frac{x^4}{\hbar^4\beta^4} = x^4 (k_B T)^4$$

$$C = \frac{3V}{2\pi^2 v^3} \frac{\hbar^2}{k_B T^2} \frac{(k_B T)^4}{\hbar^5 (k_B T)^{-1}} \int_0^{\Theta_D/T} \frac{x^4 e^x}{(e^x-1)^2}, \quad \Theta_D = \frac{\hbar\omega_D}{k_B}$$

$\longrightarrow$

$\boxed{\text{2.4 continued}}$

$$C = \frac{3V}{2\pi^2 v^3} \frac{\hbar k_B^5 T^5}{\hbar^4 k_B T^2} \int \cdots$$

$$\omega_d^3 = v^3 6\pi^2 n$$

$$\frac{\omega_d^3}{3n} = v^3 2\pi^2$$

$$C = \frac{3V}{\frac{\omega_D^3}{3n}} \frac{\hbar k_B^4 T^3}{\hbar^4} \int \cdots$$

- Coeff. only

$$\frac{3V \cdot 3\hbar n \, k_B k_B^3 T^3}{\omega_D^3 \hbar^4}, \quad \Theta_D^3 = \frac{\hbar^3 \omega_d^3}{k_B^3}$$

$$= \frac{3V \cdot 3\hbar n}{\hbar^4 (\Theta_D^3 k_B^3 / \hbar^3)} k_B k_B^3 T^3$$

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