PHY 481 & 581 Homework I

Northern Arizona University — 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.

2 Debye Model of Solids

(2.1) In class, we found a one-dimensional (1D) solid has a *density of states* given by

$$g(\omega) = \frac{L}{\pi}\frac{1}{v}, \tag{5}$$

where ω, L, and v are the frequency, length of the solid, and speed of sound, respectively. Determine the density of states in 3D. Answer:

$$g(\omega) = \frac{3V}{2\pi^2}\frac{\omega^2}{v^3}, \tag{6}$$

where V is the volume of the solid. Hint: Find the number of modes within a sphere of radius $\vec{k}$ in 3D $\vec{k}$-space, then convert to frequency, ω.

(2.2) The total energy of the the vibrations for the entire solid is given by

$$E = \frac{3V}{2\pi^2 v^3}\int \frac{\hbar\omega^3}{e^{\beta\hbar\omega} - 1} d\omega. \tag{7}$$

However, there must be a cutoff frequency, otherwise the integral goes to ∞. Assume there are $3N$ degrees of freedom in the system, where N is the number of atoms in the solid. Solve the following integral

$$\int_0^{\omega_d} g(\omega) d\omega = 3N. \tag{8}$$

to determine what the cutoff frequency, ω_d, should be.

(2.3) Now let's return to the equation for the total energy of the solid (Eq. (7)). Differentiate this expression with respect to T to get the heat capacity, C. Your answer will have an integral remaining.

(2.4) Use the following result,

$$\int_0^{\infty} \frac{x^4 e^x}{(e^x - 1)^2} dx = \frac{4\pi^4}{15}, \tag{9}$$

to express the heat capacity per atom in the form,

$$C = \frac{12\pi^4}{5} R \left(\frac{T}{\theta_b}\right)^3, \tag{10}$$

where R is the universal gas constant, and θ_d is the Dybye temperature, given by $\theta_d = \hbar\omega_d / k_b$. Notice the T^3 dependence of the heat capacity. We see now why there must be a cutoff frequency (or temp.), as the T^3 dependence can only hold for low-T.