PHY 481/581 - Solid State Physics - Quiz 1

Name: Solutions Date: 09/17/2018

Problem 1. In class, we discussed three models of solids in order to explain the origin of the heat capacity per atom, C_v: **(a)** Boltzmann (classical), **(b)** Einstein (quantum), and **(c)** Debye (quantum). Briefly describe the difference in the three models in words and how these models compare to experiments.

Problem 2. The plot in Fig. (1) shows experimental data for the molar heat capacity of diamond as the points on the plot. The dashed curve is Einstein's model of solids. Briefly explain why the curve for low temperature, T, does not match the data well. That is, the curve is below the data points at low T.

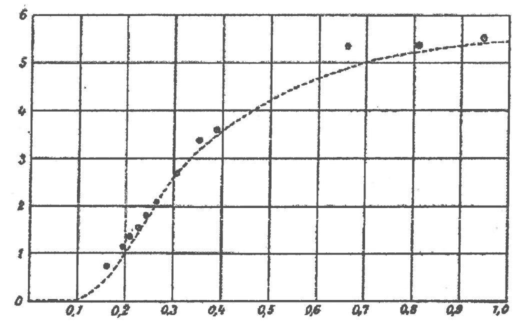

Figure 1: The molar heat capacity on the vertical axis, and the horizontal axis is normalized temperature. Data for diamond is shown as the points on the plot. The dashed line is from Einstein's model.

Problem 3. Given the expectation value of energy for the 3D quantum harmonic oscillator

$$\langle E \rangle = 3\hbar\omega\left(n_B(\beta\hbar\omega) + \frac{1}{2}\right), \tag{1}$$

where n_B is the *Bose occupation factor* given by,

$$n_B(\beta\hbar\omega) = \frac{1}{e^{\beta\hbar\omega} - 1}, \tag{2}$$

determine the heat capacity, C, per atom of a solid made from quantum harmonic oscillators.

Problem 4. Using your derived equation for C, determine what the high-T limit is.

Problem 5. For the Debye model of solids, we determined that the specific heat now takes on the form,

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

where R is the universal gas constant, and $T_d = \hbar\omega_d/k_b$ is the Debye temperature. Clearly, from Fig. (1), a temperature dependence of T^3 cannot hold for all T. Given a density of states $g(\omega) = 3V\omega^2/(2\pi v^3)$, where V and v are the volume of the solid and speed of sound, respectively, what is the maximum frequency for which the $C \propto T^3$ law holds?

(1) (a) Boltzmann: the solid consists of independent classical harmonic oscillators, of a single frequency, that can have any energy value as a continuous spectrum

(b) Einstein: the solid consists of harmonic oscillators with discrete energy values given by $E_n = \hbar\omega(n + \frac{1}{2})$, again with a single frequency.

(c) Debye: the solid consists of quantum harmonic oscillators that are coupled together thus taking on a wider range of frequencies

- Boltzmann predicts high-T well, Einstein accounts for the exponential decay of C for intermediate T, & Debye accounts for very low-T, and is the most accurate

(2) The experimental data shows the heat capacity is larger than the Einstein model predicts, thus there must be some way for a solid to absorb heat that is not accounted for by independent quantum harmonic oscillators. The larger heat capacity can be understood by considering low energy collective modes (sound waves) as a result of the coupling of the atoms to one another. These low frequency modes are able to absorb heat, thus acconting for the mismatch with the experimental data.

③ $\langle E \rangle = 3\hbar\omega\left(n_B(\beta\hbar\omega) + \frac{1}{2}\right)$

- We need to know how the energy changes with respect to a change in temperature $C = \frac{\partial \langle E \rangle}{\partial T}$

$$\langle E \rangle = 3\hbar\omega\left(\frac{1}{e^{\beta\hbar\omega}-1} + \frac{1}{2}\right)$$

$$= 3\hbar\omega\left[\left(e^{\beta\hbar\omega}-1\right)^{-1} + \frac{1}{2}\right]$$

$$= 3\hbar\omega\left[\left(e^{\hbar\omega/kT}-1\right)^{-1} + \frac{1}{2}\right]$$

$$\frac{\partial \langle E \rangle}{\partial T} = 3\hbar\omega\left[-1\left(e^{\hbar\omega/kT}-1\right)^{-2} \cdot e^{\hbar\omega/kT} \cdot \left(-T^{-2}\right) \cdot \frac{\hbar\omega}{k}\right]$$

$$= \frac{3\hbar\omega\left(\frac{\hbar\omega}{k}\right)\frac{1}{T^2}e^{\hbar\omega/kT}}{\left(e^{\hbar\omega/kT}-1\right)^2} = \boxed{\frac{3k_B(\beta\hbar\omega)^2 e^{\beta\hbar\omega}}{\left(e^{\beta\hbar\omega}-1\right)^2} = C}$$

4 let $x = \beta\hbar\omega$

$$C = \frac{3k_B x^2 e^x}{(e^x - 1)^2}$$, for high T, $x \to 0$

- expand $e^x \approx 1 + x + \ldots$ for $x \ll 1$

$$C \approx \frac{3k_B x^2 e^x}{(1+x-1)^2} = \frac{k_B x^2 e^0}{x^2} = 3k_B$$

$\boxed{C \sim 3k_B}$ for high-T

- or the classical Boltzmann model

(5) $C = \frac{12\pi^4}{5} R \left(\frac{T}{T_0}\right)^3$

- the Debye model assumes there is a cutoff frequency, ω_d, related to the total degrees of freedom of the solid
- a solid with $3N$ d.o.f. (N atoms, 3 dimensions)
- to solve for ω_d, we use the density of states

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

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

$$\frac{3V}{2\pi v^3}\left[\frac{1}{3}\omega\right]_0^{\omega_d} = 3N$$

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

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