DS 8: Phonons and Photons

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1 The Einstein solid

(a) In class, we saw how there were different models for crystals. Assuming the system to be a set of $3N$ 1D (or alternatively N 3D) uncoupled classical harmonic oscillators, Boltzmann showed in 1877 that the specific heat is given by $3N$. Show this using the principle of equipartition of energy.

This result is known as the "Dulong-Petit" law, which states that the specific heats of crystals are independent of temperature.

(b) In reality, it was found experimentally that the specific heats of crystals were, in fact, sensitive to temperature. Einstein was the first to explain this. The Einstein model considered the same system as above, but with discrete energy levels, each having an energy given by[1]

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega. \tag{1}$$

Show that in such a system, the specific heat c_V is a function of temperature.

(c) For the Einstein solid, show that a characteristic temperature T_E exists such that when $T \gg T_E$, you recover the Dulong-Petit law. Show that when $T \ll T_E$,

$$c_V \sim \left(\frac{T_E}{T}\right)^2 \exp\left(-\frac{T_E}{T}\right), \quad \text{so that} \quad c_V \to 0 \quad \text{as} \quad \frac{T}{T_E} \to 0. \tag{2}$$

2 The Debye solid

While the discovery that the specific heat could be dependent on temperature was historically very important, it was found that the low-temperature dependence of these systems was not accurate. Experimentally, it was found that $c_V \sim T^3$ at low temperatures. Debye came up with a model to explain this by assuming the oscillators were not uncoupled, but were in fact coupled. Instead of working with the individual oscillator picture, Debye considered the normal modes of the system, and assumed that it was these normal modes that were independent quantum oscillators. However, from your study of oscillations, waves, and optics, it should be clear that all these normal modes don't have the same frequency.

(a) Consider a 1D crystal lattice of some length L and some minimum spacing a. Classically, what are the possible normal modes this system can have? If c_s is the speed of sound in the material, show that the different wave-vectors k_n allowed by the system are given by

$$k_n = \frac{n\pi}{L}, \quad n = 1, 2, 3, \ldots \tag{3}$$

[1] Einstein actually did not including the zero-point energy of $1/2\hbar\omega$, but we will not omit it here.

Show that in such a system, because of the discrete lattice spacing a, there must exist some *maximum* wavenumber k_{max}.

(b) Next, from your course on oscillations, waves, and optics, you should know that such normal modes have a dispersion relation

$$\omega = c_s k, \tag{4}$$

where c_s is the speed of sound in the material. Use this to find the allowed values of ω_n, and show that there must be a maximum frequency permitted for such a system.

(c) Generalise your above results to 3D. Show that we now have a wave-vector

$$\mathbf{k} = k_x\hat{x} + k_y\hat{y} + k_z\hat{z}, \tag{5}$$

with a dispersion relation:

$$\omega = c_s|\mathbf{k}| = \frac{c_s\pi}{L}\sqrt{n_x^2 + n_y^2 + n_z^2}, \quad \text{where} \quad n_x, n_y, n_z = 1, 2, 3\ldots \tag{6}$$

(d) Now, treat these harmonic oscillators as *quantum* oscillators with different frequencies $\omega(\mathbf{k})$. Show that the total energy in this system is given by

$$E = 3\sum_{\mathbf{k}}\left(\frac{1}{2}\hbar\omega(\mathbf{k}) + \frac{\hbar\omega(\mathbf{k})}{e^{\hbar\omega(\mathbf{k})/T} - 1}\right). \tag{7}$$

(Note: The factor of 3 comes from the three spatial polarisations that these “phonons” possess.)

(e) In order to make any headway, we must now find a way to perform the sum over $\mathbf{k}$ vectors. Show that you can write

$$\sum_{\mathbf{k}} = \frac{1}{8}\int \frac{\mathrm{d}^3 k}{(\pi/L)^3} = \frac{4\pi V}{(2\pi)^3}\int_0^{k_{\text{max}}} k^2 \mathrm{d}k = \int_0^{k_{\text{max}}} g(k)\mathrm{d}k. \tag{8}$$

Where does the factor of 8 in the denominator come from? $g(k)$ is the $k-$space density of states.

(f) Use the above definition to show that

$$E = \int_0^{\omega_D} \mathrm{d}\omega \left(\frac{1}{2}\hbar\omega + \frac{\hbar\omega}{e^{\hbar\omega/T} - 1}\right) g(\omega), \tag{9}$$

where $g(\omega)$ is the $\omega-$space density of states. Argue that $g(\omega)\mathrm{d}\omega$ represents the number of normal modes in the interval $(\omega, \omega + \mathrm{d}\omega)$.

(g) We will now try to find the “maximum” frequency ω_D (the Debye frequency) by arguing that the total number of normal modes for such a system is $3N$. Using this fact, show that

$$3N = \int_0^{\omega_D} \mathrm{d}\omega\, g(\omega) \quad \Longrightarrow \quad \omega_D = c_s\left(6\pi^2\frac{N}{V}\right)^{1/3}. \tag{10}$$

(h) Use ω_D to compute E and therefore c_V. Show that

$$c_V = 9N\left(\frac{T}{T_D}\right)^3 \int_0^{T_D/T} \mathrm{d}x\, \frac{x^4 e^x}{(e^x - 1)^2}. \tag{11}$$

(i) Show that you recover the Dulong-Petit law at $T \gg T_D$, and $c_V \sim T^3$ for low temperatures.

3 Blackbody radiation

(a) Much of the above argument for phonons also works for *photons*, if we consider a blackbody to be a "box" with electromagnetic waves trapped in it. Identify what remains the same, and what changes.

(b) From our earlier results, show that the density of states of *photons* is given by

$$g(\omega) = \left(\frac{V}{\pi^2 c^3}\right)\omega^2 \tag{12}$$

(c) Use this density of states to compute the energy density of a blackbody, using the fact that the energy of a photon is $\epsilon(\omega) = \hbar\omega$.

(d) Use this to show that the energy density can be written as

$$\frac{\langle E\rangle}{V} = \frac{4\sigma}{c}T^4, \tag{13}$$

where σ is *Stephan's constant*. Derive an expression for σ in terms of the fundamental constants of Physics.