Thermal properties of the lattice - part II

1. Consider one mole (N_A) of gas consisting of monatomic molecules (i.e. point particles). Its energy would then be given by

$$E = N_A(\frac{1}{2}mv_x^2 + \frac{1}{2}mv_y^2 + \frac{1}{2}mv_z^2)$$

(a) Use the equipartition theorem to find the average energy of this gas.
(b) Use $C = \frac{\partial <E>}{\partial T}$ to find the molar heat capacity of the gas.

Suppose the gas consisted of diatomic molecules. In addition to 3D translational motion, it can rotate about 2 axes.
(c) Sketch a diatomic molecule (i.e. a barbell) and the two possible rotations it can execute.
(d) Write the energy associated with this system. Keep in mind the rotational analogs of $m \to I$ and $v \to \omega$.
(d) Find C for a diatomic molecule.

At even higher temperatures, the diatomic molecules may vibrate and with a motion modeled as SHO.
(e) Write the energy associated with this system.
(f) Find C for a diatomic molecule.

$(\frac{3}{2}N_A k_b, \frac{5}{2}N_A k_b, \frac{7}{2}N_A k_b)$

2. Experimental measurements of the heat capacity of diamond is shown below. It's given on a logarithmic scale, since the heat capacity and the temperature changes over orders of magnitude.
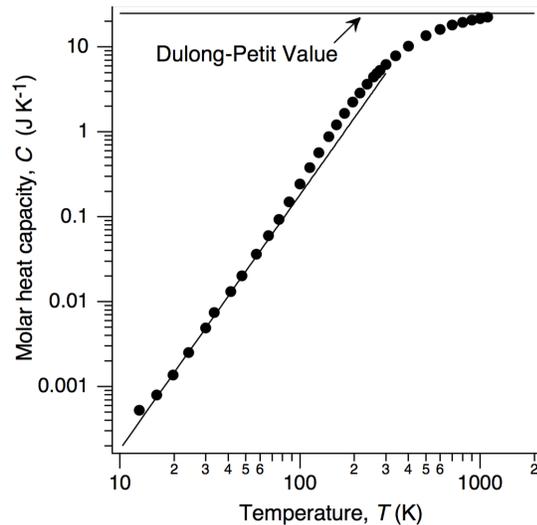
(a) Graphically determine the slope in the range 20K - 200K. That is, find the value of $\frac{\Delta(\log C)}{\Delta(\log T)}$.
(b) Use the slope to determine an expression for $C(T)$.

(figure from Hofmann... not the primary source)

3. The average energy of the system of oscillators in the Einstein model is

$$<E> = \frac{1}{2}\hbar\omega_E + \frac{\hbar\omega_E}{e^{\hbar\omega_E/k_B T} - 1}$$

4. **Periodic boundary conditions, allowed wave numbers.** One approach to handling a finite chain of atoms is to apply periodic boundary conditions: attach the ends of the chain to itself. This places the following constraint on the equation of motion

$$e^{i[kx-\omega t]} = e^{i[k(x+L)-\omega t]}$$

where $L = Na$, given that the chain has a total of N atoms and a spacing of a.

(a) Show that this means that k has the values

$$k = \frac{2\pi p}{L}$$

where p is an integer.
(b) Calculate k and λ for $p = 1$. Does this correspond to the short or long wavelength limit? Sketch what this looks like.
(c) Calculate k and λ for $p = N$. Does this correspond to the short or long wavelength limit? Sketch what this looks like.

Note: this method uses "running waves". In this case, k (and p) can take on negative values, so that the wave can travel in both $\pm$ directions.

5. **Density of states, 1D.** The 1D finite chain of atoms from above has $k = \frac{2\pi p}{L}$.

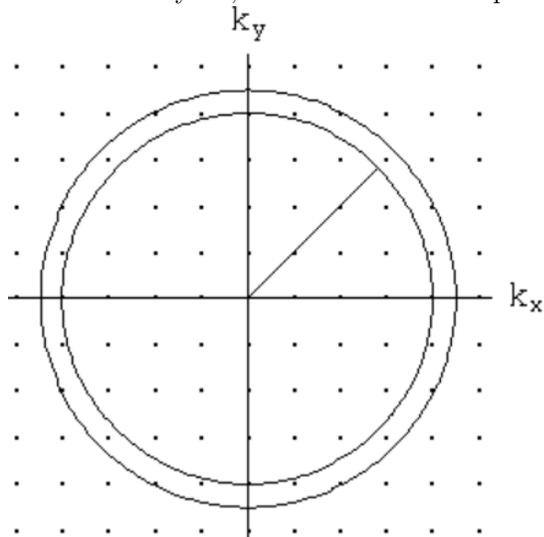(a) Consider the interval $k : \frac{2.03\pi}{L} \to \frac{10.03\pi}{L}$. Calculate $\Delta k = k_f - k_i$.
(b) Count the number of states (k-values) in this interval.
(c) Determine the density of states

$$g(k) = \frac{dN}{dk} = \frac{\text{number of states}}{\text{interval k}}$$

(d) Determine the number of states in the interval $\frac{4\pi}{L}$ to $\frac{80\pi}{L}$. Use the fact that $dN = g(k)dk$.

6. **Density of states, 2D.** The allowed states for a 2D crystal, as shown in $k-$space, is

k_y

k_x

(a) Determine $N(k)$, the number of states in a circle of radius k. To do this: determine the area of a circle of radius k. Replace k with $\frac{k}{(2\pi/L)}$ to account for the discreteness of k.

(b) Determine the density of states, $g(k) = dN/dk$.

Energy uses frequency, not wavenumber. So we need $g(\omega)$. Therefore, we need to use the dispersion relation, $\omega(k)$. Assume a linear dispersion relation, $\omega = vk$.

(c) Determine $N(\omega)$ by $\omega(k)$ into $N(k)$.

(d) Determine $g(\omega) = dN/d\omega$.

$N(k) = \frac{L^2 k^2}{4\pi}$, $g(k) = \frac{L^2 k}{2\pi}$, $N(\omega) = \frac{L^2 \omega^2}{4\pi v^2}$

7. **Density of states in 3D and the Debye frequency.** In 3D, the density of states in k-space is given by $N = \frac{4}{3}\pi \left(\frac{k}{(2\pi/L)}\right)^3$. The Debye model proposes that we use a linear dispersion relation, $\omega = vk$. From this, we find

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

It turns out that we can place a limit on ω. If we have N atoms in a 3D oscillator, there are 3N possible states. Therefore,

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

Do this integral to find ω_D, the Debye frequency.

The answer is $\omega_D = 6\pi^2 N v^3 / V$.

8. **average energy in the Debye model.** To calculate the average energy

$$< E > = \sum_i (E_i) \times (probability\ of\ E_i) \times (number\ of\ states\ at\ E_i)$$

$$= \int \frac{\hbar\omega}{e^{\hbar\omega/k_b T} - 1} g(\omega)d\omega$$

(a) Use $g(\omega)$ and the limits of ω to get

$$< E > = \frac{3V\hbar}{2\pi^2 v^3} \int_0^{\omega_D} \frac{\omega^3}{e^{\hbar\omega/k_b T} - 1} d\omega$$

(b) The above integral is easier to evaluate if we use $x = \frac{\hbar\omega}{k_b T}$ and $x_D = \frac{\hbar\omega_D}{k_b T} = \frac{\Theta_D}{T}$. In this case

$$< E > = 9Nk_b T \left(\frac{T}{\Theta_D}\right)^3 \int_0^{x_D} \frac{x^3}{e^x - 1} dx.$$

Show this is the same integral as (a). You're welcome to just sub in expressions for x, x_D and Θ_D.

9. C at high temperature. High temperature means $T \gg \Theta_D$. In this case, since $x = \ldots/T$, e^x becomes a small number.

(a) Approximate e^x as its Taylor series, use as few terms as possible that will give something with an x dependence.

(b) Find $< E >$ in the high temperature limit. That is, do the integral.

(c) Determine $C = \frac{\partial E}{\partial T}$.

This will give you the Dulong and Petit result: $3Nk_b$

10. C at low temperature. Here, low temperature means $T \ll \Theta_D$. In this case, we can approximate the upper limit as ∞.

(a) Evaluate the integral. Use Wolfram Alpha

$$\int_0^\infty \frac{x^3}{e^x - 1} dx$$

(b) Determine $< E >$.

(c) Determine $C = \frac{\partial < E >}{\partial T}$

11. **Thermal conductivity.** Diamond has a thermal conductivity of 2200 W/m·K at 295K. Other diamond properties: density 3.52×10^3 kg/m^3, molar mass 12 g/mol, speed of sound 5000 m/s, molar specific heat 5 J/mol K at 273K.

(a) Use the above values and the expression for the thermal conductivity to estimate the mean free path of phonons in diamond at 295K. *(Turton7.24)*

(b) What is meant by *mean free path*? Use text and a diagram.

12. **Thermal conductivity.** Discuss the physical reasons for a maximum in the thermal conductivity, $K(T)$.
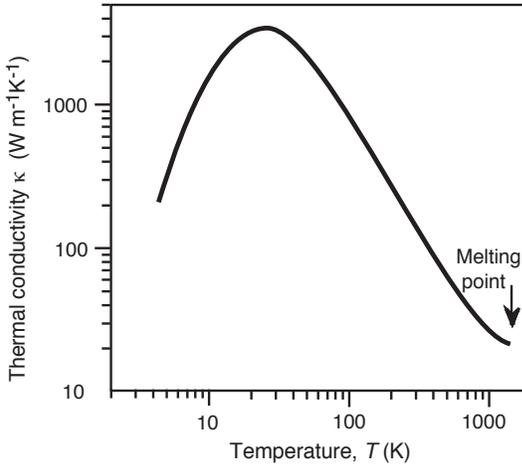
13. **Thermal conductivity.** Diamond has one of the highest thermal conductivities of all materials.

(a) Fill in the following table to see the range of Ks you can expect to see at room temperature (about 300K, 70F, 25C)

material	κ at room T, [W/m·K]
diamond	
copper	
stainless steel	
glass	
concrete	
asbestos	
styrofoam (polystyrene foam)	

(b) You're builder advising a homeowner to have a house's foundation walls insulated with 2 inches of styrofoam. To make your point, you compare it to how thick a concrete wall would have to be in order to have the same insulating effects. Calculate this thickness.

14. **Thermal expansion.** In a Bragg reflection experiment using copper, a sharp peak is observed at an angle of 25.23^o at 300K. At 500K, the same peak is observed at 25.14^o. Use this information to calculate the coefficient of linear expansion for copper. *(Hofmann 4.p9)*

15. **Thermal expansion** is often called an *anharmonic* process. (a) What does anharmonic mean? Give an equation to describe it. (b) Why is thermal expansion called an anharmonic process? Use text and a diagram in your answer. *(Hofmann 4.p14)*