

Problem 1

- a. Zero-point energy is the energy of the ground (lowest) state of a quantum system.
- b. (i) Zero-point energy is not applicable to classical systems. (ii) The energy of a 1D quantum harmonic oscillator is (ω_0 is the natural frequency of the oscillator):

$$\epsilon_n = (n + \frac{1}{2})\hbar\omega_0$$

where $n = 0, 1, 2, \dots$. For the zero-point energy $n = 0$. For the 3D case, this corresponds to:

$$\epsilon_0 = (\frac{3}{2})\hbar\omega_0$$

Problem 2

Debye theory predicts the total internal energy has:

$$U = \frac{9}{8}Nk\Theta + 9NkT \frac{T^3}{\Theta} \int_0^{\frac{\Theta}{T}} \frac{x^3}{e^x - 1} dx$$

where $x = \frac{\hbar\omega}{kT}$. The first term corresponds to the zero-point energy, therefore we can write the zero-point energy per atom as

$$\begin{aligned}\epsilon_n &= \frac{9}{8}\hbar\omega_0 \\ &= \frac{9}{8}k\Theta \\ &= 0.0089eV\end{aligned}$$

Problem 3

- a. Specific heat refers to the amount of energy that a material can contain at a given temperature. Thermal conductivity refers to the ease with which thermal energy can be transmitted through a material.
- b. Water has a relatively high specific heat capacity ($C_p = 4.181 kJ/kgK$), and can therefore extract a significant amount of thermal energy per given volume of water.

- c. The high strength of the bonds between carbon atoms indicates that the anharmonicity of the interatomic potential that is responsible for finite thermal conductivity does not manifest itself in a dominant manner. Therefore, the scattering of phonons is relatively low in contrast with other materials.