



Discussion on 13<sup>th</sup> April

Due on 20<sup>th</sup> April

**Exercise 1** *Debye temperature*

The Debye approximation is assuming a phonon dispersion with  $\omega = vk$  where  $v$  is the sound velocity.

- Calculate in two dimensions the density of state  $D(\omega)$ , the frequency cut-off  $\omega_D$  and the Debye temperature  $T_D$ .
- The sound velocity is given by  $v = \sqrt{B/\rho}$  where  $B$  is the bulk modulus and  $\rho$  is the mass density. In a previous lecture we saw how argon is bonded together through van-der-Waals interaction and take an fcc structure with nearest neighbour distance  $3.76 \text{ \AA}$ . We derived  $B \approx 75\epsilon/\sigma^3$  where (for Argon)  $\epsilon \approx 10 \text{ meV}$  and  $\sigma = 4/1.09 \approx 4 \text{ \AA}$  are the parameters of the Lennard-Jones potential. Show, using rough back-on-the-envelope approximations, that  $v \approx 1150 \text{ m/s}$ .
- With this sound velocity, evaluate the Debye temperature for this material. (Remember that opposed to (a) we are now in 3D.)

**Exercise 2** *Heat capacity - Debye approximation*

Let's again use the Debye approximation.

- Calculate in one and two dimensions the temperature dependence of the heat capacity for the limit where  $T$  is much smaller than the Debye temperature.
- The sound velocity of diamond is  $12\,000 \text{ m/s}$  whereas lead has  $2\,000 \text{ m/s}$ . For a finite fixed temperature in the limit  $T \ll T_D$ , which of the two materials will have the highest heat capacity? From our knowledge of the phonon dispersion of a mono-atomic 1D chain, give arguments as to why diamond has a higher sound velocity.

**Exercise 3** *Heat capacity - Einstein model*

Einstein derived

$$C = 3Nk_B \left( \frac{\hbar\omega_0}{k_B T} \right)^2 \frac{\exp\left(\frac{\hbar\omega_0}{k_B T}\right)}{\left[\exp\left(\frac{\hbar\omega_0}{k_B T}\right) - 1\right]^2}. \quad (1)$$

- In figure 1, the heat capacity of diamond is plotted as  $\frac{C_p}{3Nk_B}$  versus temperature. Einstein's model has just one free parameter:  $\omega_0$ . Based on these data (given below), determine the energy scale  $\hbar\omega_0$  that would give the best description of the experiment.

b) How does this energy scale compare with the energy scale of optical phonons in diamond (see figure 2)?

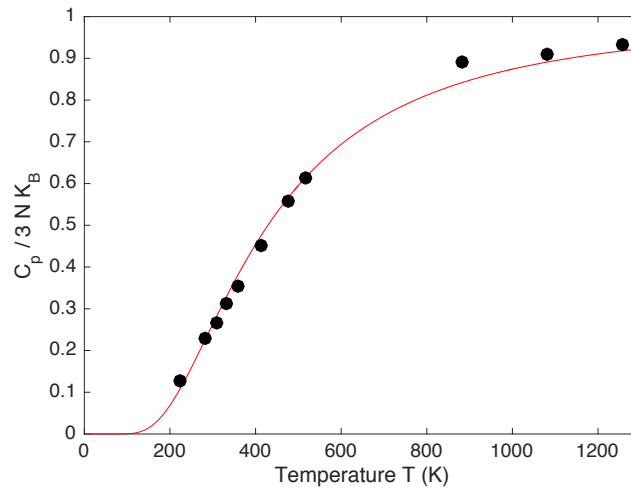


Figure 1: Heat capacity of diamond versus temperature  $T$  as of 1906. This was thus the information that Einstein had available when thinking about the problem of heat capacity.

The data points in figure 1 are:

$T$  [K] = 222, 284, 308.5, 333, 358, 411, 477, 518, 880, 1080, 1259

$\frac{C_p}{3Nk_B}$  = 0.1282, 0.2308, 0.2650, 0.3120, 0.3547, 0.4530, 0.5556, 0.6154, 0.8932, 0.9103, 0.9316

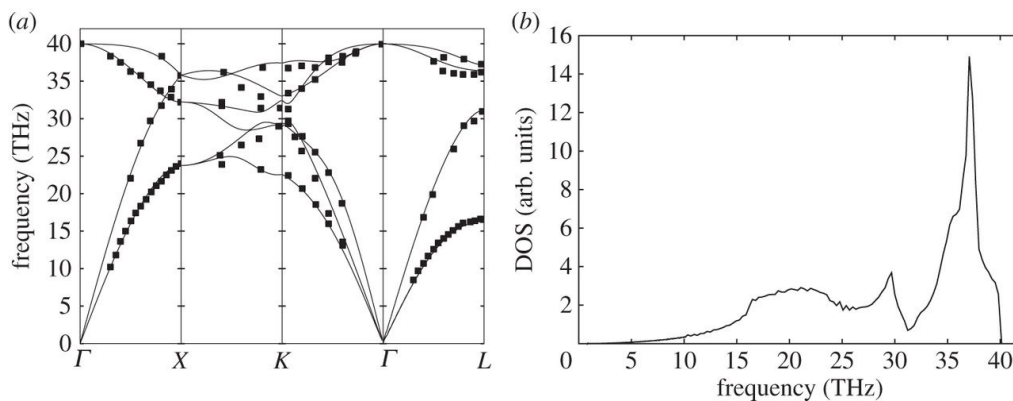


Figure 2: (a) Phonon spectrum of diamond. (b) Phonon density of states of diamond. From: <http://rspa.royalsocietypublishing.org/content/470/2169/20140371>