



Discussion on 5<sup>th</sup> April

Due on 12<sup>th</sup> April

**Exercise 1** *Neutron and photon dispersion relations*

Particles have dispersion relations. For example, the energy  $E$  of electrons and neutrons is given by:

$$E = \frac{\hbar^2 k^2}{2m} \quad (1)$$

where  $m$  is the particle mass and  $p = \hbar k$  is the momentum. Photons (light) by contrast have the following dispersion:

$$E = \hbar c k \quad (2)$$

where  $c$  is the speed of light and  $\hbar = h/(2\pi)$  with  $h$  being Planck's constant.

- a) For a neutron moving with 2 km/s, what is its kinetic energy  $E$  (in meV)? (Hint: look up the mass of a neutron) What is its wavelength  $\lambda = 2\pi/k$ ? Derive the following relation for neutrons:

$$\lambda[\text{\AA}] = \frac{9.045}{\sqrt{E[\text{meV}]}} \quad (3)$$

- b) With the wavelength calculated in (a), calculate the energy of a photon.
- c) To experimentally study excitations such as phonons, meV energy resolution is needed. Let the instrumental resolving power be defined by  $\Delta E/E$  where  $\Delta E$  is the energy resolution. If  $\Delta E = 1$  meV, what is the resolving power of neutrons and photons with a wavelength of 4 \AA.

**Exercise 2** *Measuring phonons*

In a previous lecture, we discussed the recent discovery of high-temperature superconductivity in H<sub>2</sub>S. We found that under the high pressure needed to crystallize this gas, the crystal structure is bcc.

- a) Is the (200) Bragg peak allowed (non-zero) or forbidden (zero) by the structure factor for a monoatomic crystal?
- b) If the conventional lattice parameter is 3 \AA, and we use neutrons moving with 2 km/s, what is the scattering angle of the (200) Bragg peak (hint: use Bragg's law) and what is the energy of the scattered neutrons?
- c) What is the expectation for the phonon branches (dispersions) of a mono atomic bcc lattice? Can we expect optical phonons? What is the expectation for H<sub>2</sub>S?

- d) Let's assume that the phonon velocity of an acoustic branch is 4 meV per reciprocal lattice unit ( $2\pi/a$ ) in the long wavelength limit  $k \rightarrow 0$ . What is the phonon energy at  $\mathbf{Q} = (2.1, 0, 0)$  (where  $\mathbf{Q}$  is in reciprocal units)?
- e) If we fix the analyser at our triple axis instrument to measure neutrons with energy 7 meV, what should be the energy of the incident neutrons to measure the phonon at  $\mathbf{Q} = (2.1, 0, 0)$ ?

**Exercise 3** *Singularity in density of states*

- a) From the dispersion relation derived in the lecture for a monoatomic linear lattice of  $N$  atoms with nearest neighbour interactions, show that the density of modes is

$$D(\omega) = \frac{2N}{\pi} \cdot \frac{1}{\sqrt{\omega_m^2 - \omega^2}}, \quad (4)$$

where  $\omega_m$  is the maximum frequency.

- b) Make a plot of equation (4).
- c) Suppose that an optical phonon branch has the form  $\omega(K) = \omega_0 - AK^2$ , near  $K = 0$  in three dimensions. Show that  $D(\omega) = \left(\frac{L}{2\pi}\right)^3 \left(\frac{2\pi}{A^{3/2}}\right) (\omega_0 - \omega)^{\frac{1}{2}}$  for  $\omega < \omega_0$  and  $D(\omega) = 0$  for  $\omega > \omega_0$ . Here the density of modes is discontinuous.