Condensed Matter Physics: Weekly Problem 3

These problems are to be formatively self-assessed by you, the student. Students taking part in the peer-marking pilot scheme will also be required to mark one of their peer's weekly problems. A mark scheme, out of 10, will be provided with each solution to aid your assessment before your timetabled weekly workshop. Information underlined/boxed in red in the model solutions is required for marks to awarded.

Summary: In this problem, we will explore vibrations in solids using phonons as a model for describing the transmission of sound in crystalline solids. You will need to refer to Lecture 6.

Na 5K	Mg	
bcc	hcp	← Crystal structure →
4.225	3.21	← a lattice parameter, in Å →
	5.21	← c lattice parameter, in Å →

K 5K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
bcc	fcc	hcp	hcp	bcc	bcc	cubic	bcc	hcp	fcc	fcc	hcp
5.225	5.58	3.31	2.95	3.03	2.88	complex	2.87	2.51	3.52	3.61	2.66
		5.27	4.68					4.07			4.95

a. The metal iron has a bcc structure with the unit cell length of $a = 0.287$ nm (Kittel Table 1.3, page 20). Calculate the speed of sound propagating along the [100] axis where the spring constant is $C = 5.00$ N m^{-1}. **[3 marks]**

b. At what wavelength would the speed fall to 50 % of the speed calculated above? **[1 mark]**

c. Explain physically why the speed drops. **[1 mark]**

d. What is the maximum frequency that can be generated along the [100] axis? **[2 marks]**

e. Describe the Debye approximation. Would the value for (d) above be lower or higher if the Debye approximation were used? Illustrate your answer with a sketch of the phonon dispersion curve in the first Brillouin zone. **[3 marks]**

Condensed Matter Physics: Weekly Problem 3 - Solutions

When completing your assessment please enter the numerical marks for each question. Please also give information on any parts which you found difficult, as this will allow me to go over any common issues in the workshops. The workshops also provide the opportunity to individually talk to myself, and other staff members about any issues you faced when solving the problem.

a. The speed of sound is determined using the phonon dispersion relationship applied at the long-wavelength limit (very small wavevector) where $Ka \ll 1$.

We know that the phonon dispersion relation is given by:

$$\boxed{\omega(K) = \left(\frac{4C}{M}\right)^{1/2} \left|\sin\frac{1}{2}Ka\right|}$$

[1 mark]

The speed of sound is determined from the group velocity:

$$\boxed{v_g = \frac{\partial\omega}{\partial K} = \left(\frac{Ca^2}{M}\right)^{1/2} \cos\frac{1}{2}Ka}$$

[1 mark]

(You need to find out the mass of Fe which is 55.8 u).

Evaluating this at $K = 0$ (the long wavelength limit) at the centre of the Brillouin zone gives:

$$\boxed{v_g = \left(\frac{Ca^2}{M}\right)^{1/2} = \left(\frac{5 \times (0.287 \times 10^{-9})^2}{55.8 \times 1.66 \times 10^{-27}}\right)^{1/2} = 2.11 \times 10^3 \text{ m s}^{-1}}$$

[1 mark]

b. The value falls to 50 % when $\boxed{\cos\frac{1}{2}Ka = 0.5}$, which occurs when $\boxed{\frac{1}{2}Ka = \pi/3}$.
This gives $K = 7.298 \times 10^9 \text{m}^{-1}$ and $\lambda = 2\pi/K = 8.61 \times 10^{-10}\text{m} = 0.861 \text{ nm}$. **[1 mark]**

(This shows that at very short wavelengths (approaching the lattice spacing) the speed drops. This is a characteristic of a dispersive medium).

c. The wavelength at which the speed drops to 50 % is 0.861 nm, equivalent to 3 times the lattice spacing. At such small wavelengths (large wavevectors) adjacent atoms are close to being displaced out of phase. This requires more energy and slows the wave down. **[1 mark]**

d. The maximum frequency occurs at the Brillouin zone boundary when $K = \pi/a$.

Substituting this into the expression for $\omega(K)$ gives $\omega(K = \pi/a) = (4C/M)^{1/2}$. **[1 mark]**

For the wave concerned this gives:

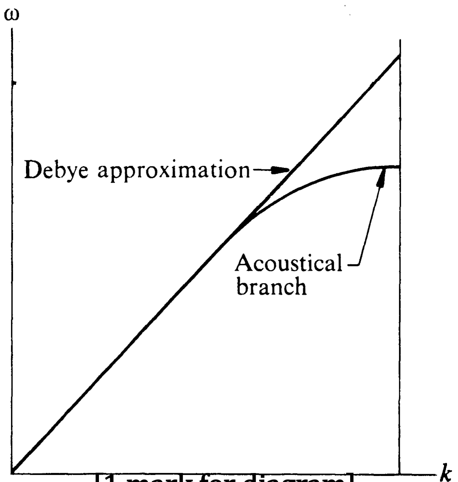
$$\omega(K) = \left(\frac{4 \times 5}{55.8 \times 1.66 \times 10^{-27}}\right)^{1/2} = 1.469 \times 10^{13}\ \text{rads s}^{-1}$$
$$= 2.338 \times 10^{12}\text{Hz}$$

[1 mark]

e. The Debye approximation assumes that the dispersion relation is linear $\omega = vK$, that the velocity is constant throughout the Brillouin zone and given by the long-wavelength limit approximation. **[1 mark]**

For this case, the group velocity remains constant across the Brillouin zone from $K = 0$ to $K = \pi/a$. As is shown in the sketch the maximum frequency in this model (the Debye frequency) is slightly higher than the value in (d). **[1 mark]**

(You will see that the result obtained in part (a) is less than the values generally quoted for the speed of sound in Fe. This is because the spring constants are different in different crystal directions. Think about the bcc structure and you will see that the constant along the [111] axis is different from the [100] axis. This is detail not covered in this course).



[1 mark for diagram]