

This series of homework is based on the covered chapters of Introduction to solid state physics by Charles Kittel. Before answering the problems, make sure to study the related materials thoroughly from the two primary references. You may think and work on problems with your classmates, but **you must submit the answers you only write**; otherwise, you will receive no points. The last two questions are for bonus points.

---

### Problem 1

Consider a row of equidistant atoms having alternative masses  $m$  of species  $Z_1$  and  $M$  of species  $Z_2$  Relative to the origin situated on one of these atoms, the average position of atoms from species  $Z_1$  is  $2na$  with  $n$ : integer. The Hooke's approximation is used and only is taken into account the action of nearest neighbors characterized by a force constant  $b$ .

(a) Starting from the equation of motion of these two types of atoms, find the dispersion relation for vibrations that propagate along the row with solutions of the form:

$$u_{2n} = A \exp i[\omega t - 2kna], u_{2n+1} = B \exp i[\omega t - (2n + 1)ka].$$

(b) Find the expressions for  $\omega$  and for the ratio  $U = u_{2n+1}/u_n$  in the following cases:

(i)  $k \ll \pi/a$

(ii) The extremity of  $k$  is in contact to the first BZ

(c) In each of the two situations above (i, ii), draw the elongation of several atoms as a function of their position:  $u = f(x)$ .

(d) What is the velocity of sound  $v_s$  along the row?

(e) Find the evolution of the dispersion curve, which has two branches toward the curve that has only 1 as the value for  $M$  is progressively changed toward that of  $m$ .

(f) *Numerical application to NaCl:*

Taking  $a \approx 2.8 \text{ \AA}$  and  $b \approx 42 \text{ N/m}$ , find the numerical value of  $v_s$  and that of  $\omega$  at characteristic points [ $m (\text{Na}) = 23, M (\text{Cl}) = 35.5$ ]. (N)

---

### Problem 2

Consider a linear lattice with parameter  $a$  formed from identical atoms of mass  $m$ . Each atom is submitted to a force constant  $\beta_1$  by its nearest neighbors and to  $\beta_2$  from its second nearest neighbors.

(a) Find the equation governing the displacement of atom  $n$ , given by  $u_n$  (compared to its equilibrium position), as a function of  $u_{n+1} u_{n-1} u_{n+2} u_{n-2}$

(b) Find the dispersion relation of longitudinal phonons,  $\omega = f(k)$ , starting from the solution in the form of a plane wave of type:  $u_n = A \exp i(\omega t - kx) \approx A \exp i(\omega t - kna)$ . In this relation highlight the corrective factor  $S(k)$ , related to the influence of second nearest neighbors.

(c) Find the expression for the velocity of sound. Indicate the characteristics of the dispersion curve by considering successively the hypothesis  $\beta_2 > 0$  and  $\beta_2 < 0$  ( $\beta_1$  is necessarily  $> 0$ ). Also sketch the reference curve  $\beta_2 = 0$ . Show the displacement of atoms  $u_{n+j}$  as a function of their coordinates  $x_{n+j}$  for  $k = \pi/2a$  and  $k = \pi/a$ . Explain what happens when  $\beta_2 = -\beta_1/4$ .

---

### Problem 3

Exercises 8.1, 8.2 from Simon.

---

### Problem 4

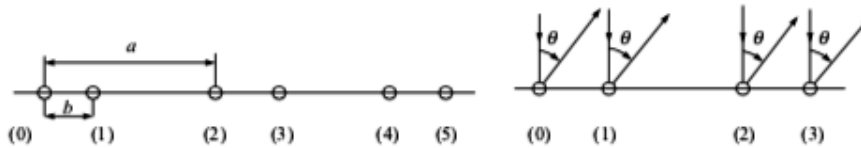
Exercises 9.1, 9.2 from Simon.

---

**Bonus Problems**


---

1) Consider the linear chain of carbon atoms shown in the figure below. This structure could easily be a chain of hydrocarbons with alternating single and double bonds such as  $-C=C-C=C-$ .



- a) What is the lattice vector? What is the basis? Specify using the conventional notation with  $b = \frac{a}{4}$ .
- b) Monochromatic X-rays of wavelength  $\lambda$  illuminate the chain.
- Evaluate the path difference between the waves diffracted in the angle  $\theta$  by the atom positioned at the origin (O) and the atom placed in the position (2). Indicate the possible values of  $\theta$  ( or of one of its trigonometric function) observed by diffraction assuming that the chain consists only of atom pairs (crystal diffraction). Show that the addition of odd atoms accentuates the diffracted intensity in certain directions while diminishing it in others ( always assuming that  $b=a/4$ ). Find the result using the structure factor.
  - Numerical Application:*  $\lambda=0.5 \text{ \AA}$ ,  $a=0.5 \text{ \AA}$ , determine the table of increasing values from  $0 \leq \theta \leq \pi/2$ , for which the diffraction conditions are satisfied. State the values corresponding to the intensities  $I_T/I_f$  in which  $I_T$  the diffracted intensity of the group of the atoms of the chain and  $I_f$  is the diffracted intensity of the atoms only situated at the lattice points.
- 

2) We continue the same structure from the previous problem, but now assume that the linear chain of atoms has a finite length with the basis repeated  $N$  times.

- Find the expression for the intensity due only to the lattice as a function of  $\theta$ .
- Find the expression for the intensity due to the crystal structure(lattice + basis) assuming that  $b = \frac{a}{4}$
- Apply the results to the case when  $\lambda=0.5 \text{ \AA}$ ,  $a=0.5 \text{ \AA}$  and  $N=10$ . What is the angular width of the first reflection ( $n=1$ )?