Assessment

Solid-state physics

Assignment 5: One-dimensional solids (welcome to the diatomic party), crystals

Compiled: August 2, 2023

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Due: 1700, October 2, 2023

Exercise 1 *Dispersion* (11 points)

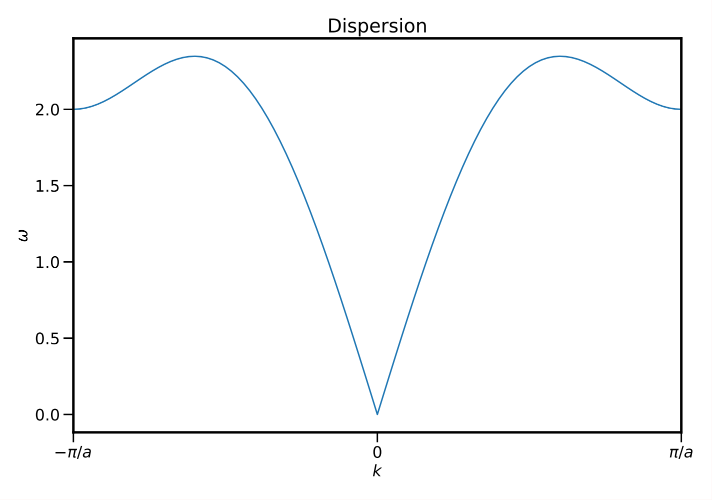
During our study of vibrations in one dimension, we arrived the dispersion relation for normal modes of the system.

(i) Use the dispersion relation to compute the group velocity v_g

(ii) What is the relationship between the group velocity v_g and the density of states $g(\omega)$? Use this to calculate $g(\omega)$.

(iii) Sketch or plot both v_g and $g(\omega)$

(iv) Consider the dispersion curve below



This script used to produce this plot is available here.

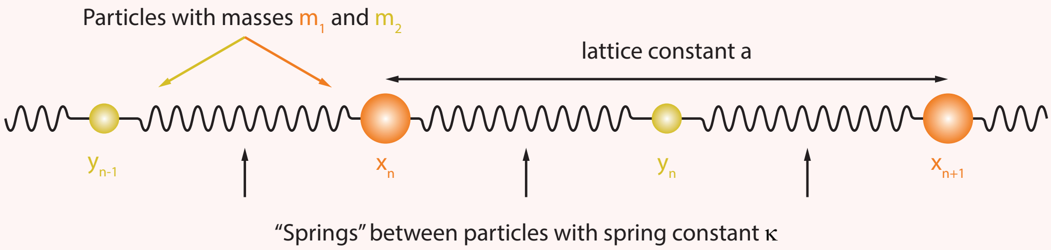
(a) Sketch the group velocity $v_g(k)$

(b) Produce a visualisation (e.g. a plot or histogram) of the density of states $g(\omega)$

Exercise 2 *Normal modes of a one-dimensional diatomic chain* (15 points)

(i) What is the difference between an acoustic mode and optical mode? Describe the motion of adjacent particles in both cases.

(ii) Derive the dispersion relation for the longitudinal oscillations of a one-dimensional diatomic mass-and-spring crystal with unit cell length a and where each unit cell contains one atom of mass m_1 and one atom of mass m_2 connected by a spring with spring constant κ.



(iii) Determine the frequencies of the acoustic and optical modes at $k = 0$ and at the Brillouin zone boundary

(iv) Determine the sound velocity, and show that the group velocity is zero at the zone boundary

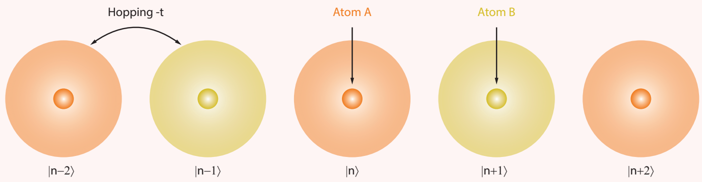
(v) Sketch or plot the dispersion in both the reduced and extended zone scheme

(vi) Assuming that there are N unit cells, how many different normal modes are there? And how many branches of excitation are there?

(vii) What happens when $m_1 = m_2$

Exercise 3 *Diatomic tight binding chain* (8 points)

We have seen the both the diatomic chain and the tight-binding chain, so we are going to combine the two. Consider the system shown below



Suppose that the *onsite* energy of atom A is different for atom B, that is $\langle n|H|n\rangle = \epsilon_A$ for $|n\rangle$ being on site A and $\langle n|H|n\rangle = \epsilon_B$ for $|n\rangle$ being on site B. We assume that the hopping $-t$ is unchanged from the monatomic case.

(i) Derive the dispersion curve for electrons

(ii) Sketch or plot the above dispersion relation in both the reduced and extended zone schemes

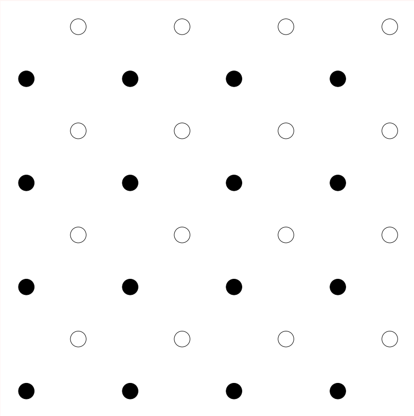
(iii) What is the effective mass of an electron near the bottom of the lower band?

(iv) If each atom (A and B) are monovalent, is the system a conductor or insulator? Justify your response

(v) Consider the material LiF, and use the above results to justify why it is observed to be an excellent insulator.

Exercise 4 *Two-dimensional crystal structure* (9 points)

Consider the following two-dimensional diatomic crystal:

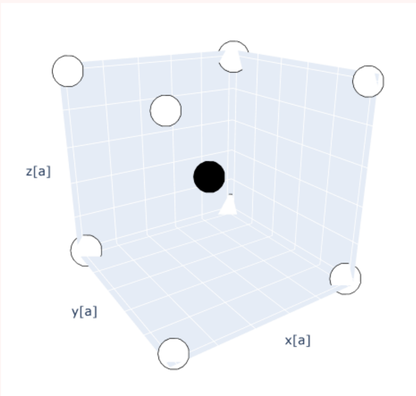


(i) Sketch the Wigner-Seitz unit cell and two other possible primitive unit cells of the crystal

(ii) If the distance between the filled circles is $a = 2.8\,\text{Å}$, what is the area of the primitive unit cell? How would this area change if all the empty circles and the filled circles were identical?

(iii) Write down one set of primitive lattice vectors and the basis for this crystal. What happens to the number of elements in the basis if all empty and filled circles were identical?

(iv) Imagine expanding the lattice into the perpendicular direction z. We can define a new three-dimensional crystal by considering a periodic structure in the z direction, where the filled circles have been displaced by $\frac{a}{2}$ in both the x and y direction from the empty circles. The figure below shows the new arrangement of the atoms.

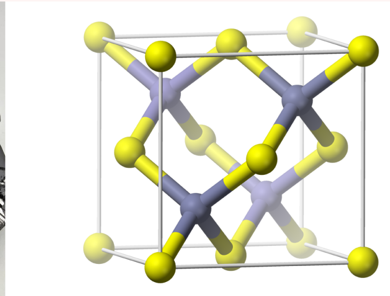


What lattice do we obtain? Write down the basis of the three-dimensional crystal.

(v) If we consider all atoms to be the same, what lattice do we obtain?

Exercise 5 *Three-dimensional crystal structure* (6 points)

The image below shows the three dimensional structure of zincblende (ZnS) (zinc atoms are yellow, sulphur atoms are grey).



(i) How many atoms are in the unit cell?

(ii) Draw the plan view of the unit cell

(iii) Identify the lattice type of zincblende

(iv) Describe the basis for zincblende

(v) Given the unit cell length $a = 5.41\,\text{Å}$, calculate the nearest-neighbour Zn-Zn, Zn-S, and S-S distances