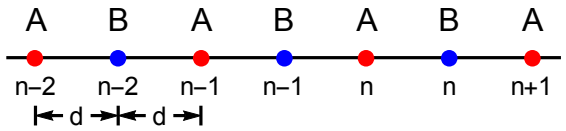
# Solid State Physics I

PY 741

Homework 2

(1) One-dimensional model of ionic solids




A composite 1-dimensional crystal of period $a = 2d$ consisting of two types of atoms



The periodic arrangement of the two types of atoms shown in the above figure is the simplest 1-dimensional model of an ionic solid. Each atom has one orbital and one electron, with atom $A$ being the cation and $B$ the anion ($\epsilon_A > \epsilon_B$).



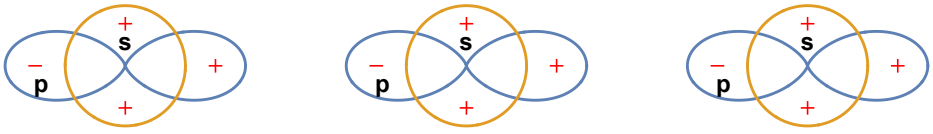
Setting

$$\begin{aligned}
\langle \psi_A | \mathcal{H} | \psi_A \rangle &= \epsilon_A \\
\langle \psi_B | \mathcal{H} | \psi_B \rangle &= \epsilon_B \\
\langle \psi_{A,n} | \mathcal{H} | \psi_{B,n} \rangle &= \langle \psi_{B,n} | \mathcal{H} | \psi_{A,n+1} \rangle = V
\end{aligned}$$



Derive an expression for the energy dispersion of its electronic bands. Plot the corresponding band dispersions.

(2) One-dimensional solid with 2 electrons per primitive cell




1-dimensional solid with $sp$ hybrids

Let us consider a 1-dimensional solid, of period $a$, consisting of a single atom type, but now each atom has a single $s$ and a single $p$ orbital, with 2 electrons per atom.

Setting

$$\begin{aligned}
\langle \psi_{np} | \mathcal{H} | \psi_{np} \rangle &= \epsilon_p, \\
\langle \psi_{ns} | \mathcal{H} | \psi_{ns} \rangle &= \epsilon_s \\
\langle \psi_{np} | \mathcal{H} | \psi_{n\pm1,p} \rangle &= V_{pp\sigma} > 0 \\
\langle \psi_{ns} | \mathcal{H} | \psi_{n\pm1,s} \rangle &= V_{ss\sigma} < 0 \\
\langle \psi_{ns} | \mathcal{H} | \psi_{n+1,p} \rangle &= -\langle \psi_{ns} | \mathcal{H} | \psi_{n-1,p} \rangle = V_{sp\sigma} > 0
\end{aligned}$$

(a) Construct the Bloch functions associated with the $s$ and $p$ orbitals.

(b) Determine the set of coupled equations obtained by minimizing the energy expectation value, assuming that orbitals on different sites are orthogonal.

(c) Derive an expression for the dispersion of the electronic bands, and plot the dispersion curves for the two sets of parameters:

1. Parameter set I

$$\epsilon_s = -10.725 \text{ eV},\ \epsilon_p = -3.525 \text{ eV},\ V_{ss\sigma} = -2.08 \text{ eV},\ V_{pp\sigma} = 3.49 \text{ eV},\ V_{sp\sigma} = 2.24 \text{ eV}$$

Identify the maximum energy of occupied states.

2. Parameter set II

$$\epsilon_s = -9.725 \text{ eV},\ \epsilon_p = -4.525 \text{ eV},\ V_{ss\sigma} = -4.294 \text{ eV},\ V_{pp\sigma} = 5.2 \text{ eV},\ V_{sp\sigma} = 2.24 \text{ eV}$$

Identify the the valence band maximum and conduction band minimum in set II.

(3) In the example of s-p basis on a square lattice with nearest-neighbor interactions ($a = 2\,\mathring{A}$), extend the interactions to next-nearest neighbor.