

**Physics 460 Problem Set 7; Due Friday, March 29**

**1) Tight-binding model for a one-dimensional crystal with two atoms per primitive cell**

Consider a one-dimensional crystal in the form of a zig-zag, of period  $2a$ . The hopping matrix element for nearest neighbors is  $t$ , and that for next nearest neighbors is  $t'$ , so that the dispersion relation is

$$\varepsilon(k) = -2t \cos ka - 2t' \cos 2ka.$$

- a) For  $t = t' = 1/2$ , plot  $\varepsilon(k)$  in the first and second Brillouin zones.
- b) Plot the two energy bands in the first Brillouin zone.
- c) If this crystal consists of atoms with a single valence electron, so that there are two valence electrons per primitive cell, is the crystal a metal or an insulator?

**2) Donor States in Silicon**

A single pentavalent atom (impurity) in a silicon crystal can take the place of one of the tetravalent Si atoms in the crystal structure. Four of its five valence electrons will participate in covalent bonds with its four Si neighbors, and the remaining electron is weakly bound by the resultant positive ion. The Schrödinger equation describing this bound state is

$$\left[ -\frac{\hbar^2}{2m^*} \nabla^2 - \frac{e^2}{\epsilon|\mathbf{r}|} \right] \Psi(\mathbf{r}) = E\Psi(\mathbf{r}),$$

where  $m^* = 0.2m$  is the effective mass in the conduction band of silicon ( $m$  being the free electron mass) and  $\epsilon = 11.7$  is the static dielectric constant of silicon.

- a) Show that the effective Bohr radius of the bound state is

$$a_d = \frac{\epsilon \hbar^2}{m^* e^2}.$$

Give the numerical value for  $a_d$  in Si.

- b) Show that the ionization energy of the donor is

$$E_d = \frac{e^4 m^*}{2\epsilon^2 \hbar^2}.$$

Give the value of  $E_d$  in eV for Si.

- c) Consider a crystal of silicon with a density  $n_d$  of pentavalent donor impurities per unit volume. If the mean spacing between impurities is much greater than  $a_d$ , then each donor electron will be bound to its parent impurity, as discussed above. However, above a critical density  $n_c$ , the donor electrons will be delocalized, forming an *impurity band*. Such a material is referred to as an n-type semiconductor, and behaves like a semimetal. Estimate  $n_c$  in silicon. Give your answer in units of  $\text{m}^{-3}$ .