

PH102: Modern Physics Homework 4 (Due: 2/21//2014)

1. (12 points) Semiconductor

(a) (2 points) Write Si's atomic configuration and draw a diagram for atomic energy levels at $T=0$. (Note that Li's atomic configuration can be written as $1s^2 2s^1$.)

(b) (2 points) Si Crystal is a semiconductor with the energy band gap of 1.11 eV. When Si atoms form a tetrahedral crystal, a covalent bond is created between two neighboring Si atoms. In this process, how Si's atomic orbitals change? How can molecular bonding between two Si atoms explain conduction and valence energy bands of Si crystal?

(c) (2 points) Consider a cube with a side length 2 and the origin at the center. The eight vertices of the cube are given by $(\pm 1, \pm 1, \pm 1)$. Choose four vertices of the cube so that any pair of vertices are diagonally connected to each other on a face of the cube that can form a tetrahedron. Draw the cube and the tetrahedron. The four vertices should be where Si atoms are located in Si Crystal.

(d) (3 points) Consider the atomic wave functions of Si (i.e. $\psi_s, \psi_x, \psi_y, \psi_z$) related to 3s and 3p ($3p_x, 3p_y, 3p_z$) orbitals, respectively. These four wave functions are orthogonal. That is

$$\int dV \psi_\alpha^* \psi_\alpha = 1 \text{ and } \int dV \psi_\alpha^* \psi_\beta = 0$$

where $\alpha, \beta = s, x, y, z$.

Four new orbitals can be constructed using the coordinates (x_i, y_i, z_i) of each of the four vertices in the tetrahedron.

$$\psi_i = \frac{1}{2} \psi_s + \frac{1}{2} (x_i \psi_x + y_i \psi_y + z_i \psi_z)$$

Pick one vertex and construct a new wave function related to the vertex. Show that

$$\int dV \psi_i^* \psi_i = 1$$

(e) (3 points) Pick two vertices and construct two new wave functions related to the two vertices. Show that

$$\int dV \psi_i^* \psi_j = 0$$

2. (5 points) Textbook: Harris, Chapter 10 Conceptual Question #7

3. (5 points) Textbook: Harris, Chapter 10 Conceptual Question #11

4. (5 points) Textbook: Harris, Chapter 10 Conceptual Question #16

5. (10 points) Textbook: Harris, Chapter 10 Exercises #39

6. (5 points) Textbook: Harris, Chapter 10 Exercises #44

7. (5 points) Textbook: Harris, Chapter 10 Exercises #48