# MASSACHUSETTS INSTITUTE OF TECHNOLOGY

Physics of Solids II —6.732

PROBLEM SET # 1

Issued: September 7, 2001 Due: September 14, 2001

1. This problem is a review of the nearly free electron approximation.

   (a) Write a general expression for the $E(\vec{k})$ relations for the empty lattice (i.e., $V(\vec{r}) = 0$) for a two dimensional square lattice.

   (b) Find $E(\vec{k})$ explicitly along $\Gamma - X$ and $X - L$ for the lowest 3 energy levels including the degeneracies of each level. Plot $E(\vec{k})$ for these levels using MATLAB, preferably. Note: the $\Gamma$ point is $(\pi/a)(0,0)$; the $X$ point is $(\pi/a)(1,0)$; and the $L$ point is $(\pi/a)(1,1)$.

   (c) Suppose that small carrier pockets are formed in the energy bands about points $\Gamma$, X and L of the square lattice Brillouin Zone. In each case, indicate the shape of this carrier pocket and the number of equivalent full carrier pockets that are formed.

   (d) Find the wave functions corresponding to the three lowest $X$ point energy levels in the empty lattice model.

   (e) Using first order degenerate perturbation theory, find the effect of a small periodic potential $V(\vec{r})$ on producing band gaps for these $X$ point energy levels according to the nearly free electron approximation. Which degeneracies in (d) are lifted?

2. This problem is to review the tight binding approximation.

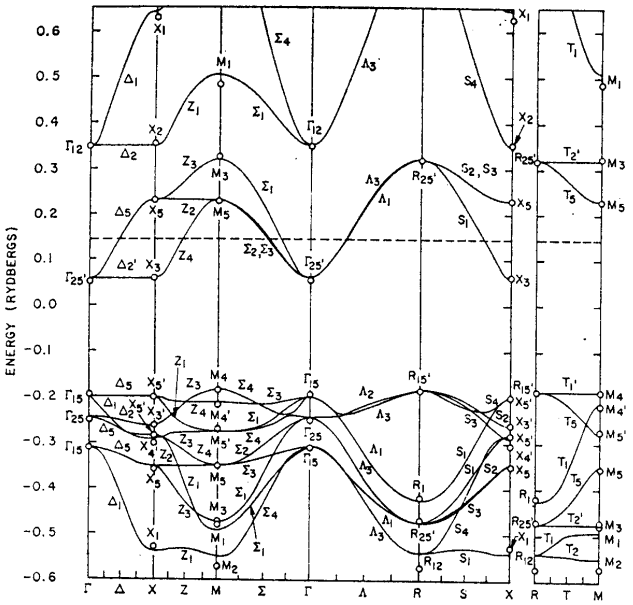
   (a) Suppose that the overlap integral for the electrons on adjacent sites vanishes ($s = 0$). Sketch the effect of taking $s = 0$ on the dispersion relations (Fig. 1.9 of class notes). This approximation is sometimes used in research (e.g., carbon nanotubes).

   (b) To satisfy the bonding requirements of carbon, polyacetylene has alternating single and double bonds with bond lengths of 1.7Å and 1.3Å, respectively (see §1.2.4 of class notes Part I). Please clarify why single and double bonds are needed from a chemical point of view. What modification to the electronic dispersion relations does this bond alternation give rise to (see Fig. 1.9 of class notes)? Sketch the effect on Fig. 1.9 of introducing these differences in the bond length.

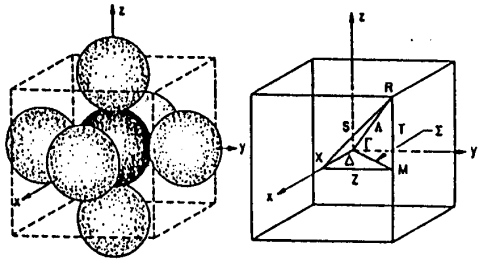
   (c) In this treatment the effect of the hydrogen atoms has been ignored. What physical argument can you give to justify this approximation?

3. Consider the diagram for the electronic dispersion relations $E(k)$ for $ReO_3$ shown below. The atomic configuration for Re is $4f^{14}5d^{5}6s^{2}$

and for O is $2s^2 2p^4$, and the $ReO_3$ unit cell and Brillouin zone are shown below.




LCAO energy bands for $ReO_3$.




(a) (b)

$ReO_3$ unit cell and Brillouin zone.

(a) How many atoms per unit cell are there (see diagram)?

(b) Which bands are associated with the Re and which with the oxygen?

(c) Is $ReO_3$ a semiconductor or a metal?

(d) Identify the *d*-bands on the band diagram. Are these associated with the oxygen atoms? If not, where are the oxygen *d*-bands? (atomic number for oxygen = 8)

(e) Where are the carrier pockets? Estimate the effective masses for the carriers qualitatively.

(f) How many electrons are contained in the carrier pockets?

(g) What is the shape of Fermi surface?

(h) Where in the Brillouin zone does the lowest energy optical transition occur? Is this transition expected to be strong or weak? Why?