## MASSACHUSETTS INSTITUTE OF TECHNOLOGY

# Physics Department

8.231, Physics of Solids I

Due on Wed., Nov. 15.

#### Problem set #8

# 1. Band structure for periodic $\delta$ -potential in 1D:

A mass m particle moves in a periodic potential V(x):

$$V(x) = V_0 \sum_{n = -\infty}^{+\infty} \delta(x - na)$$

where a is the period. In this problem, we assume  $\hbar = m = a = 1$ .

(a) Find the dispersion  $\epsilon(k)$  for the first band in the following two limits: (1)  $V_0 = 0$  and (2)  $V_0 \gg 1$ .

(Hint: across a  $\delta$ -potential  $V_0\delta(x-a)$ , we have the following boundary condition for the wave function:  $\psi(a^+) - \psi(a^-) = 0$ ,  $\psi'(a^+) - \psi'(a^-) = \frac{2mV_0}{\hbar^2}\psi(a)$ .)

(b) (Optional) Plot the dispersion  $\epsilon(k)$  for the first and the second band for the following three cases: (1)  $V_0 = 0$ , (2)  $V_0 = 5$ , and (3)  $V_0 = 100$ . (Hint: choose a set of energies  $\{E_i\}$  and find the corresponding set of wave vectors  $\{k_i\}$ . Then plot E as a function of k.)

## 2. Band structure for an 1D tight binding model with two orbits per unit cell:

In the lecture (see also the lecture note on the class homepage), we discuss an 1D tight binding model where the hoping between sites are described by the following picture.



We show that the dispersions of the two bands can be obtained from the following k dependent 2 by 2 matrix

$$M(k) = -t \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - t' e^{i2ak} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} - t' e^{-i2ak} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

(In the lecture, we have assumed 2a = 1.)

- (a) Find the dispersions of the two bands,  $\epsilon_1(k)$  and  $\epsilon_2(k)$ .
- (b) Find  $\epsilon_1(k)$  and  $\epsilon_2(k)$  for (1) t = t' and (2)  $t' \ll t$ .
- (c) Find the energy gap  $\Delta$  between the two bands.
- (d) Assume the lower band is filled. Find the effective mass  $m_e$  of the electrons at the bottom of the upper band. Find the effective mass  $m_h$  of the hole at the top of the lower band.

(e) Assume the lower band is filled by spin-up and spin-down electrons at T = 0. When  $T \neq 0$ , some particles and holes are excited. Find the density of the particles  $n_p$  and holes  $n_h$  in the low temperature limit. (Note  $n_p = n_h$ .) Express you answer in term of  $m_e$ ,  $m_h$  and  $\Delta$ .