Assignment 7

1. (a) In this question, we are only assuming one-dimensinal solids. Show that $V(x) = \sum_G V_G e^{iGx}$ is a periodic fuction wilh period a.

   (b) Using the above description of the periodic $V(x)$, show that if $V(x)$ is real, we have $V_{-G} = V_G^*$.

   (c) Conider the eigenstates for the free electron

$$\langle x \mid k \rangle = \frac{1}{\sqrt{L}} e^{i\mathrm{kx}}$$

   where L is the length of the solid and $L \gg 1/\mathrm{k}$. Show that the matrix element $\langle k'|V(x)|k\rangle$ is non-zero only when $G = k - k'$.

   (d) Consider k values at the first zone boundaries, i.e. at $k = -\pi/a$ and $k = -\pi/a + G = -\pi/a + 2\pi/a = \pi/a$. Hence these states can be written as $|k\rangle$ and $|k+G\rangle$. Write the Hamiltonian in the $\{|k\rangle, |k+a\rangle\}$ basis and diagonalize. This will provide the energies at the zone boundaries. Show that they are

$$\varepsilon = \frac{\hbar^2\pi^2}{2ma^2} + V_0 \pm V_{2\pi/a}. \tag{1}$$

   What is the band gap between the first and second Brillouin zones?

2. (a) The dispersion relationship for elections in a metal is given by

$$\varepsilon = 2A\sin^2(ka/2), \tag{2}$$

where a is the lattice spacing. If for small k, $k << 1$, the effective mass m^* is equal the the free electron mass m, find the constant A.

(b) Show that $\partial\varepsilon/\partial k = 0$ at the zone boundary $k = \pm\pi/a$.

(c) If $m^* = \hbar^2/(\partial^2\varepsilon/\partial k^2)$ plot the variation of the effective mass of the electrons in the FBZ.