Assignment 7 : Solution

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.

Solution:

$$V(x) = \sum_G V_G\, e^{iGx} \tag{1}$$

$$\begin{aligned} V(x+a) &= \sum_G V_G\, e^{iG(x+a)} \\ &= \sum_G V_G\, e^{iGx}\, e^{iGa}. \end{aligned} \tag{2}$$

Uisng $Ga = \frac{2\pi}{a}.a = 2\pi$, we obtain

$$V(x+a) = V(x). \tag{3}$$

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

Solution:

$$\begin{aligned} V^*(x) = V(x) &= \sum_G V_G^*\, e^{-iGx} \\ &= \sum_{-G} V_G^*\, e^{i(-G)x} \end{aligned} \tag{4}$$

In equation (1), we can replace G by $-G$, since the sum is over all $G's$.

$$V(x) = \sum_{-G} V_{-G}\ e^{i(-G)x} \tag{5}$$

By comparing (2) and (3), we have

$$V_{-G} = V_G^*.$$

(c) Conider the eigenstates for the free electron

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

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 $G = k - k'$.

Solution:

$$\begin{aligned}
\langle k^{'} \mid V \mid k\rangle &= \frac{1}{L}\int_0^L dx\ e^{-ik^{'}x}\ V(x)\ e^{ikx}, \\
&= \frac{1}{L}\int_0^L dx\ V(x)\ e^{i(k-k^{'})x}, \\
&= \frac{1}{L}\sum_G \int_0^L dx\ V_G\ e^{iGx}\ e^{i(k-k^{'})x}, \\
&= \frac{1}{L}\sum_G V_G \int_0^L dx\ e^{i(G+k-k^{'})x}, \\
&= V_G\ \delta_{G,k-k'}.
\end{aligned}$$

(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

$$\varepsilon = \frac{\hbar^2\pi^2}{2ma^2} + V_0 \pm V_{2\pi/a}. \tag{6}$$

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

Solution:

$$\begin{aligned} \mid \psi\rangle &= A \mid k\rangle + B \mid k+G\rangle \\ \psi(x) &= \frac{1}{L}(A\ e^{ikx} + B\ e^{i(k+G)x}) \end{aligned}$$

Hamiltonian of the system will be,

$$H = \frac{p^2}{2m} + V(x)$$

The matrix in the $\mid \psi\rangle, \mid \psi\rangle$ space is found by determing the following matrix elements.

$$\begin{aligned} \langle k \mid H \mid k\rangle &= \varepsilon(k) + V_G, \\ &= \varepsilon(k = -\pi/a) + V_G, \\ &= \frac{\hbar^2}{2m}(\frac{\pi^2}{a^2}) + V_o, \\ &= \frac{\hbar^2\pi^2}{2ma^2} + V_o. \end{aligned}$$

Similarly,

$$\langle k+G \mid H \mid k+G\rangle = \frac{\hbar^2\pi^2}{2ma^2} + V_o.$$

$$\langle k+G \mid H \mid k+G\rangle = V_G = V_{2\pi/a}.$$

$$\langle k+G \mid H \mid k+G\rangle = V_{-G} = V_{-2\pi/a}.$$

Noted that for $G \neq 0$

$$\langle k+G \mid H_o \mid k\rangle = \langle k \mid H_o \mid k+G\rangle = 0$$

Since the free plane waves are orthogonal to one another the Hamiltonian can be written in matrix form as

$$\begin{aligned} H &= \begin{pmatrix} \frac{\hbar^2\pi^2}{2ma^2} + V_o & V_{2\pi/a} \\ V_{-2\pi/a} & \frac{\hbar^2\pi^2}{2ma^2} + V_o \end{pmatrix} \\ &= \begin{pmatrix} \frac{\hbar^2\pi^2}{2ma^2} + V_o & V_{2\pi/a} \\ V_{-2\pi/a} & \frac{\hbar^2\pi^2}{2ma^2} + V_o \end{pmatrix} \end{aligned}$$

Let $\alpha = \frac{\hbar^2\pi^2}{2ma^2} + V_o$. The eigenvalues are found as:

$$\begin{aligned} \begin{vmatrix} \alpha-\lambda & V_g \\ V_g^* & \alpha-\lambda \end{vmatrix} &= (\alpha-\lambda)^2 - |V_g|^2 = 0 \\ (\alpha-\lambda)^2 &= |V_g|^2 \\ \alpha-\lambda &= \pm V_g \\ \lambda &= \alpha \mp V_g \end{aligned}$$

$$\lambda_{1,2} = \frac{\hbar^2\pi^2}{2ma^2} + V_o \mp V_{2\pi/a}$$

It can also be shown that the eigenstates are proportional to $\mid k\rangle + \mid k+G\rangle$ and $\mid k\rangle - \mid k+G\rangle$, i.e,

$$\mid v_{1,2}\rangle = \frac{1}{\sqrt{2}}(\mid k\rangle \pm \mid k+G\rangle).$$

$$\begin{aligned}\langle x \mid v_1\rangle &= \frac{1}{\sqrt{2}\sqrt{L}}(e^{ikx} + e^{i(k+G)x}) \\ &= \frac{e^{ikx}}{\sqrt{2}\sqrt{L}}(1 + e^{iGx}) \\ &= \frac{e^{ikx}\ e^{iGx/2}}{\sqrt{2}\sqrt{L}}(e^{iGx/2} + e^{-iGx/2}) \\ \langle x \mid v_1\rangle &\propto \cos(Gx/2) = \cos(\pi x/2)\end{aligned}$$

and

$$\langle x \mid v_2\rangle \propto \sin(Gx/2) = \sin(\pi x/2)$$

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

$$\varepsilon = 2A\sin^2(ka/2), \tag{7}$$

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.

Solution:

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

For small k,

$$\begin{aligned}\varepsilon &= 2A\ \left(\frac{ka}{2}\right)^2 \\ &= \frac{2Ak^2a^2}{4} = \frac{Ak^2a^2}{2} \\ \frac{\hbar^2k^2}{2m} &= \frac{Ak^2a^2}{2m}\end{aligned}$$

We obtain,

$$A = \frac{\hbar^2}{ma^2}$$

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

Solution:

$$\begin{aligned}\frac{\partial \varepsilon}{\partial k} &= 2A\frac{a}{2}2\sin(ka/2)\cos(ka/2) \\ &= Aa\sin(ka)\end{aligned}$$

At the zone boundary, $k = \pm\frac{\pi}{a}$

$$\frac{\partial \varepsilon}{\partial k} = 0.$$

So, the dispersion curve hits the zone boundary perpendicularly.

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

Solution:

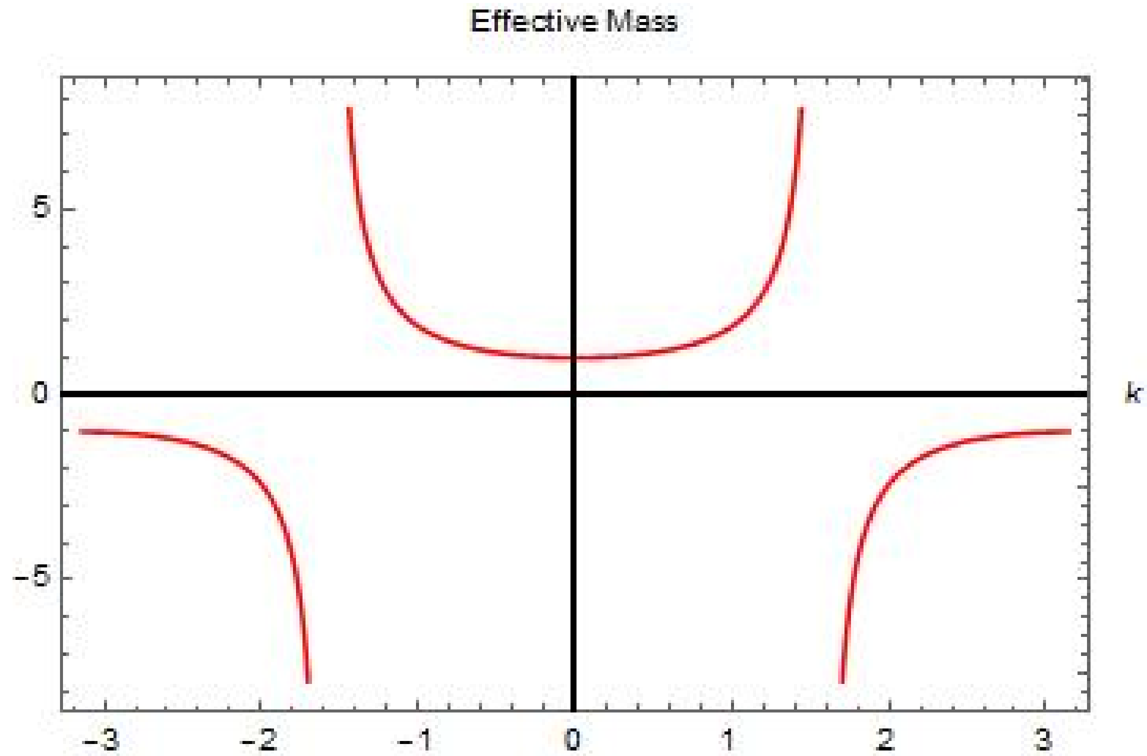
$$m^* = \frac{\hbar^2}{\partial^2\varepsilon/\partial k^2}.$$

$$\frac{\partial \varepsilon}{\partial k} = Aa\sin(ka).$$

$$\frac{\partial^2 \varepsilon}{\partial k^2} = Aa^2\cos(ka).$$

$$m^* = \frac{\hbar^2}{Aa^2\cos(ka)}$$

$$\left(\frac{m^*}{\hbar^2/Aa^2}\right) = \frac{1}{\cos(ka)}$$


Effective Mass
5
0
-5
k
-3
-2
-1
0
1
2
3