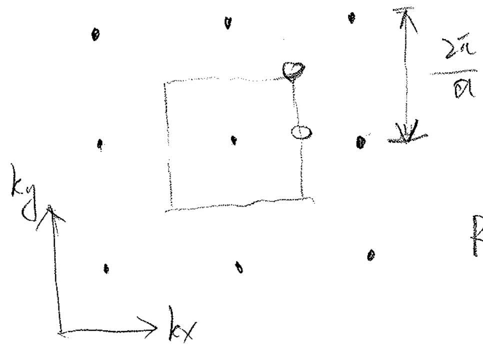
Problem Set # 7 Solution

Problem 1

(a) In a 2D simple squre lattice, the first Brillouin zone is like



Randomly choose one corner and midpoint

$$\vec{k}_{corner} = \left(\frac{\pi}{a}, \frac{\pi}{a}\right), \quad \vec{k}_{midpoint} = \left(\frac{\pi}{a}, 0\right)$$

Since $E(k) = \frac{\hbar k^2}{2m}$

$$\frac{E_{corner}}{E_{midpoint}} = \frac{\frac{\hbar^2}{2m}\left(\sqrt{2}\frac{\pi}{a}\right)^2}{\frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2} = 2$$

(b) In 3D

$$\vec{k}_{corner} = \left(\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a}\right), \quad \vec{k}_{midpoint} = \left(\frac{\pi}{a}, 0, 0\right)$$

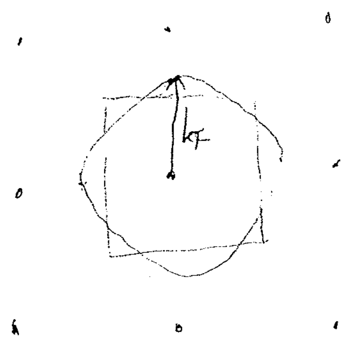
then $$\frac{E_{corner}}{E_{midpoint}} = \frac{\frac{\hbar^2}{2m}\left(\sqrt{3}\frac{\pi}{a}\right)^2}{\frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2} = 3$$

(c). For divalent metals with simple cubic structure

$$n = \frac{2}{a^3}$$

$$k_F = (3\pi^2 n)^{\frac{1}{3}} = \left(\frac{6\pi^2}{a^3}\right)^{\frac{1}{3}} \simeq \frac{3.9}{a}$$

while $|\vec{k}_{corner}| = \sqrt{3}\frac{\pi}{a} = \frac{5.44}{a}$, $\quad |\vec{k}_{midpoint}| = \frac{\pi}{a} = \frac{3.14}{a}$

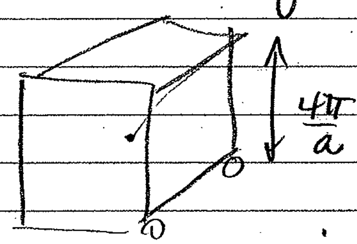


$E_{midpionit} < E_F < E_{corner}$.

states at midpoint are occupied, while we have unoccupied state at corner, which indicates both lower and upper band are partilly filled, therefore it's a conductor even at $T=0K$.

Problem #2

FCC band edge in the ⟨111⟩ directions at



$$\frac{1}{2}\left[\frac{\sqrt{3}}{2}\frac{4\pi}{a}\right] = \frac{\sqrt{3}\pi}{a}$$

$$\therefore \quad E_{\text{band edge}} = \frac{\hbar^2}{2m}\left[\frac{\sqrt{3}\pi}{a}\right]^2 = \frac{\hbar^2 3\pi^2}{2ma^2}$$

Need to plot to 6× this energy

In reciprocal space this is a BCC lattice

$$\vec{b}_1 = \frac{2\pi}{a}(-\hat{x}+\hat{y}+\hat{z}) \quad \vec{b}_2 = \frac{2\pi}{a}(\hat{x}-\hat{y}+\hat{z}) \quad \vec{b}_3 = \frac{2\pi}{a}(\hat{x}+\hat{y}-\hat{z})$$

$$E = \frac{\hbar^2}{2m}\left[(k_x+G_x)^2 + (k_y+G_y)^2 + (k_z+G_z)^2\right]$$

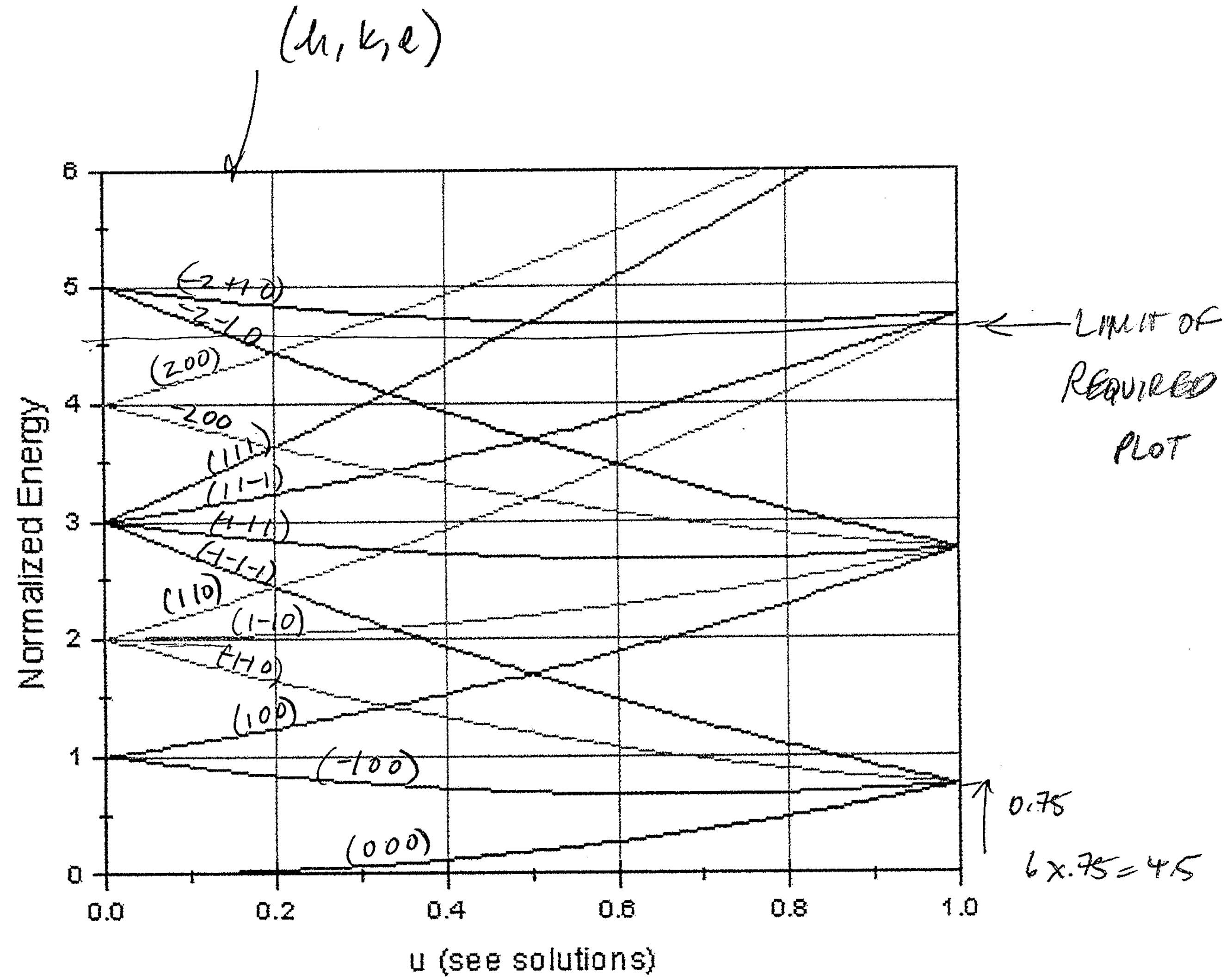
$$\text{for} \quad \vec{k} = \frac{2\pi}{a}u\left(\frac{\hat{x}}{2}+\frac{\hat{y}}{2}+\frac{\hat{z}}{2}\right) \quad -1 < u \le 1$$

$$\vec{G} \text{ in general} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$$

$$= \frac{2\pi}{a}(-h+k+l)\hat{x} + \frac{2\pi}{a}(h-k+l)\hat{y} + \frac{2\pi}{a}(h+k-l)\hat{z}$$

$$\therefore \quad E = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2\left[\left(\frac{u}{2}-h+k+l\right)^2 + \left(\frac{u}{2}+h-k+l\right)^2 + \left(\frac{u}{2}+h+k-l\right)^2\right]$$

(See plot)


(h,k,l)
Normalized Energy
u (see solutions)
(2-1 0)
-2-1 0
(200)
200
(111)
(11-1)
(-1-11)
(-1-1-1)
(110)
(1-10)
(-1-10)
(100)
(-100)
(000)
LIMIT OF REQUIRED PLOT
0.75
6x.75=4.5

Problem 3.

$$\frac{P}{Ka}\sin Ka + \cos Ka = \cos ka \qquad \text{from Kittle}$$

(a) For $k=0 \Rightarrow \cos ka = 1$

Since $P \ll 1 \Rightarrow K \to 0$

Expand $\sin Ka$ and $\cos Ka$ about $K=0$

$$\frac{P}{Ka}\left[Ka + \left(1 - \frac{(Ka)^2}{2}\right)\right] = 1$$

$$\Rightarrow K^2 = \frac{2P}{a^2}$$

$$\epsilon = \frac{\hbar^2 K^2}{2m} = \frac{\hbar^2 P}{ma}$$

(b) For $k = \frac{\pi}{a}$, $\cos ka = -1$

Ka must also be close to π

Let $Ka = \pi + \delta$, $\delta \ll 1$, then

$$\frac{P}{\pi+\delta}\sin(\pi+\delta) + \cos(\pi+\delta) = -1$$

$$\Rightarrow \frac{P}{\pi+\delta}(-\sin\delta) - \cos\delta = -1$$

$$\frac{P}{\pi+\delta}(-\delta) - \left(1 - \frac{\delta^2}{2}\right) = -1$$

$$\pi \gg \delta \Rightarrow \frac{-P}{\pi}\delta - 1 + \frac{\delta^2}{2} = -1$$

$$\Rightarrow \frac{P\delta}{\pi} = \frac{\delta^2}{2} \rightarrow \delta = \begin{cases} 0 \\ \frac{2P}{\pi} \end{cases}$$

$\delta = 0$, $Ka = \pi$

$$E_A = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2$$

$\delta = \frac{2P}{\pi}$, $Ka = \pi + \frac{2P}{\pi}$

$$E_B = \frac{\hbar^2}{2m}\left(\frac{\pi}{a} + \frac{2P}{\pi a}\right)^2$$

The gap at $k = \frac{\pi}{a}$ is

$$\Delta = E_B - E_A = \frac{\hbar^2}{2m}\left[\left(\frac{\pi}{a} + \frac{2P}{a}\right)^2 - \left(\frac{\pi}{a}\right)^2\right]$$

$$= \frac{2\hbar^2}{ma^2}\left(P + \frac{P^2}{\pi^2}\right)$$