MS1230 - Physics of Solids

1. (a) Cu - K_α : $\lambda = 1.5406 \mathring{A}$

We use Braggs Law : $\boxed{n\lambda = 2d\sin\theta}$, where

(i) $2\theta = 22.88° \Rightarrow \theta = 11.44°$

$\sin(11.44°) = 0.198$

$$\boxed{\therefore d = \frac{\lambda}{2\sin\theta} = 3.89 \mathring{A}}$$

Similarly,

2θ	d-spacing $\left[\frac{\lambda}{2\sin\theta}\right]$
22.88	3.89 Å
32.54	2.749 Å
40.1	2.246 Å
46.6	1.947 Å
52.48	1.742 Å
57.92	1.59 Å
67.94	1.38 Å
72.68	1.29 Å
77.3	1.233 Å

$$\left\{ d = \frac{\lambda}{2\sin\theta} \right\}$$

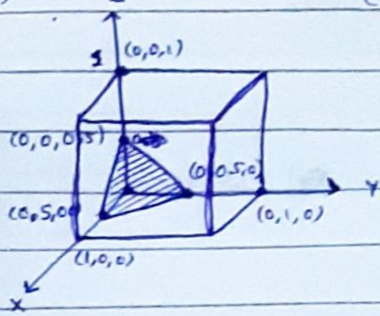
(b) If Fe - K_α with $\lambda = 1.93604 \mathring{A}$ was used,

d-spacing	$2\theta°$ (Peak)
3.89 Å	28.7
2.749 Å	41.25
2.246 Å	51.02
1.947 Å	59.52
1.742 Å	67.5
1.59 Å	~~74.9~~ 75
1.38 Å	89.2
1.29 Å	96.3
1.233 Å	103.2

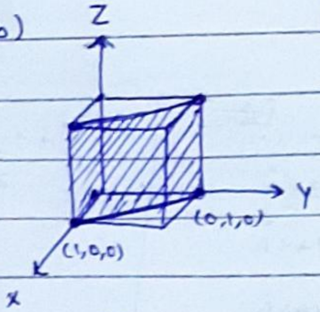
$$\cancel{\left\{ d = \frac{\lambda}{\sin\left(\frac{2\theta}{2}\right)} \right\}}$$

$$\left\{ \theta = \sin^{-1}\left(\frac{\lambda}{2d}\right) \right\}$$

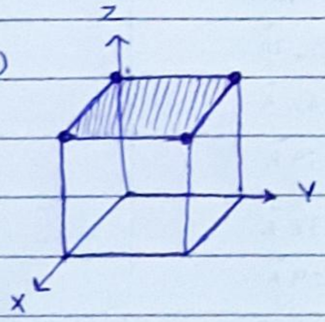
2. (a) (2 2 2)



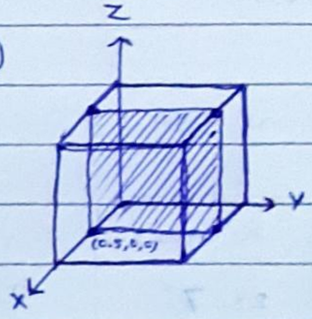
(b) (1 1 0)



(c) (0,0 1)



(d) (2 0 0)



3. (i) The planes belong to the family (0,0,K) $0 \le K < 1$

(ii) (1 1 0)

(iii) $(1 1 \bar{1})$

4. (a) Tossing a single coin gives rise to 2 eigen states.

If coins are <u>distinguishable</u>

→ No. of eigen states of tossing 3 coins simultaneously = 8

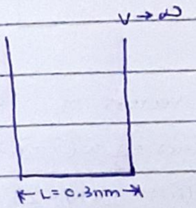
(H H H), (H H T), (H T H), (T H H), (H T T), (T H T), (T T H)
(T T T)

If coins are <u>indistinguishable</u>

→ No. of eigen states = 4

(HHH), (HHT), (HTT), (TTT)

(b) No. of degenerate states = (HHH) & (TTT)
$= \boxed{4}$

5. 

We know, in a potential well,

$$E = \frac{n^2 h^2}{8 m L^2}$$

$$E_{ground\ state} = \frac{h^2}{8mL^2} \quad [n=1]$$

$$\Rightarrow E_{gs} = \frac{(6.63\times10^{-34})^2}{8\times 9.1\times10^{-31}\times(0.3\times10^{-9})^2}$$

$$= 6.7089\times10^{-19}\ J$$

$$= 4.193\ eV$$ = KE of e^- in ground state $[v=0]$.

⇒ 2^{nd} excited state : $n = 3$

$\therefore E_3 = 9E_1$

$$\therefore \nu = \frac{E_3 - E_1}{h} = \frac{8E_1}{h} = \frac{8\times 6.7089\times10^{-19}}{6.63\times10^{-34}}$$

$$= \boxed{8.0952\times10^{15}\ Hz}$$

6. (a) Fermi-Dirac Statistics are used.

$$\therefore f(E) = \frac{1}{1 + e^{(E-E_F)/k_B T}}$$

$E = 8eV = 8\times1.6\times10^{-19}\ J$
$E_F = 7eV = 7\times1.6\times10^{-19}\ J$

$E - E_F = 1.6\times10^{-19}\ J$
$T = 298.15\ K$
$K_B = 1.38\times10^{-23}\ J/K$

$$\therefore \frac{E - E_F}{K_B T} = 38.887$$

$$\boxed{\therefore f(E) = \frac{1}{7.734\times10^{16}} = 1.293\times10^{-17}}$$

(b) If $f(E) = 0.3$,

$$0.3 = \frac{1}{1+e^{\frac{11594.2}{T}}}$$

$$e^{\frac{11594.2}{T}} = 2.333$$

$$\boxed{T = \frac{11594.2}{\ln(2.333)} = 13,683.74\ K}$$

7. Basis vectors of BCC:

$$\bar{a}_1 = \frac{1}{2}a(\bar{x}+\bar{y}-\bar{z})$$

$$\bar{a}_2 = \frac{1}{2}a(-\bar{x}+\bar{y}+\bar{z})$$

$$a_3 = \frac{1}{2}a(\bar{x}-\bar{y}+\bar{z})$$

Basis vectors of FCC:

$$\bar{a}_1(\text{FCC}) = \frac{1}{2}a(\bar{x}+\bar{y})$$

$$\bar{a}_2(\text{FCC}) = \frac{1}{2}a(\bar{y}+\bar{z})$$

$$\bar{a}_3(\text{FCC}) = \frac{1}{2}a(\bar{z}+\bar{x})$$

Vectors in reciprocal lattice

$$\bar{b}_1 = \bar{a}_1^* = \frac{2\pi(\bar{a}_2\times\bar{a}_3)}{[\bar{a}_1\ \bar{a}_2\ \bar{a}_3]}$$

$$\bar{b}_2 = \bar{a}_2^* = \frac{2\pi(\bar{a}_3\times\bar{a}_1)}{[\bar{a}_1\ \bar{a}_2\ \bar{a}_3]}$$

$$\bar{b}_3 = \bar{a}_3^* = \frac{2\pi(\bar{a}_1\times\bar{a}_2)}{[\bar{a}_1\ \bar{a}_2\ \bar{a}_3]}$$

$$\left\{\begin{aligned} &[\bar{a}_1\ \bar{a}_2\ \bar{a}_3] = \bar{a}_1\cdot(\bar{a}_2\times\bar{a}_3) \\ &\bar{x}\times\bar{y} = \bar{z} \\ &\bar{y}\times\bar{z} = \bar{x} \\ &\bar{z}\times\bar{x} = \bar{y} \end{aligned}\right\}$$

$$\bar{a}_2\times\bar{a}_3 = \frac{1}{4}a^2\left[\cancel{(\bar{x}\times\bar{y})} - (\bar{x}\times\bar{z}) + \cancel{(\bar{y}\times\bar{x})} + (\bar{y}\times\bar{z}) + (\bar{z}\times\bar{x}) - \cancel{(\bar{z}\times\bar{y})}\right]$$

$$= \frac{1}{2}a^2[\bar{x}+\bar{y}]$$

$$\bar{a}_3\times\bar{a}_1 = \frac{1}{4}a^2\left[(\bar{x}\times\bar{y}) - (\bar{x}\times\bar{z}) - (\bar{y}\times\bar{x}) + \cancel{(\bar{y}\times\bar{z})} + (\bar{z}\times\bar{x}) + \cancel{(\bar{z}\times\bar{y})}\right]$$

$$= \frac{1}{2}a^2[\bar{z}+\bar{y}]$$

$$\bar{a}_1\times\bar{a}_2 = \frac{1}{4}a^2\left[(\bar{x}\times\bar{y}) + \cancel{(\bar{x}\times\bar{z})} - (\bar{y}\times\bar{x}) + (\bar{y}\times\bar{z}) + \cancel{(\bar{z}\times\bar{x})} - (\bar{z}\times\bar{y})\right]$$

$$= \frac{1}{2}a^2[\bar{z}+\bar{x}]$$

$[a_1\ a_2\ a_3] = \cancel{\frac{1}{2}} \frac{1}{4} a^3 (\bar{x}+\bar{y}-\bar{z}).(\bar{x}+\bar{y})$

$= \frac{1}{2} a^3$

$$\boxed{\begin{array}{lll} \therefore \bar{b}_1 = \frac{2\pi}{a}(\bar{x}+\bar{y}) & \bar{b}_2 = \frac{2\pi}{a}(\bar{y}+\bar{z}) \ \& & \bar{b}_3 = \frac{2\pi}{a}(\bar{z}+\bar{x}) \\ = k\bar{a}_1 (FCC) & = k\bar{a}_2 (FCC) & = k\bar{a}_3 (FCC) \\ & \{k \text{ being a constant}\} & \end{array}}$$

$\therefore$ The reciprocal lattice of BCC is FCC.

8\. (a) Group velocity of a wave packet $v_g = \frac{d\omega}{dk}$

→ We know $E = \hbar\omega$. Differentiating wrt k,

$$\frac{dE}{dk} = \hbar \frac{d\omega}{dk} \Rightarrow \boxed{\frac{d\omega}{dk} = \frac{1}{\hbar}\frac{dE}{dk} = v} \rightarrow (1)$$

~~→ Also, $E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$. Differentiating wrt k,~~

$$\cancel{\boxed{\frac{dE}{dk} = \frac{\hbar^2 k}{m}}} \rightarrow (2)$$

$$\cancel{\boxed{v = \frac{1}{\hbar}\frac{dE}{dk} = \frac{\hbar k}{m}}} \rightarrow (3)$$

→ On applying an electric field $\vec{E}$, the e^- gets accelerated.

$$\boxed{\text{Force} = m^* a} \rightarrow (4)$$

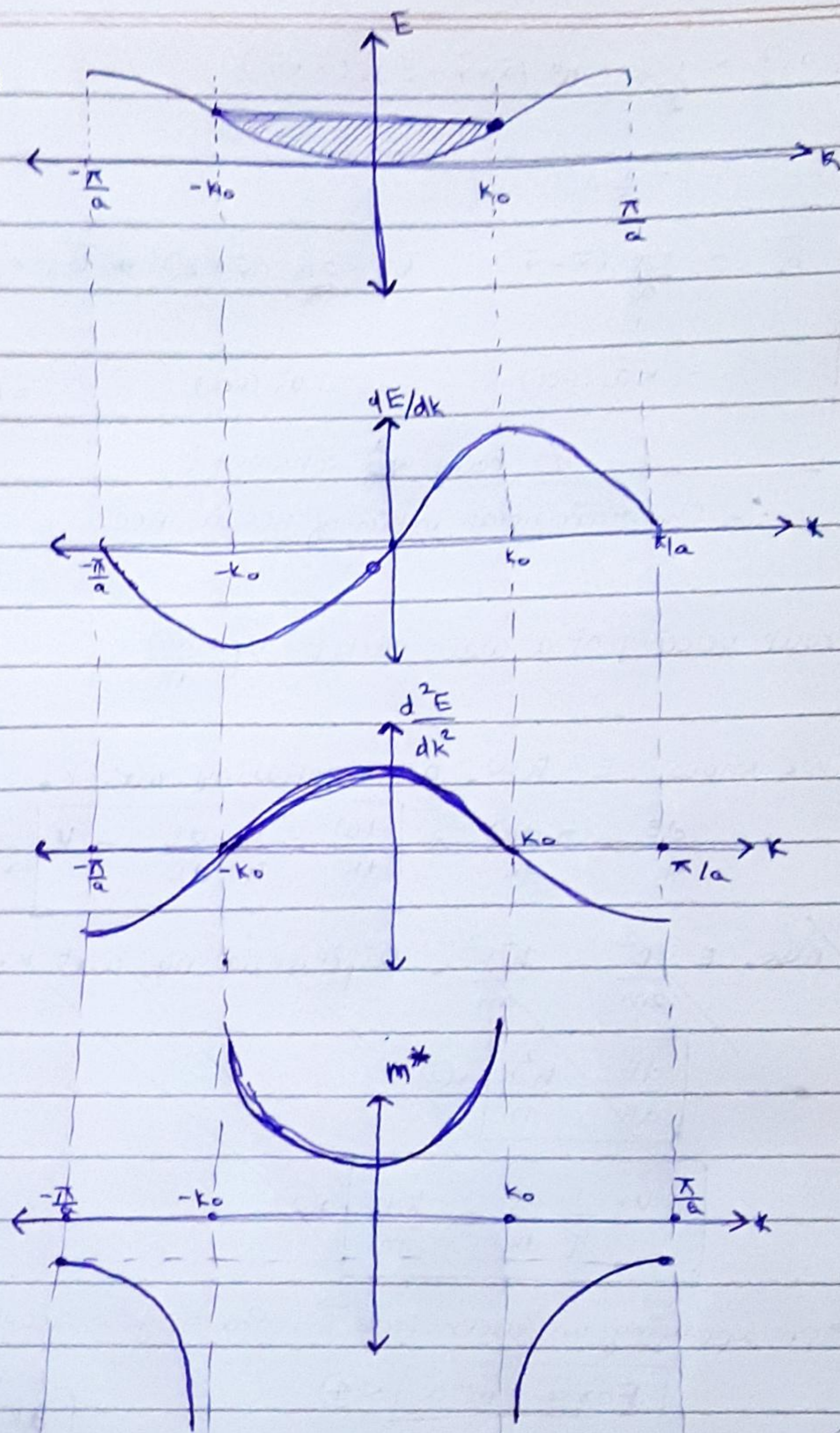
$$\left\{ \frac{dk}{dt} = \frac{1}{\hbar}\frac{dP}{dt} = \frac{F}{\hbar} \right\}$$

$$a = \frac{d}{dt}\left(\frac{1}{\hbar}\frac{dE}{dk}\right) = \frac{1}{\hbar}\frac{dk}{dt} \cdot \frac{d^2E}{dk^2}$$

$$= \frac{F}{\hbar^2}\frac{d^2E}{dk^2}$$

$$\boxed{\frac{F}{m^*} = \frac{F}{\hbar^2}\frac{d^2E}{dk^2} \Rightarrow m^* = \frac{\hbar^2}{\left(\frac{d^2E}{dk^2}\right)}}$$

(b)


E
k
$-\frac{\pi}{a}$
$-k_0$
k_0
$\frac{\pi}{a}$
dE/dk
k
$-\frac{\pi}{a}$
$-k_0$
k_0
π/a
$\frac{d^2E}{dk^2}$
$-\frac{\pi}{a}$
$-k_0$
k_0
π/a
k
m^*
$-\frac{\pi}{a}$
$-k_0$
k_0
$\frac{\pi}{a}$
k

9. In the lower portions of E-k graph, $\left(\frac{d^2E}{dk^2}\right)$ is positive. [$\therefore m^*$ is positive]

With the increase in k, m^* attains a maximum positive value at the inflection point after which $\frac{d^2E}{dk^2}$ becomes negative [$k \to \pi/a$].

→ This happens when the e^- approaches the zone boundary. However, the external force is still positive.

→ Physically, this means that the electron responds to the electric field OPPOSITE to how a free electron would respond. This happens because the e^- must reflect off the zone boundary, and hence it ~~dec~~ decellerates.

10. ~~For Lithium~~,

$$E_F = \frac{50.1\,eV}{\left(\frac{r_s}{a_0}\right)^2}$$, where a_0 is the Bohrs radius.

→ For Li, $\frac{r_s}{a_0} = 3.25$

$\therefore \boxed{E_F = 4.743\,eV}$

For Na, $\frac{r_s}{a_0} = 3.93$

$\boxed{E_F = 3.244\,eV}$