Problem Set 4 Soln's

1. A&M 8.2

a) show 8.63 $\rightarrow$ $D(\varepsilon_F) = \dfrac{m k_F}{\hbar^2 \pi^2}$

8.63: $$D(\varepsilon) = \int_S \frac{1}{4\pi^3} \frac{1}{|\nabla \varepsilon_k|} \, dS$$

Constant Energy Surface is sphere: $dS = k^2 \sin\theta \, d\theta \, d\phi$

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

$$\nabla_k \varepsilon_k = \frac{\hbar^2 k}{m}$$

$$\therefore \; D(\varepsilon) = \int_0^{\pi}\int_0^{2\pi} \frac{1}{4\pi^3} \frac{m}{\hbar^2 \cancel{k}} k^{\cancel{2}} \sin\theta \, d\theta \, d\phi$$

$$= \frac{4\pi m k}{4\pi^3 \hbar^2} = \frac{m k}{\hbar^2 \pi^2}$$

$$\therefore \; D(\varepsilon_F) = \frac{m k_F}{\hbar^2 \pi^2}$$

b) $\varepsilon(k) = \varepsilon_0 + \frac{\hbar^2}{2}\left(\frac{k_x^2}{m_x} + \frac{k_y^2}{m_y} + \frac{k_z^2}{m_z}\right)$

show $D(\varepsilon) \propto (\varepsilon - \varepsilon_0)^{1/2}$

$$D(\varepsilon) = \frac{1}{4\pi^3} \int d\vec{k}\; \delta(\varepsilon - \varepsilon_k)$$

$$= \frac{1}{4\pi^3} \int dk_x\, dk_y\, dk_z\; \delta\left(\varepsilon - \varepsilon_0 - \frac{\hbar^2}{2}\left(\frac{k_x^2}{m_x} + \frac{k_y^2}{m_y} + \frac{k_z^2}{m_z}\right)\right)$$

let $k_x' = \frac{k_x}{\sqrt{m_x}}$; $k_y' = \frac{k_y}{\sqrt{m_y}}$; $k_z' = \frac{k_z}{\sqrt{m_z}}$

$$dk_x' = \frac{1}{\sqrt{m_x}}\, dk_x$$

$$\Rightarrow D(\varepsilon) = \frac{\sqrt{m_x m_y m_z}}{4\pi^3} \underbrace{\int dk_x'\, dk_y'\, dk_z'}\; \delta\left(\varepsilon - \varepsilon_0 - \frac{\hbar^2}{2m} k'^2\right)$$

where $k'^2 = k_x'^2 + k_y'^2 + k_z'^2$

transform to spherical, integrate over θ & φ.

$\Rightarrow 4\pi k'^2\, dk'$

let $\sqrt{m_x m_y m_z} = \sqrt{m}$

$$D(\varepsilon) = \frac{\sqrt{m}}{4\pi^2} \int k'^2 \, \delta\left(\varepsilon - \varepsilon_0 - \frac{\hbar^2 k'^2}{2}\right) dk'$$

let $u = \frac{\hbar^2}{2} k'^2 \qquad du = \hbar^2 k' \, dk' = \sqrt{\frac{2u}{\hbar^2}} \, dk'$

$$D(\varepsilon) = \frac{\sqrt{m}}{\pi^2} \int \frac{2u}{\hbar^2} \left(\frac{\hbar^2}{2u}\right)^{1/2} \frac{du}{\hbar^2} \, \delta(\varepsilon - \varepsilon_0 - u)$$

$\Rightarrow$ δ evals @ $\varepsilon - \varepsilon_0 = u$.

$$\therefore \; D(\varepsilon) = \frac{\sqrt{m}}{\pi^2} \frac{1}{\hbar^3} \sqrt{2u} = \frac{\sqrt{2}\sqrt{m_x m_y m_z}}{\hbar^3 \pi^2} (\varepsilon - \varepsilon_0)^{1/2}$$

$D(\varepsilon_F)$

integrate over band.

$$\hookrightarrow \quad n = \int_{\varepsilon_0}^{\varepsilon_F} D(\varepsilon) \, d\varepsilon = \int_{\varepsilon_0}^{\varepsilon_F} A (\varepsilon - \varepsilon_0)^{1/2} d\varepsilon$$

$$n = \frac{2}{3} A (\varepsilon_F - \varepsilon_0)^{3/2}$$

$$D(\varepsilon_F) = A(\varepsilon_F - \varepsilon_0)^{1/2}$$

$$\therefore \; n = \frac{2}{3} D(\varepsilon_F)(\varepsilon - \varepsilon_0)$$

$$D(\varepsilon_F) = \frac{3}{2} n \left(\frac{1}{\varepsilon - \varepsilon_0}\right)$$

2. Important Notes NFEM

-> Far from degeneracies & B.Z. boundary, FE disp. curves ($\mathcal{E} \propto k^2$)

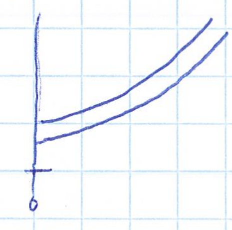
-> @ B.Z. boundaries => bandgap.

For 2 level degen. $\Delta \mathcal{E} = 2|V_k|$

-> For multiple degen levels (bands), splitting results from det of $m \times m$ matrix, for m-degeneracies.

-> Far from B.Z., degen levels ~~c~~an split by const. amount, otherwise following FEM.

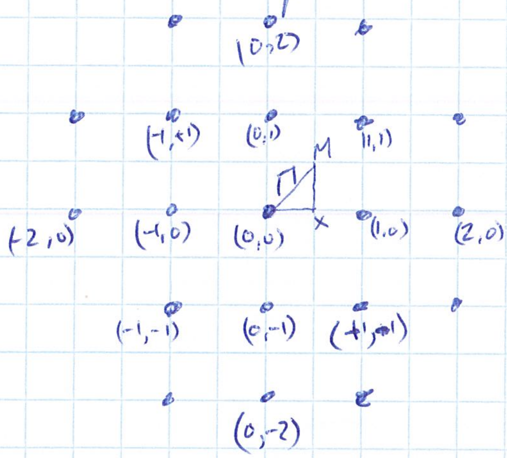
e.g.



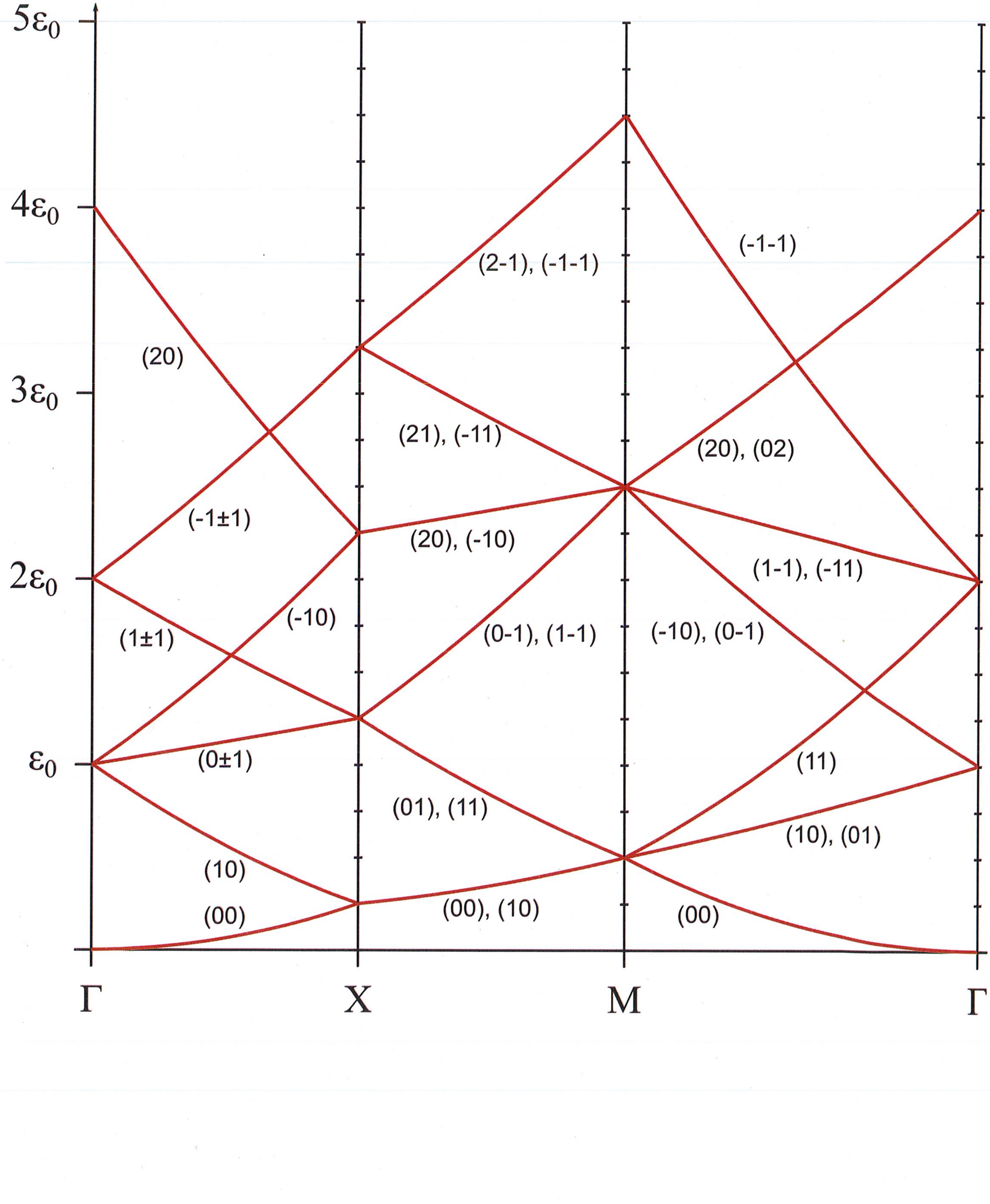
-> @ BZ. bounderies, multiple ~~xxx~~ degens. can form multiple band gaps or crossings (depends on soln from matrix).

-> see real BCC structures for examples.

3. Follow ~~proc~~ procedure given for nearby recip. lattice pts.



=> See attached for soln.


$5\varepsilon_0$
$4\varepsilon_0$
$3\varepsilon_0$
$2\varepsilon_0$
ε_0
(20)
(-1±1)
(1±1)
(-10)
(0±1)
(10)
(00)
(2-1), (-1-1)
(21), (-11)
(20), (-10)
(0-1), (1-1)
(01), (11)
(00), (10)
(-1-1)
(20), (02)
(1-1), (-11)
(-10), (0-1)
(11)
(10), (01)
(00)
Γ
X
M
Γ