731 Homework #8

Points

Due November 10th, 2006

1. A&M, problem 9.1	a) 8 pts	b) 7 pts	→	15
2. A&M, problem 9.3	a) 8 pts	b) 7 pts	→	15
3. A&M, problem 9.5	a) 8 pts	b) 7 pts	→	15
			Total =	45

Solution ~~II~~ 8

9.1

a) in the Bragg plane

$$\mathcal{E} = \mathcal{E}^0_{K/2} + \frac{\hbar^2 K_\perp^2}{2m} - |\vec{v}_K| \qquad \text{lower band}$$

$$\mathcal{E} = \mathcal{E}^0_{K/2} + \frac{\hbar^2 K_\perp^2}{2m} + |\vec{v}_K| \qquad \text{upper band}$$

$$\Rightarrow \begin{cases} \mathcal{E} > \mathcal{E}^0_{K/2} \Leftrightarrow |\vec{v}_K\rangle & \text{lower band} \\ \mathcal{E} > \mathcal{E}^0_{K/2} + |\vec{v}_K| & \text{upper band} \end{cases}$$

$$0 < \Delta < 2|\vec{v}_K|$$

$$\mathcal{E}_F > \mathcal{E}_{min\text{-}lower}$$

$$\mathcal{E}_F < \mathcal{E}_{min\text{-}upper}$$

$\Rightarrow$ Fermi surface lies entirely in lower band. $K_\perp = \beta_1$

$$\mathcal{E}^0_{\vec{K}/2} + \frac{\hbar^2 \beta_1^2}{2m} - |\vec{v}_K| = \mathcal{E}^0_{K/2} - |\vec{v}_K| + \Delta$$

$$\Rightarrow \beta_1 = \sqrt{\frac{2m\Delta}{\hbar^2}}$$

b) $\Delta > |2V_{\vec{k}'}|$

$\varepsilon_F > \varepsilon_{min-lower}$ → ϵ_F lies in both bands

$\varepsilon_F > \varepsilon_{min-upper}$

$$\varepsilon^0_{k/2} + \frac{\hbar^2 g_2^2}{2m} - |V_k| = \varepsilon^0_{k/2} - |V_k| + \Delta$$

$$\varepsilon^0_{k/2} + \frac{\hbar^2 g_1^2}{2m} + |V_k| = \varepsilon_{k/2} - |V_k| + \Delta$$

$$\rightarrow \quad \pi\left(g_2^2 - g_1^2\right) = \frac{4m|V_k|}{\hbar^2}$$

9.3

9.18 A and M textbook

$$\left(\varepsilon - \varepsilon^0_{\vec{k}'-\vec{k}_1}\right) C_{\vec{k}'-\vec{k}_1} = \sum_{j=1} V_{\vec{k}_j-\vec{k}_1} C_{\vec{k}'-\vec{k}_j} \quad (1)$$

$\vec{k}_1 = 0 \quad k_2 = \frac{2\pi}{a}(1,1,1) \quad k_3 = \frac{2\pi}{a}(1,1,1) \quad , \quad k_4 = \frac{2\pi}{a}(2,0,0)$

apply to (1)

$$\Rightarrow \quad \left(\varepsilon^0_1 - \varepsilon\right) C_{\vec{k}'-\vec{k}_1} + V_{\vec{k}_2-\vec{k}_1} C_{\vec{k}'-\vec{k}_2} + V_{\vec{k}_3-\vec{k}_1} C_{\vec{k}'-\vec{k}_3} + V_{\vec{k}_4-\vec{k}_1} C_{\vec{k}'-\vec{k}_4} = 0$$

$$V_{\vec{k}_1-\vec{k}_2} C_{\vec{k}'-\vec{k}_1} + \left(\varepsilon^0_2 - \varepsilon\right) C_{\vec{k}'-\vec{k}_2} + V_{\vec{k}_3-\vec{k}_2} C_{\vec{k}'-\vec{k}_3} + V_{\vec{k}_4-\vec{k}_2} C_{\vec{k}'-\vec{k}_4} = 0$$

$$V_{\vec{k}_1-\vec{k}_3} C_{\vec{k}'-\vec{k}_1} + V_{\vec{k}_2-\vec{k}_3} C_{\vec{k}'-\vec{k}_2} + \left(\varepsilon^0_3 - \varepsilon\right) C_{\vec{k}'-\vec{k}_3} + V_{\vec{k}_4-\vec{k}_3} C_{\vec{k}'-\vec{k}_4} = 0$$

$$V_{\vec{k}_1-\vec{k}_4} C_{\vec{k}'-\vec{k}_1} + V_{\vec{k}_2-\vec{k}_4} + V_{\vec{k}_3-\vec{k}_4} C_{\vec{k}'-\vec{k}_3} + \left(\varepsilon^0_4 - \varepsilon\right) C_{\vec{k}'-\vec{k}_4} = 0$$

By setting v_1 v_1 ...

$$\begin{vmatrix} \varepsilon_1^\circ - \varepsilon & v_1 & v_1 & v_2 \\ v_1 & \varepsilon_2^\circ - \varepsilon & v_2 & v_1 \\ v_1 & v_2 & \varepsilon_3^\circ - \varepsilon & v_1 \\ v_2 & v_1 & v_1 & \varepsilon_4^\circ - \varepsilon \end{vmatrix} = 0$$

~~Rewritten~~

$$\Leftrightarrow \begin{vmatrix} \varepsilon_w - \varepsilon & \text{———} \\ 0 & \text{———} \\ 0 & \text{———} \\ 0 & \text{———} \end{vmatrix} = 0$$

We can get $\varepsilon = \varepsilon_w - v_2$

$\varepsilon = \varepsilon_v + v_2 \pm 2v_1$

b) $\varepsilon_1^0 = \hbar^2/2m\, k^2 \qquad \varepsilon_2^0 = \frac{\hbar^2}{2m}\left(k - \frac{2\pi}{a}(111)\right)^2$

$\varepsilon_3^0 = \frac{\hbar^2}{2m}\left(k' - \frac{2\pi}{a}(200)\right)^2$

$k_1 = 0 \qquad k_2 = \frac{2\pi}{a}(111) \qquad k_3 = \frac{2\pi}{a}(200)$

apply to (1).

$$\begin{vmatrix} \varepsilon_v - \varepsilon & v_1 & v_2 \\ v_1 & \varepsilon_v - \varepsilon & v_1 \\ v_2 & v_1 & \varepsilon_v - \varepsilon \end{vmatrix}$$

$\Leftrightarrow$

$$\begin{vmatrix} \varepsilon_v - \varepsilon & v_1 & v_2 \\ 0 & (\varepsilon_v - \varepsilon) - \frac{v_1^2}{\varepsilon_v - \varepsilon} & v_1 - \frac{v_1 v_2}{\varepsilon_v - \varepsilon} \\ 0 & v_1 - \frac{\varepsilon_v - \varepsilon}{v_1} v_2 & \varepsilon_v - \varepsilon - v_2 \end{vmatrix} = 0$$

$\Rightarrow$ get

$$\varepsilon = \varepsilon_v - v_2$$

$$\varepsilon = \varepsilon_v + \frac{v_2}{2} \pm \frac{1}{2}\sqrt{v_2^2 + 8v_1^2}$$

9.5. F : Full P : partially empty

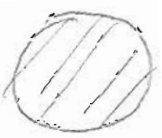
E : Empty

a)

m / Zone	1	2	3	4	5	6	7	8	9	10	11	12
I	P	P	P	F	F	F	F	F	F	F	F	F
II	E	P	P	P	P	P	F	F	F	F	F	F
III	E	E	E	P	P	P	P	F	F	F	F	F
IV	E	E	E	P	P	P	P	P	P	F	E	F
V	E	E	E	E	E	E	P	P	P	P	P	P
VI	E	E	E	E	E	E	E	P	P	P	P	P
VII	E	E	E	E	E	E	E	E	E	P	P	P

b)

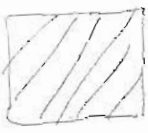
$m = 1$ Zone 1



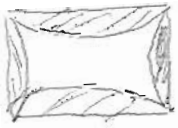
$m = 2$ Z_1

Z_2

$m = 3$ Z_1

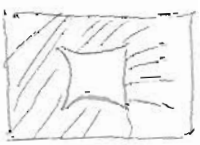


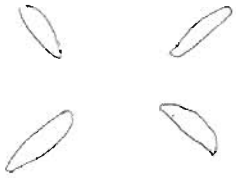
Z_2



m_4 Z_1

Z_2



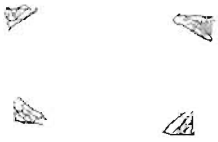
z_3 

z_4 

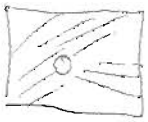
$m = 5$ 

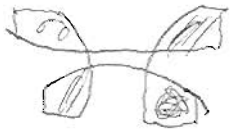
z_2 

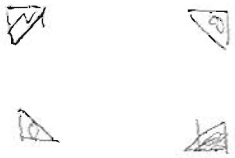
z_3 

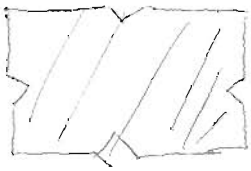
z_4 

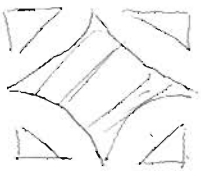
$m = 6$ 

z_2 

z_3 

z_4 

$m = 7$ z_3 

z_4 

z_5