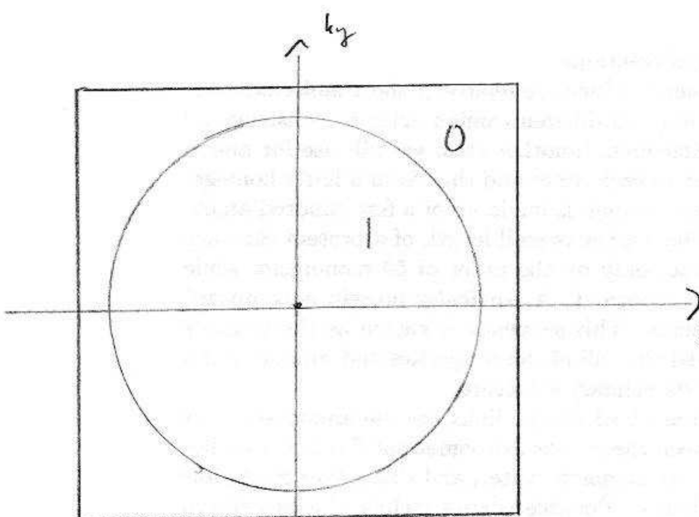
Physics 481: Solid State Physics - Homework Solutions 10

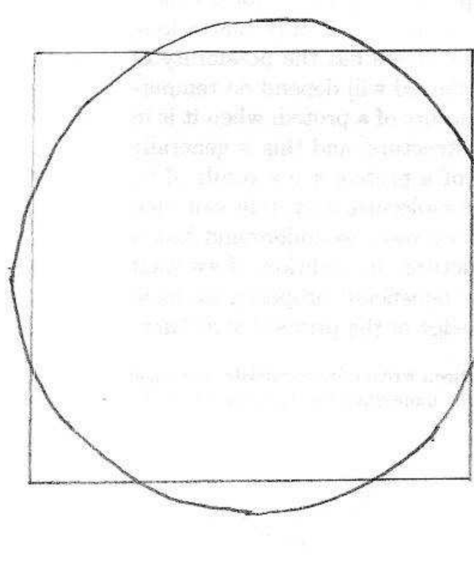
Problem 1

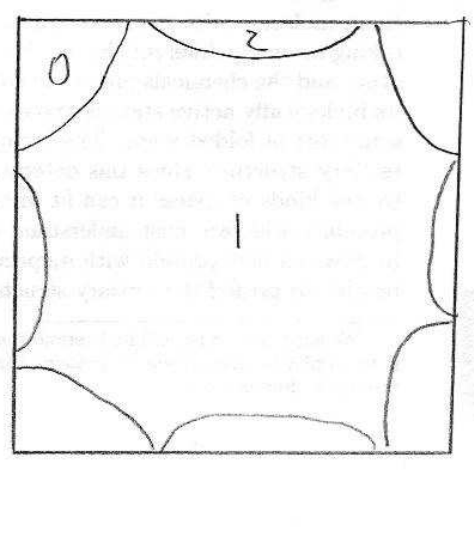
$$\frac{1}{(2\pi)^2}\;\underset{\text{spin}}{2}\;\pi k_F^2 = \frac{N}{A}$$

$$k_F^2 = 2\pi \frac{N}{A} \qquad k_F = \frac{1}{a}\begin{cases} 2.51 & N=1 \\ 3.54 & N=2 \\ 4.34 & N=3 \\ 5.60 & N=5 \end{cases}$$



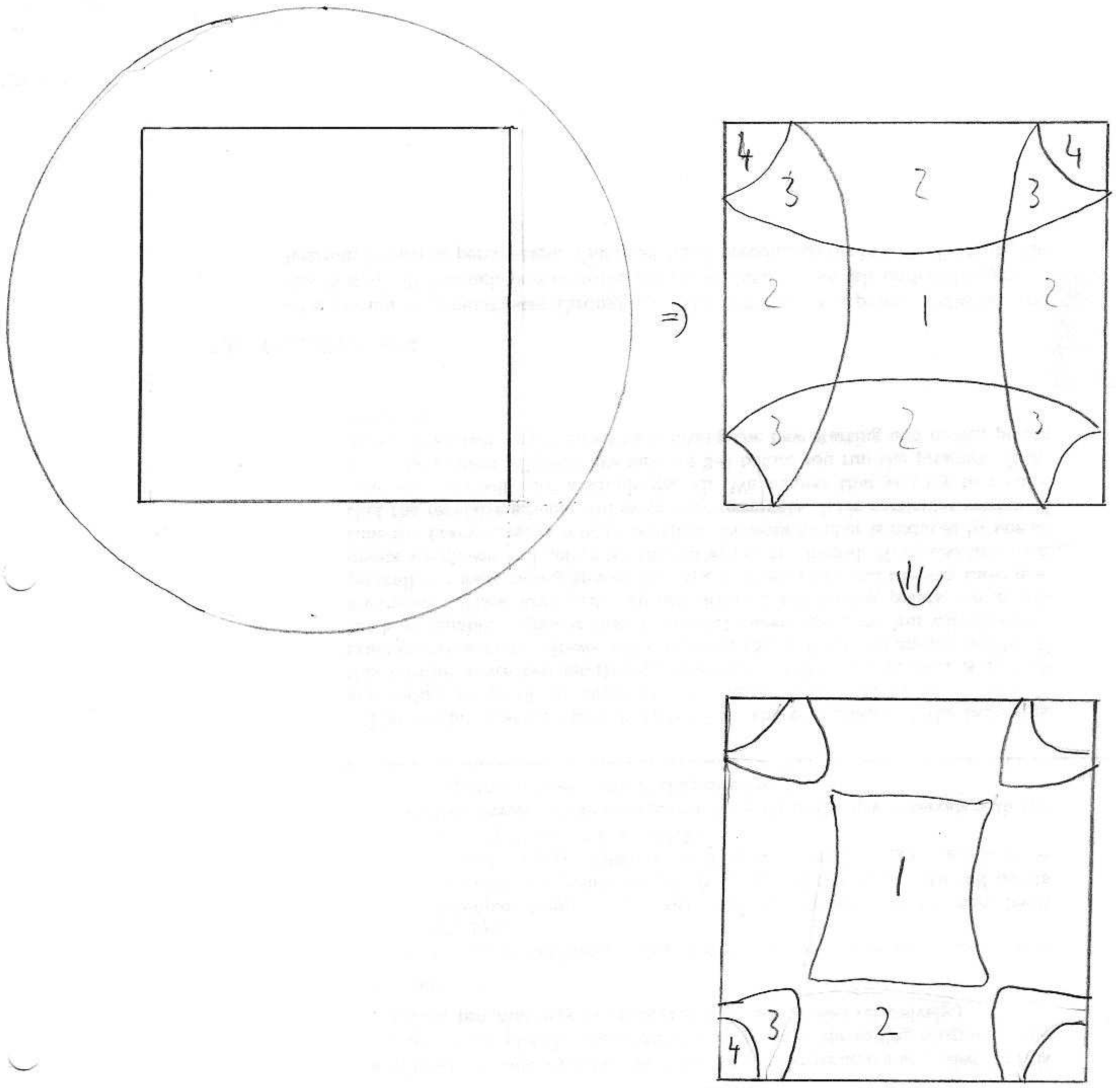
N=1



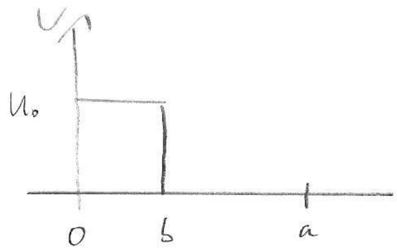


N=2

N=3 as analogous to N=2


4
3
2
3
4
2
1
2
3
2
3
1
3
2
4

Problem 2



$\downarrow$ no i $(E<U_0)$

$$\psi = A_1 e^{q_1 x} + B_1 e^{-q_1 x} \quad (0<x<b)$$

$$\psi = A_2 e^{iq_2 x} + B_2 e^{-iq_2 x} \quad (b<x<a)$$

$$\frac{\hbar^2 q_1^2}{2m} = U_0 - E \quad , \quad \frac{\hbar^2 q_2^2}{2m} = E$$

boundary conditions

$x=b$:

$$A_1 e^{q_1 b} + B_1 e^{-q_1 b} = A_2 e^{iq_2 b} + B_2 e^{-iq_2 b}$$

$$q_1 A_1 e^{q_1 b} - q_1 B_1 e^{-q_1 b} = iq_2 A_2 e^{iq_2 b} - iq_2 B_2 e^{-iq_2 b}$$

$x=a$

$$A_2 e^{iq_2 a} + B_2 e^{-iq_2 a} = (A_1 + B_1) e^{ika}$$

$$iq_2 A_2 e^{iq_2 a} - iq_2 B_2 e^{-iq_2 a} = (q_1 A_1 - q_1 B_1) e^{ika}$$

coefficient determinant must vanish

$$\begin{vmatrix} e^{q_1 b} & e^{-q_1 b} & -e^{iq_2 b} & -e^{-iq_2 b} \\ q_1 e^{q_1 b} & -q_1 e^{-q_1 b} & -iq_2 e^{iq_2 b} & +iq_2 e^{-iq_2 b} \\ e^{ika} & e^{ika} & -e^{iq_2 a} & -e^{-iq_2 a} \\ q_1 e^{ika} & -q_1 e^{ika} & -iq_2 e^{iq_2 a} & +iq_2 e^{-iq_2 a} \end{vmatrix} = 0$$

Use Maple for determinant

$$0 = \cos ka - \Big(\frac{1}{4}\, e^{q_1 b + iq_2 b - iq_2 a} + e^{q_1 b - iq_2 b + iq_2 a} + e^{-q_1 b + iq_2 b - iq_2 a} + e^{-q_1 b + iq_2 a - iq_2 b}\Big)$$

$$- \frac{i(q_1^2 - q_2^2)}{8 q_1 q_2}\Big(e^{q_1 b + iq_2 a - iq_2 b} - e^{q_1 b + iq_2 b - iq_2 a} + e^{-q_1 b + iq_2 b - iq_2 a} - e^{-q_1 b + iq_2 a - iq_2 b}\Big)$$

$$\cos ka = \cosh(q_1 b)\cos\big(q_2(a-b)\big) + \frac{q_1^2 - q_2^2}{2q_1 q_2}\sinh(q_1 b)\sin q_2(a-b)$$

c) $b \to 0$, $U_0 \to \infty$ $\qquad U_0 b \to \frac{W_0 \hbar^2}{ma}$

$$q_1 b \to 0 \qquad (q_1 \sim \sqrt{U_0})$$

$$\frac{q_1^2 - q^2}{2q_1 q_2}\sin(q_1 b) \to \frac{q_1^2 - q_2^2}{2q_2}\, b \to \frac{2mU_0}{\hbar^2}\frac{b}{2q_2}$$

$$\to \frac{W_0}{a q_2}$$

$$\boxed{\cos ka = \cos(q_2 a) + \frac{W_0}{a q_2}\sin q_2 a}$$

d) plots can be produced by calculating k as function of $\varepsilon = \frac{\hbar^2 q_2^2}{2m}$

Problem 3

$$\varepsilon = -2t\left(\cos k_x a + \cos k_y a\right)$$

a) see picture below

b)
$$\frac{\varepsilon}{2t} = -\cos k_x a - \cos k_y a$$

$$\cos k_y a = -\frac{\varepsilon}{2t} - \cos k_x a$$

$$k_y a = \arccos\left(-\frac{\varepsilon}{2t} - \cos k_x a\right)$$

plot see picture below

c) look at $k_x = \frac{\pi}{a}$, expand k_y about this point

assume $\varepsilon > 0$

$$k_y a = \arccos\left(-\frac{\varepsilon}{2t} + 1 - \frac{1}{2}(\Delta k_x a)^2\right) \qquad \Delta_{k_x} = k_x - \frac{\pi}{a}$$

$$= \arccos\left(1 - \frac{\varepsilon}{2t}\right) - \frac{1}{2}(\Delta k_x a)^2 \left.\frac{1}{\sqrt{1-x^2}}\right|_{x = 1 - \frac{\varepsilon}{2t}}$$

$\Rightarrow$ as long as $x = 1 - \frac{\varepsilon}{2t} \neq 1$,

the coefficient of $(\Delta k_x a)^2$ is finite

$\Rightarrow$ horizontal tangent

$\Rightarrow$ exception is $\varepsilon = 0$

d) one electron per site $\hat{=}$ half filling

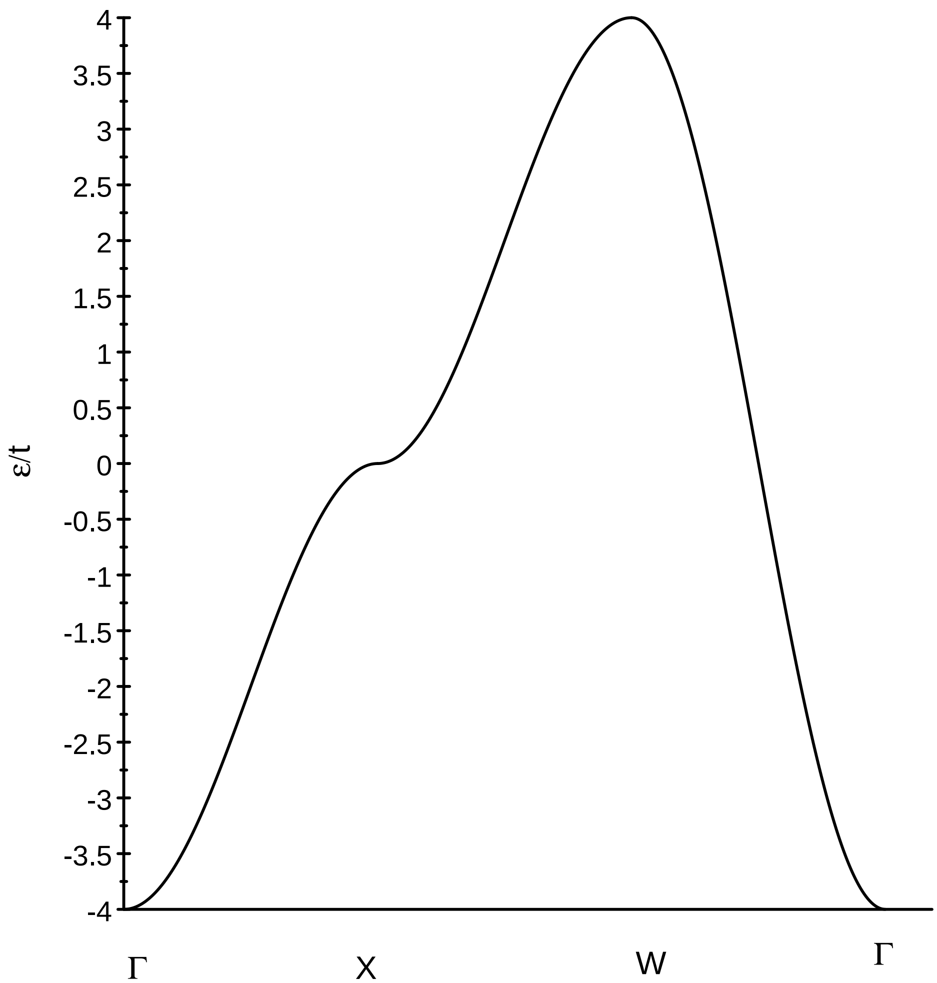
$\Rightarrow$ $\varepsilon_F = 0$ by symmetry

Fermi surface see picture of $\varepsilon = 0$ line

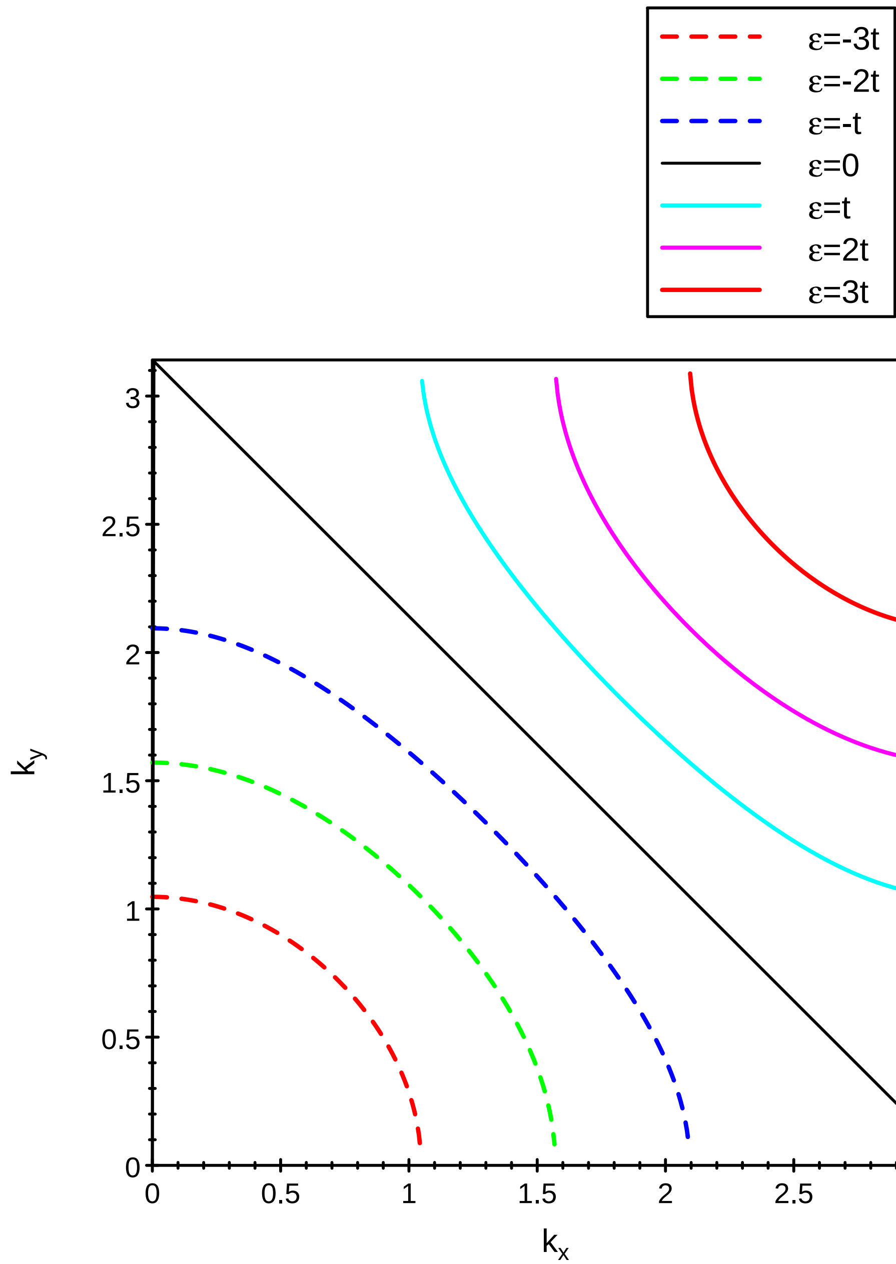
$\Rightarrow$ half-filled band $\Rightarrow$ metal

e) two e^- per site $\hat{=}$ band full

$\varepsilon_F = 4t$, insulator



ε/t
4
3.5
3
2.5
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-2.5
-3
-3.5
-4
Γ
X
W
Γ



ε=-3t
ε=-2t
ε=-t
ε=0
ε=t
ε=2t
ε=3t
k_y
k_x
0
0.5
1
1.5
2
2.5
3