Homework 1 - Solutions

Problem 1 - Free Electron Fermi Surface

Consider a hypothetical two dimensional solid with a single type of atom on a hexagonal lattice, with lattice spacing a. Suppose there are two electrons per atom

(a) What is the radius of the free electron circular Fermi surface in reciprocal space?

For the free electron model, we can calculate the area of the Fermi surface by counting the number of filled states in reciprocal space, and setting that equal to the number of states in real space (equal to the total number of particles), noting that we can only two electrons occupying the same momentum state.

We have the formula

$$2\frac{A_{\text{f.s.}}}{V_{\text{k space}}} = N \tag{1}$$

Where $A_{\text{f.s.}} = \pi k_F^2$ is the area enclosed by the circular Fermi surface. $V_{\text{k space}} = (2\pi)^2/V_{\text{unit cell}}$ is the 2d volume per state in k-space.

$$\Rightarrow \qquad 2\pi k_F^2 \frac{V}{(2\pi)^2} = N \tag{2}$$

$$k_F = \sqrt{2\pi\frac{N}{V}} = \sqrt{2\pi\frac{2}{\frac{\sqrt{3}}{2}a^2}} = \sqrt{\frac{8\pi}{\sqrt{3}a^2}} \tag{3}$$

where above I used that the volume (area) of the primitive unit cell is for the hexagonal lattice with basis vectors $\vec{a}_1 = a(1,0)$ and $\vec{a}_2 = a(\frac{1}{2}, \frac{\sqrt{3}}{2})$ is $V = |\vec{a_1} \times \vec{a_2}| = \frac{\sqrt{3}}{2}a^2$, plus the fact that there is one atom per unit cell (since there is 1/4 of an atom at the 4 corners of the primitive unit cell) and two electrons per atom so that $N = 2$.

(b) Draw the free electron Fermi surface in the reduced zone scheme

We can see immediately from Eq. (1) that for $N = 2$, the area of the first Brillouin zone in k-space is equal to the area enclosed by the Fermi surface $A_{\text{f.s.}} = V_{\text{k space}}$. Since the Fermi surface is circular and the 1st Brillouin zone is hexagonal, we also expect the Fermi surface to extend past the 1st Brillouin in some places.

The basis vectors in reciprocal space are the vectors $\vec{b}_i$ satisfying the condition $\vec{b}_i \cdot \vec{a}_j = 2\pi\delta_{i,j}$. From this relationship we can convince ourselves that the vectors $\vec{b}_i$ are given by:

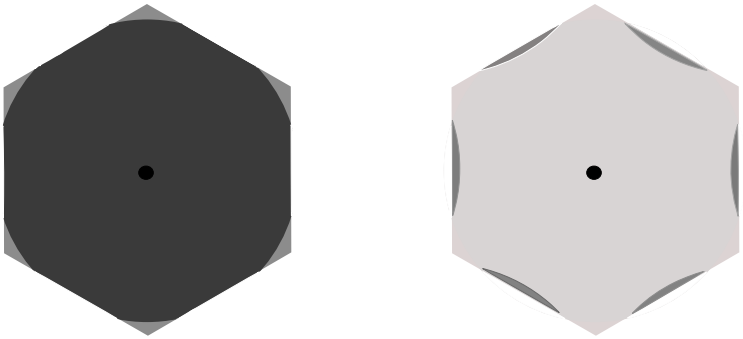
$$\vec{b}_1 = \frac{2\pi}{a}(\frac{1}{\sqrt{3}}, 1) \quad \text{and} \quad \vec{b}_1 = \frac{2\pi}{a}(\frac{-1}{\sqrt{3}}, 1) \tag{4}$$

The 1st B.Z. is then given by bisecting the vectors $\{\pm\vec{b}_1, \pm\vec{b}_2, \pm(\vec{b}_1 + \vec{b}_2)\}$ The distance the edge of the B.Z. is given by $|b_i/2| = \frac{2\pi}{a}\sqrt{(1/3)+1} = \frac{2\pi}{\sqrt{3}a} \approx 3.628/a$

The distance to the corner is the side length ℓ of the equilateral triangle in the 1st B.Z. whose height is given by $\vec{b}_1/2$ with $|b_i|/2 = \frac{2\pi}{\sqrt{3}a}$ Then,

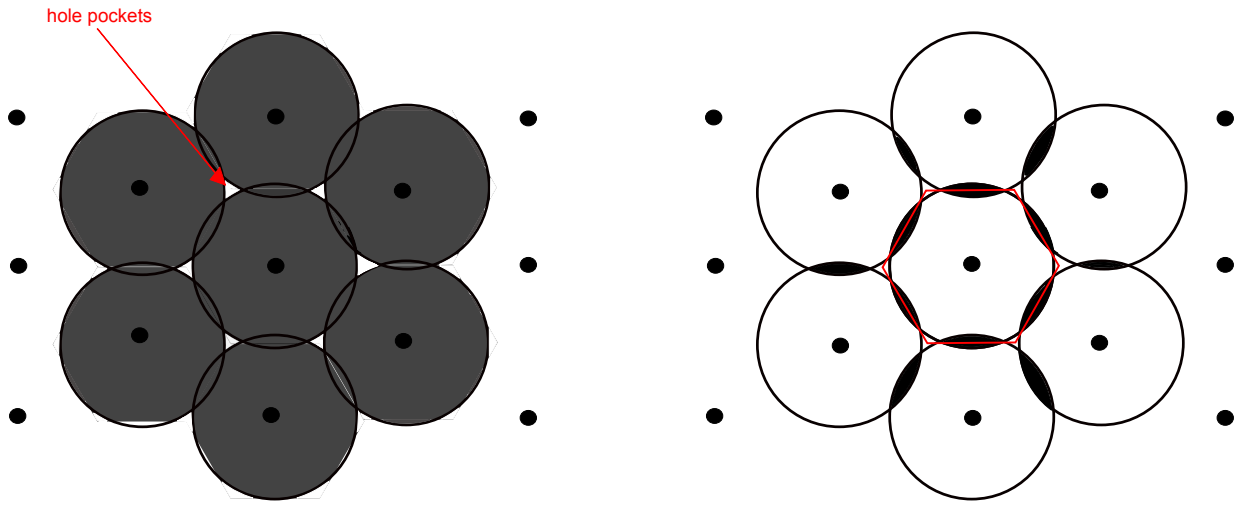
$$(\frac{\ell}{2})^2 + (\frac{2\pi}{\sqrt{3}a})2 = \ell^2 \Rightarrow \ell = \sqrt{\frac{4}{3}(\frac{2\pi}{\sqrt{3}a})^2} = \frac{4\pi}{3a} \approx 4.186/a \tag{5}$$

From before we see l that $k_F \approx 3.81/a$. This verifies that the Fermi surface is partly within the 1st B.Z. (since $k_F < \ell$ the corner length of the B.Z.) , and goes outside the B.Z. at the sides. We can draw this in the reduced zone scheme as



(c) Draw the free electron Fermi surface in the extended/periodic zone scheme

To draw the Fermi surface in the extended zone scheme, we just need the draw the second Brillouin zone by extending the lines which bisect the basis vectors $\vec{b}_1$ and $\vec{b}_2$, and draw the closed star shaped surface. Note that the 2nd B.Z. has the same area as the 1st B.Z.. Then, the figure on the left below is the first Brillouin zone in the reduced scheme, where you can clearly see the hole pockets which are formed by the unfilled states in the first B.Z. The second figure shows the second B.Z. in the periodic scheme, where the black area shows the filled states in the second zone, which when repeated shows the shape of the electron pockets.



(d) What is the area of the electron and hole pockets, i.e. the density of electrons and holes

From part (b), we see the there are unfilled states in the 1st B.Z., and filled states in the 2nd B.Z., which correspond to pockets and holes respectively. To find the area of these we first need to find where the Fermi surface intersects the 1st B.Z..

The distance to a side of the B.Z. is $|b_i|/2 = \frac{2\pi}{\sqrt{3}}$. So, we can center the circular Fermi surface (with radius k_F) at the point $y = -2\pi/\sqrt{3}$ and see where it intersects the line $y = 0$.

$$x^2 + (y + \frac{2\pi}{\sqrt{3}})^2 = \frac{8\pi}{\sqrt{3}} \tag{6}$$

$$\text{set } y = 0 \Rightarrow \qquad x = \pm\sqrt{\frac{8\pi}{\sqrt{3}} - \frac{4\pi^2}{3}} \approx \pm 1.162 \tag{7}$$

The angle between the plus and minus solutions of this is given by

$$\theta/2 = \arccos\left(\frac{2\pi}{3}\sqrt{\frac{\sqrt{3}}{8\pi}}\right) = 0.310 \quad \Rightarrow \theta - 0.6201 \tag{8}$$

Then, this fraction of the Fermi circle has an area equal to $A_{\text{slice}} = \pi k_F^2 \frac{\theta}{2\pi} = \frac{8\pi^2}{\sqrt{3}} \frac{0.6201}{2\pi} = 4.4989$

The portion of the slice which is in the 1st B.Z. is the area of the triangle with base length $2x = 2 * 1.162$ from above and height equal to $|\vec{b}_i|/2 = \frac{2\pi}{\sqrt{3}}$ so that $A_{\text{triangle}} = \frac{1}{2}(2 * 1.162)(\frac{2\pi}{\sqrt{3}}) = 4.215$

Then, the area of one electron pocket in the 2nd B.Z. is just given by $A_{\text{slice}} - A_{\text{triangle}} = 0.2836$ The total area of the electron pockets is 6 times this so $A_{\text{electron}} = 6 * 0.2836 = 1.701$ Since the area of the Fermi surface equals the area of the 1st B.Z., this implies

$$A_{\text{hole}} = A_{\text{electron}} = 1.701 \tag{9}$$

Compare this to the area of the Fermi surface $A_{\text{F.S.}} = 45.59$ to find the electron and hole density

Problem 2 - Cuprate Fermi Surface

(a) Show/ argue that the energy band is described by the function $\varepsilon(k) = -2\gamma(\cos k_x a + \cos k_y a) - 2\gamma'(\cos(k_x + k_y)a + \cos(k_x - k_y)a$

Following the arguments from class we can write the discrete Schrdinger equation for the tight binding model as

$$\varepsilon_0 \psi_R - \sum_{R'} \gamma_{R,R'} \psi_{R'} = \varepsilon \psi_R \tag{10}$$

Then, assuming that $\psi_R = \bar{\psi} e^{i\vec{k}\cdot\vec{R}}$, Eq. (10) gives

$$\begin{aligned} \varepsilon\bar{\psi}e^{i\vec{k}\cdot\vec{R}} = \varepsilon_o\bar{\psi}e^{i\vec{k}\cdot\vec{R}} &- \bar{\psi}\gamma(e^{i\vec{k}\cdot(\vec{R}+\hat{x})} + e^{i\vec{k}\cdot(\vec{R}-\hat{x})} + e^{i\vec{k}\cdot(\vec{R}+\hat{y})} + e^{i\vec{k}\cdot(\vec{R}-\hat{y})}) \\ &-\bar{\psi}\gamma'(e^{i\vec{k}\cdot(\vec{R}+(\hat{x}+\hat{y}))} + e^{i\vec{k}\cdot(\vec{R}-(\hat{x}-\hat{y}))} + e^{i\vec{k}\cdot(\vec{R}+(\hat{x}-\hat{y}))} + e^{i\vec{k}\cdot(\vec{R}-(\hat{x}-\hat{y}))} \end{aligned} \tag{11}$$

$$\Rightarrow \qquad \varepsilon = \varepsilon_0 - 2\gamma(\cos k_x a + \cos k_y a) - 2\gamma'(\cos(k_x + k_y)a + \cos(k_x - k_y)a) \tag{12}$$

Where to get to the last line I canceled out the terms $\bar{\psi}e^{i\vec{k}\cdot\vec{R}}$ and used $e^{ix} + e^{-ix} = 2\cos(x)$

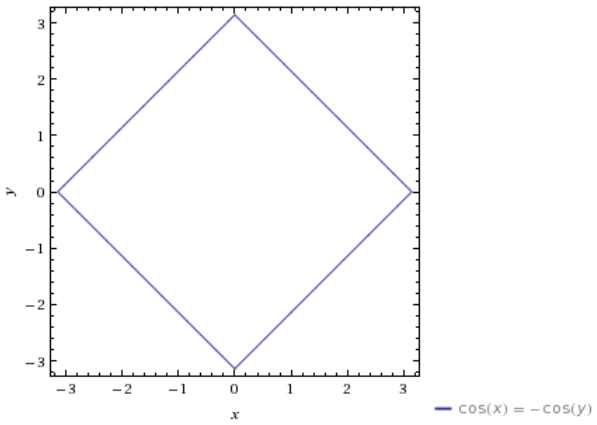
(b) Suppose the Fermi energy (with the above definition of the zero of energy) is zero. What is the density of electrons, per site?

Set the unimportant constant $\varepsilon_0 = 0$ in the equation above. Then, we want the find the surface in the first B.Z. where $\varepsilon(k) = \varepsilon_F = 0$, when $\gamma' = 0$.

$$0 = -2\gamma(\cos k_x a + \cos k_y a) \tag{13}$$

$$\Rightarrow \qquad \cos k_y a = -\cos k_x a \tag{14}$$

$$\Rightarrow \qquad k_y = \pm k_x \pm \frac{\pi}{a} \tag{15}$$



We can easily calculate the area enclosed by this Fermi surface.

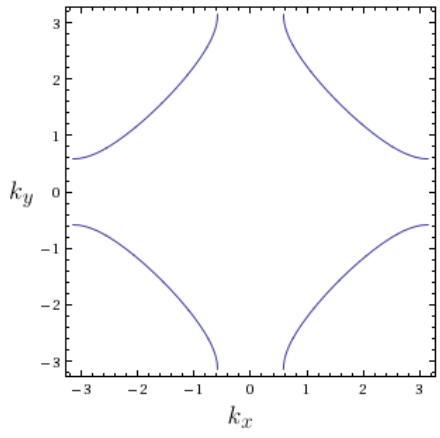
$$A_{\text{F.S.}} = 2 \times \frac{1}{2}\frac{2\pi}{a} * \frac{\pi}{a} = \frac{2\pi^2}{a^2} \tag{16}$$

Now, using the formula

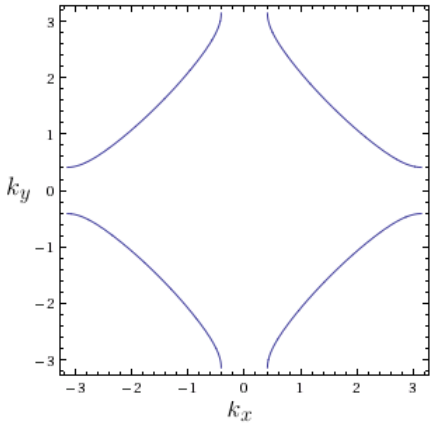
$$2A_{\text{F.S.}} \times \frac{V}{(2\pi)^2} = N \quad \Rightarrow 2\frac{2\pi^2}{a^2}\frac{1}{(2\pi)^2} = \frac{N}{V} \quad \Rightarrow \frac{N}{V} = 1 \tag{17}$$

Therefore, there number density $N/V = 1$, so that there is one electron per site on the lattice.

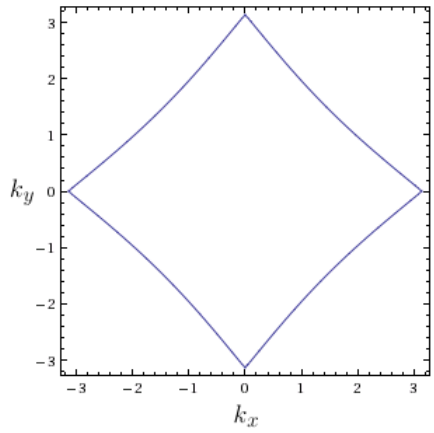
(c) Take $\gamma = 1$ and $\gamma' = -0.1$. Sketch the Fermi surfaces for Fermi energies corresponding to 0, -0.2, -0.4, -0.6. Lowering the Fermi energy corresponds to "hole doping"



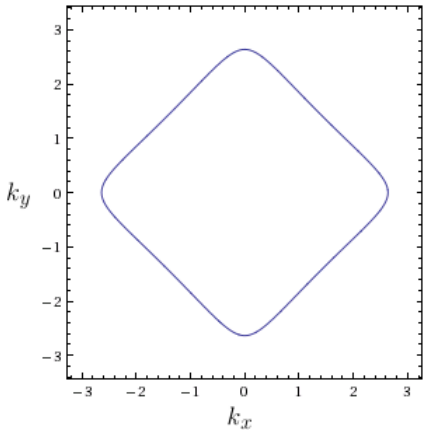
(i)



(ii)



(iii)



(iv)

The Fermi surface in the first Brillouin zone corresponding to Fermi energies **(i)** $\varepsilon = 0$, **(ii)** $\varepsilon = -0.2$, **(iii)** $\varepsilon = -0.4$ and **(iv)** $\varepsilon = -0.6$