<u>Problem 2</u> - 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

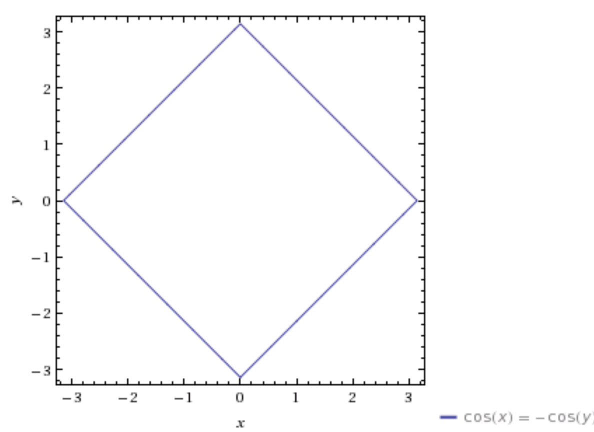
$$\begin{aligned}\varepsilon \bar{\psi} e^{i\vec{k}\cdot\vec{R}} &= \varepsilon_o \bar{\psi} e^{i\vec{k}\cdot\vec{R}} - \bar{\psi}\gamma(e^{i\vec{k}\cdot(\vec{R}+\hat{x})} + e^{i\vec{k}\cdot(\vec{R}-\hat{x})} + e^{i\vec{k}\cdot(\vec{R}+\hat{y})} + e^{i\vec{k}\cdot(\vec{R}-\hat{y})}) \\ &\quad -\bar{\psi}\gamma'(e^{i\vec{k}\cdot(\vec{R}+(\hat{x}+\hat{y}))} + e^{i\vec{k}\cdot(\vec{R}-(\hat{x}-\hat{y}))} + e^{i\vec{k}\cdot(\vec{R}+(\hat{x}-\hat{y}))} + e^{i\vec{k}\cdot(\vec{R}-(\hat{x}-\hat{y}))} \qquad (11) \\ \Rightarrow \quad \varepsilon &= \varepsilon_0 - 2\gamma(\cos k_x a + \cos k_y a) - 2\gamma'(\cos(k_x + k_y)a + \cos(k_x - k_y)a) \qquad (12)\end{aligned}$$

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 $\gamma' = 0$.

$$\begin{aligned} & 0 = -2\gamma(\cos k_x a + \cos k_y a) && (13) \\ \Rightarrow \quad & \cos k_y a = -\cos k_x a && (14) \\ \Rightarrow \quad & k_y = \pm k_x \pm \frac{\pi}{a} && (15)\end{aligned}$$



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

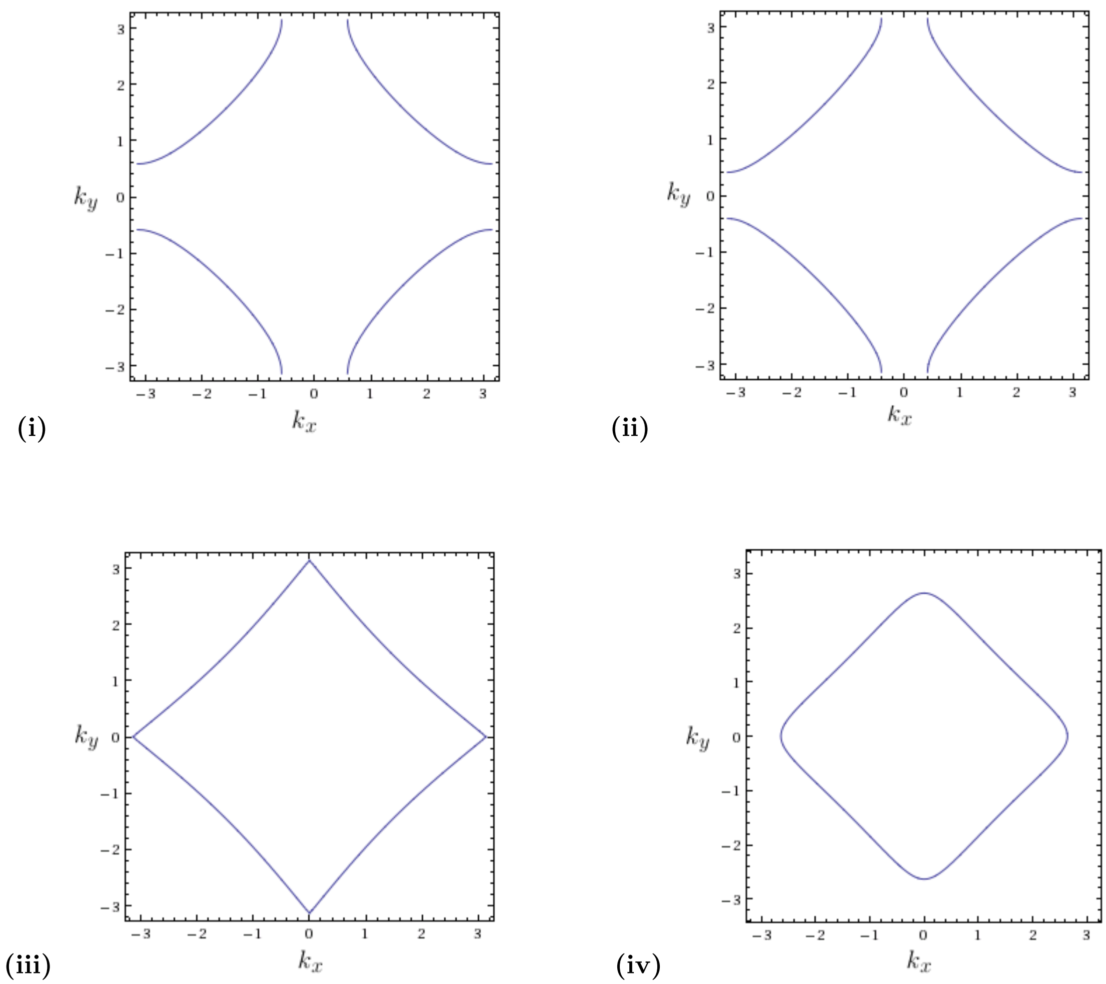
$$A_{\text{F.S.}} = 2 \times \frac{1}{2}\frac{2\pi}{a} * \frac{\pi}{a} = \frac{2\pi^2}{a^2} \tag{16}$$

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"



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)** $\varepsilon = -0.6$