Homework 3
Due Monday, October 19 in class

1. Assume electrons are moving on a two-dimensional triangular lattice with lattice constant a. The Hamiltonian in the Wannier representation, restricted to the lowest band, has the form:

$$H = -t \sum_{\mathbf{R},\boldsymbol{\lambda},\sigma} c^{\dagger}_{\mathbf{R}\sigma} c_{\mathbf{R}+\boldsymbol{\lambda}\sigma},$$

where $\mathbf{R}$ label the lattice sites, $\boldsymbol{\lambda}$ are the nearest-neighbor vectors, and $t > 0$ is the overlap integral. As was mentioned in class, this Hamiltonian describes electrons, tunneling between nearest-neighbor lattice sites.

   (a) Find reciprocal lattice basis vectors for the triangular lattice. Construct the first Brillouin zone.

   (b) Diagonalize this Hamiltonian by transforming from Wannier to Bloch basis and find the band dispersion $\epsilon(\mathbf{k})$.

   (c) Plot the dispersion, expressing the band energy in units of t and momenta in units of the lattice constant a. Make a density plot of the dispersion and draw the first Brillouin zone on this plot.

   (d) Find the effective mass near the bottom of the band.

   (e) Draw the Fermi surface $\epsilon(\mathbf{k}) = \epsilon_F$ for several values of ϵ_F, going from a nearly empty to a nearly full band, and observe how the Fermi surface evolves as the band is filled (use contour plot of the band dispersion for guidance). What is the most significant difference between the Fermi surfaces of a nearly empty and nearly full band?

   (f) Find the Fermi energy (in units of t), corresponding to electron density of 1/3 per lattice site. You can use the effective mass approximation near the bottom of the band for the band dispersion.

(a) Basis vectors of the triangular lattice:

$$\vec{a}_1 = a\hat{x}\ ,\quad \vec{a}_2 = a\left(\frac{1}{2}\hat{x} + \frac{\sqrt{3}}{2}\hat{y}\right)$$

$$\vec{b}_i \cdot \vec{a}_j = \delta_{ij}$$

The above condition gives:

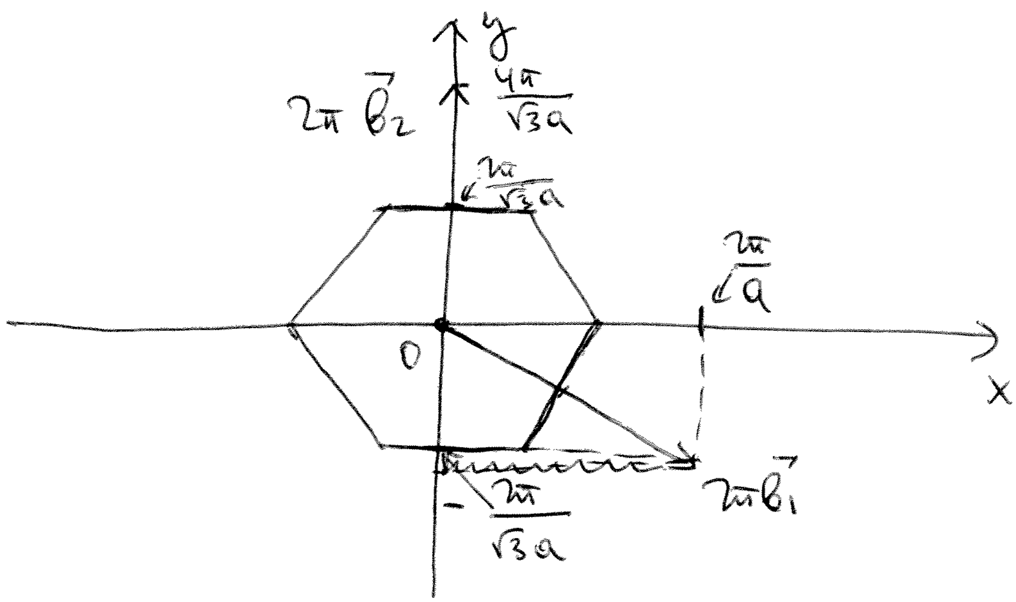
$$\vec{b}_1 = \frac{1}{a}\left(\hat{x} - \frac{1}{\sqrt{3}}\hat{y}\right)$$

$$\vec{b}_2 = \frac{2}{\sqrt{3}a}\hat{y}$$

$\vec{b}_1, \vec{b}_2$ are basis vectors of the reciprocal lattice.

$$\vec{k} = k_1\vec{b}_1 + k_2\vec{b}_2$$

First BZ is defined by $-\pi \le k_{1,2} < \pi$.



(b) $$H = -t \sum_{\vec{R},\vec{\lambda},\sigma} c^{+}_{\vec{R}\sigma} c_{\vec{R}+\vec{\lambda}\sigma}$$

$$c^{+}_{\vec{R}\sigma} = \frac{1}{\sqrt{N}} \sum_{\vec{k}} c^{+}_{\vec{k}\sigma} e^{-i\vec{k}\cdot\vec{R}}$$

$$H = -\frac{t}{N} \sum_{\vec{R},\vec{\lambda},\sigma} \sum_{\vec{k}\vec{k}'} c^{+}_{\vec{k}\sigma} c_{\vec{k}'\sigma} e^{-i\vec{k}\cdot\vec{R}} e^{i\vec{k}'\cdot(\vec{R}+\vec{\lambda})}$$

$$\frac{1}{N} \sum_{\vec{R}} e^{-i(\vec{k}-\vec{k}')\cdot\vec{R}} = \delta_{\vec{k},\vec{k}'}$$

$$H = -t \sum_{\vec{k},\vec{\lambda},\sigma} c^{+}_{k\sigma} c_{k\sigma} e^{i\vec{k}\cdot\vec{\lambda}} =$$

$$= -t \sum_{\vec{k}\vec{\lambda}\sigma} c^{+}_{k\sigma} c_{k\sigma} \cos(\vec{k}\cdot\vec{\lambda})$$

Thus $\varepsilon_k = -t \sum_{\vec{\lambda}} \cos(\vec{k}\cdot\vec{\lambda})$

Triangular lattice has 6 nearest-neighbor vectors:

$\vec{\lambda} = \pm\vec{a}_1, \pm\vec{a}_2, \pm(\vec{a}_1-\vec{a}_2)$

Thus we obtain:

$$\varepsilon_k = -2t \left[\cos(\vec{k}\cdot\vec{a}_1) + \cos(\vec{k}\cdot\vec{a}_2) + \cos(\vec{k}\cdot(\vec{a}_1-\vec{a}_2))\right]$$

$$\varepsilon_k = -2t\left[\cos(k_x a) + \cos\left(\frac{k_x a}{2} + \frac{k_y a\sqrt{3}}{2}\right) + \cos\left(\frac{k_x a}{2} - \frac{k_y a\sqrt{3}}{2}\right)\right]$$

(d) Bottom of the band is at $\vec{k}=0$.

Expand ε_k near $\vec{k}=0$.

$$\varepsilon_k = -2t\left[1 - \frac{(k_x a)^2}{2} + 1 - \frac{1}{2}\left(\frac{k_x a}{2} + \frac{k_y a\sqrt{3}}{2}\right)^2 + 1\right.$$

$$\left. - \frac{1}{2}\left(\frac{k_x a}{2} - \frac{k_y a\sqrt{3}}{2}\right)^2\right] =$$

$$= -6t + t\left[(k_x a)^2 + \frac{(k_x a)^2}{2} + \frac{3(k_y a)^2}{2}\right] =$$

$$= -6t + \frac{3t}{2}k^2 a^2$$

By definition of the effective mass:

$$\frac{\hbar^2}{2m^*} = \frac{3ta^2}{2} \Rightarrow m^* = \frac{\hbar^2}{3ta^2}$$

(f) $\varepsilon_k \triangleq \frac{\hbar^2 k^2}{2m^*}$

Fermi surface is circular in this approximation.

Fermi momentum k_F is related to the density as:

$$\pi k_F^2 \cdot 2 \cdot \frac{1}{(2\pi)^2} = n$$

$$k_F^2 = 2\pi n$$

$$\varepsilon_F = -6t + \frac{\hbar^2 k_F^2}{2m^*} = -6t + \frac{\pi \hbar^2}{m^*} n$$

Density of 1/3 per lattice site means that:

$$n = \frac{1}{3\Omega}$$

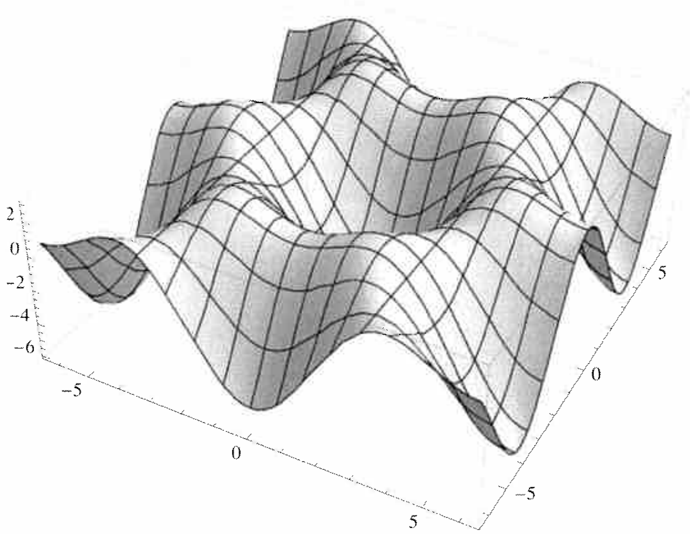
$$\Omega = |\vec{a}_1 \times \vec{a}_2| = \frac{\sqrt{3} a^2}{2}$$ – unit cell area of triangular lattice.

$$n = \frac{2}{3\sqrt{3} a^2}$$

$$\varepsilon_F = -6t + \pi \hbar^2 \cdot \frac{3ta^2}{\hbar^2} \cdot \frac{2}{3\sqrt{3} a^2} = -6t + \frac{2\pi t}{\sqrt{3}}$$

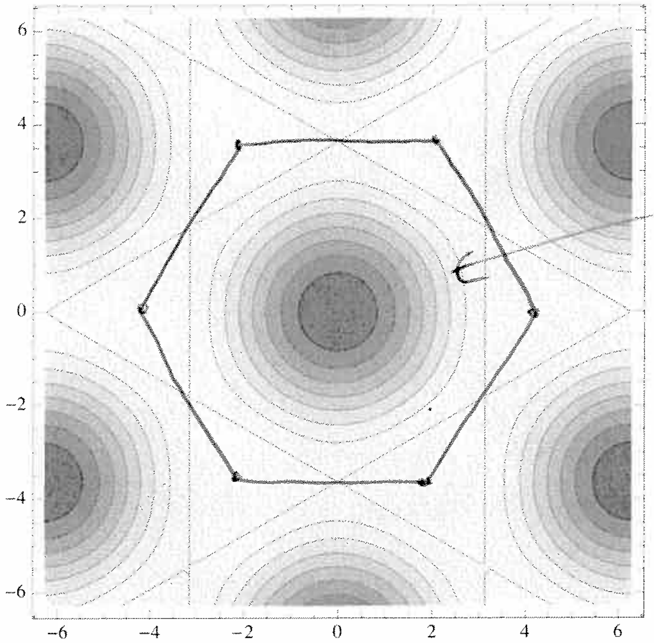
```
In[1]:= ϵ[k1_, k2_] := -2 * (Cos[k1] + Cos[k2] + Cos[-k1 + k2]);
        Plot3D[ϵ[kx, Sqrt[3] * ky / 2 + kx / 2], {kx, -2 * Pi, 2 * Pi}, {ky, -2 * Pi, 2 * Pi}]
        (*ContourPlot[ϵ[kx,Sqrt[3]*ky/2+kx/2]==2.5,{kx,-2*Pi,2*Pi},{ky,-2*Pi,2*Pi}]*)
        (*ContourPlot[-2*(Cos[kx]+Cos[ky])== 1,{kx,-2*Pi,2*Pi},{ky,-2*Pi,2*Pi}]*)
```

Out[2]=



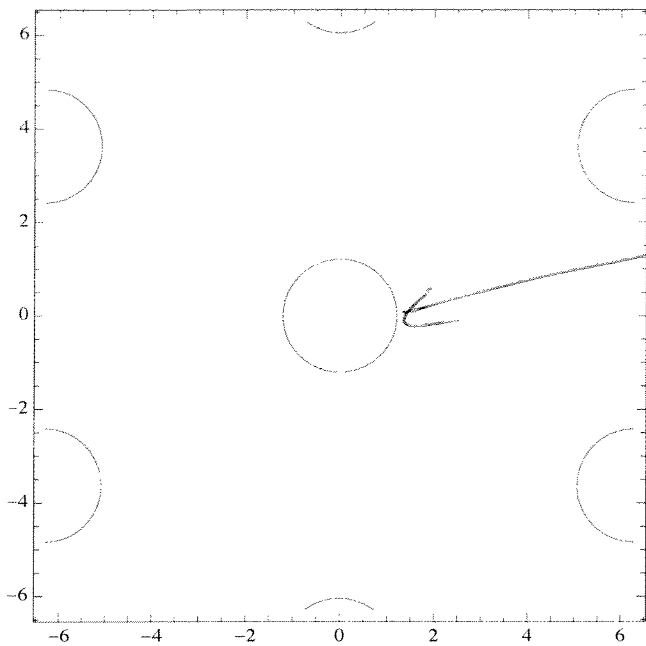
```
In[3]:= ϵ[k1_, k2_] := -2 * (Cos[k1] + Cos[k2] + Cos[-k1 + k2]);
ContourPlot[ϵ[kx, Sqrt[3] * ky / 2 + kx / 2], {kx, -2 * Pi, 2 * Pi}, {ky, -2 * Pi, 2 * Pi}]
(*ContourPlot[ϵ[kx,Sqrt[3]*ky/2+kx/2]==2.5,{kx,-2*Pi,2*Pi},{ky,-2*Pi,2*Pi}]*)
(*ContourPlot[-2*(Cos[kx]+Cos[ky])== 1,{kx,-2*Pi,2*Pi},{ky,-2*Pi,2*Pi}]*)
```

Out[4]=



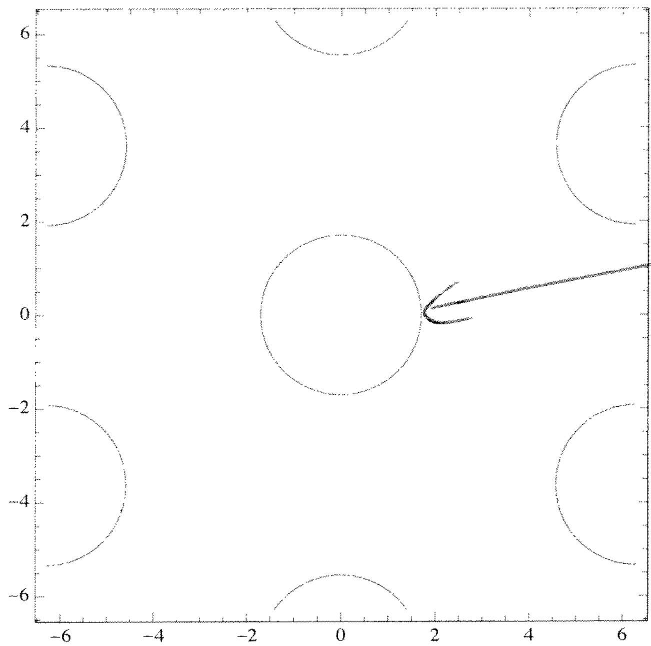
first BZ

```
ϵ[k1_, k2_] := -2 * (Cos[k1] + Cos[k2] + Cos[-k1 + k2]);
(*ContourPlot[ϵ[kx,Sqrt[3]*ky/2+kx/2],{kx,-2*Pi,2*Pi},{ky,-2*Pi,2*Pi}]*)
ContourPlot[ϵ[kx, Sqrt[3] * ky / 2 + kx / 2] == -4, {kx, -2 * Pi, 2 * Pi}, {ky, -2 * Pi, 2 * Pi}]
(*ContourPlot[-2*(Cos[kx]+Cos[ky]) == 1,{kx,-2*Pi,2*Pi},{ky,-2*Pi,2*Pi}]*)
```



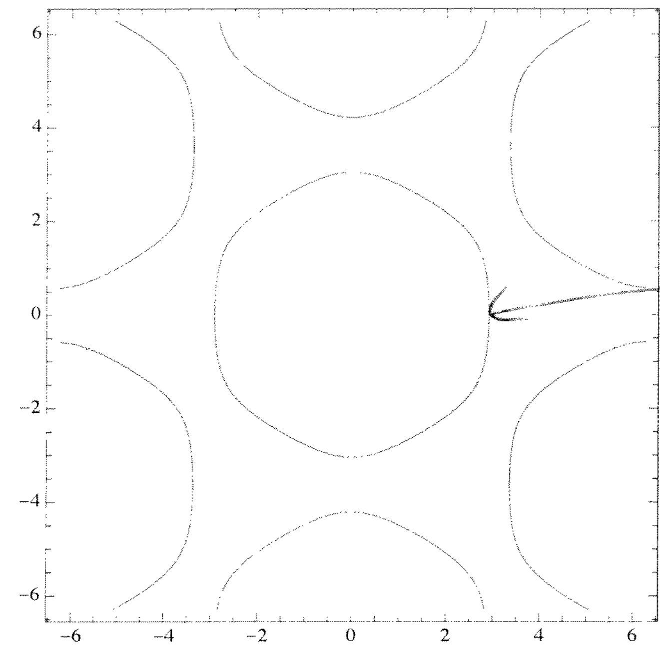
Fermi surface for $\varepsilon_F = -4t$ - lightly filled band.
FS is circular, effective mass approximation is good.

```
ϵ[k1_, k2_] := -2 * (Cos[k1] + Cos[k2] + Cos[-k1 + k2]);
(*ContourPlot[ϵ[kx,Sqrt[3]*ky/2+kx/2],{kx,-2*Pi,2*Pi},{ky,-2*Pi,2*Pi}]*)
ContourPlot[ϵ[kx, Sqrt[3] * ky / 2 + kx / 2] == -6 + 2 * Pi / Sqrt[3],
 {kx, -2 * Pi, 2 * Pi}, {ky, -2 * Pi, 2 * Pi}]
(*ContourPlot[-2*(Cos[kx]+Cos[ky])== 1,{kx,-2*Pi,2*Pi},{ky,-2*Pi,2*Pi}]*)
```



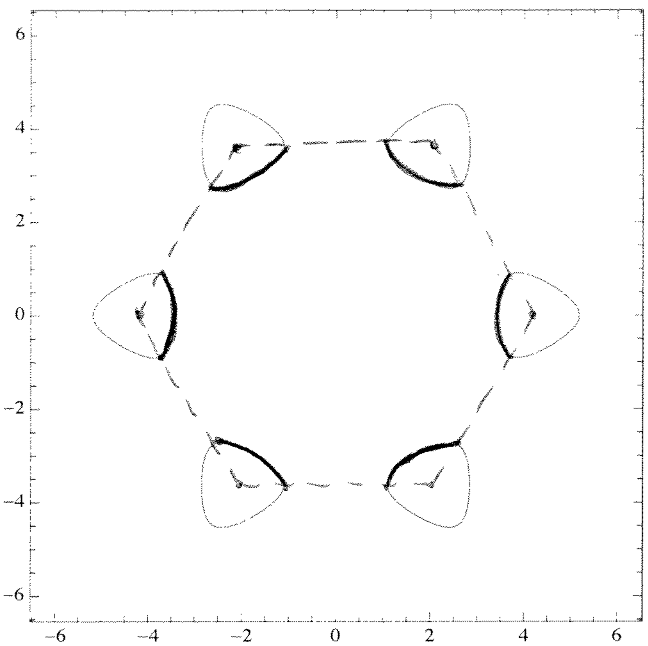
FS for $\varepsilon_F = -6t + \frac{2\pi t}{\sqrt{3}}$, corresponding to the density of 1/3 per site. FS is still circular and effective mass approx. is good

```
ϵ[k1_, k2_] := -2 * (Cos[k1] + Cos[k2] + Cos[-k1 + k2]);
(*ContourPlot[ϵ[kx,Sqrt[3]*ky/2+kx/2],{kx,-2*Pi,2*Pi},{ky,-2*Pi,2*Pi}]*)
ContourPlot[ϵ[kx, Sqrt[3] * ky / 2 + kx / 2] == 1.5, {kx, -2 * Pi, 2 * Pi}, {ky, -2 * Pi, 2 * Pi}]
(*ContourPlot[-2*(Cos[kx]+Cos[ky])== 1,{kx,-2*Pi,2*Pi},{ky,-2*Pi,2*Pi}]*)
```



FS for $\varepsilon_F = 1.5\,t$
Not circular anymore, effective mass approx. isn't as good.

```
ϵ[k1_, k2_] := -2 * (Cos[k1] + Cos[k2] + Cos[-k1 + k2]);
(*ContourPlot[ϵ[kx,Sqrt[3]*ky/2+kx/2],{kx,-2*Pi,2*Pi},{ky,-2*Pi,2*Pi}]*)
ContourPlot[ϵ[kx, Sqrt[3] * ky / 2 + kx / 2] == 2.5, {kx, -2 * Pi, 2 * Pi}, {ky, -2 * Pi, 2 * Pi}]
(*ContourPlot[-2*(Cos[kx]+Cos[ky])== 1,{kx,-2*Pi,2*Pi},{ky,-2*Pi,2*Pi}]*)
```



FS for $\varepsilon_F = 2.5t$ - almost filled band. FS is multiply-connected now, i.e. topologically distinct from FS for lightly-filled band.