Homework 4
Due Wednesday, October 28 in class

1. Assume electrons are moving on a two-dimensional square lattice with lattice constant a. The tight-binding band dispersion is

$$\epsilon(\mathbf{k}) = -2\gamma[\cos(k_x a) + \cos(k_y a)],$$

where γ is the overlap integral.

   (a) Draw Fermi surfaces in three cases: almost empty band, exactly half-filled band, and nearly full band. What is the electron density corresponding to half-filled band?

   (b) Calculate effective masses near the bottom and near the top of the band.

   (c) Assume a constant magnetic field is applied in the z-direction, i.e. perpendicular to the plane in which electrons move. Write down quasiclassical equations of motion. Using these, prove that the energy is a constant of motion (this can be proven generally, without using the explicit form of the band dispersion). This means that electron trajectories in momentum space trace out constant energy contours. Find trajectories numerically (use Maple) in three cases: electrons with energy near the bottom of the band, in the middle of the band and near the top of the band. Compare with your Fermi surface sketches.

   (d) Solve quasiclassical equations of motion analytically near the bottom of the band, using effective mass approximation for the band dispersion.

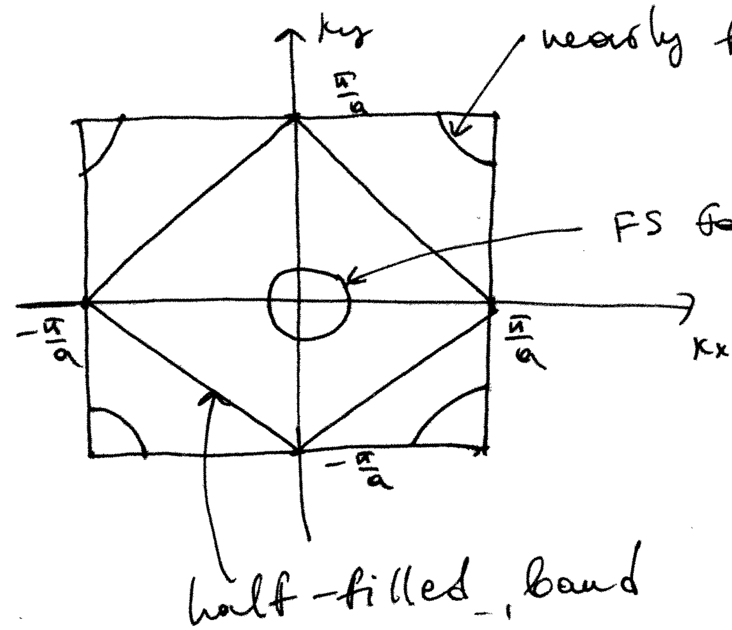
2. For the square lattice tight-binding band from Problem 1 calculate the conductivity for half-filled band. Use the general expression for the conductivity we obtained in class:

$$\sigma = \frac{e^2\tau}{4\pi^2\hbar}\int d\ell_F \; v_{\mathbf{k}},$$

and the Fermi surface for half-filled band you found in Problem 1. Compare the result with what you would get if you used effective mass approximation near the bottom of the band for the dispersion.

Problem 1

(a)



Electron density for half-filled band is:

$n = \frac{1}{a^2}$ – one electron per unit cell

(b) $\varepsilon(\vec{k}) = -2\gamma\left[\cos(k_x a) + \cos(k_y a)\right]$

Near the bottom of the band (i.e. near $\vec{k} = 0$):

$$\varepsilon(\vec{k}) \approx -4\gamma + \gamma\left[(k_x a)^2 + (k_y a)^2\right] =$$

$$= -4\gamma + \gamma a^2 k^2$$

$$\gamma a^2 = \frac{\hbar^2}{2m^*} \Rightarrow m^* = \frac{\hbar^2}{2\gamma a^2}$$

Band maxima occur at $\vec{k} = \left(\pm\frac{\pi}{a}, \pm\frac{\pi}{a}\right)$.

Take $\vec{k_0} = \left(\frac{\pi}{a}, \frac{\pi}{a}\right)$. To find effective mass expand the dispersion near $\vec{k} = \vec{k_0}$.

$$\varepsilon(\vec{k}) = \varepsilon(\vec{k} - \vec{k_0} + \vec{k_0}) = -\varepsilon(\vec{k} - \vec{k_0})$$ – here I've used $\cos(x+\pi) = -\cos x$

Thus, near the top of the band:

$$\varepsilon(\vec{k}) \approx 4\gamma - \gamma a^2 (\vec{k} - \vec{k}_0)^2$$

$\cancel{m^* = -\frac{\hbar^2}{2\gamma a^2}}$ ~~- effective mass~~

$$m^* \doteq -\frac{\hbar^2}{2\gamma a^2}$$ - same by magnitude but opposite in sign to the effective mass of the bottom of the band.

(c) Quasiclassical equations of motion in magnetic field are:

$$\begin{cases} \dot{\vec{r}} = \dfrac{1}{\hbar} \dfrac{\partial \varepsilon(\vec{k})}{\partial \vec{k}} \\ \hbar \dot{\vec{k}} = -\dfrac{e}{c} \dot{\vec{r}} \times \vec{H} \end{cases}$$

Explicitly, in components:

$$\begin{cases} \dot{x} = \dfrac{2\gamma a}{\hbar} \sin k_x a \\ \dot{y} = \dfrac{2\gamma a}{\hbar} \sin k_y a \\ \dot{k}_x = -\dfrac{eH}{\hbar c} \dfrac{2\gamma a}{\hbar} \sin k_y a \\ \dot{k}_y = \dfrac{eH}{\hbar c} \dfrac{2\gamma a}{\hbar} \sin k_x a \end{cases}$$

Using $m^* = \dfrac{\hbar^2}{2\gamma a^2}$ and $\omega_c^* = \dfrac{eH}{m^* c}$ - cyclotron frequency near the bottom of the band we can rewrite these equations as:

$$\begin{cases} \dot{x} = \dfrac{\hbar}{m^* a} \sin k_x a \\ \dot{y} = \dfrac{\hbar}{m^* a} \sin k_y a \\ \dot{k}_x = -\dfrac{\omega_c^*}{a} \sin k_y a \\ \dot{k}_y = \dfrac{\omega_c^*}{a} \sin k_x a \end{cases}$$

To prove that the band energy is a constant of motion, consider its time derivative:

$$\frac{d\varepsilon(\vec{k})}{dt} = \frac{d\varepsilon(\vec{k})}{d\vec{k}} \cdot \frac{d\vec{k}}{dt} = \hbar \vec{v} \cdot \left(-\frac{e}{\hbar c} \vec{v} \times \vec{H} \right) = 0,$$

since $\vec{v} \cdot (\vec{v} \times \vec{H}) = 0.$

(d) Near the bottom of the band we can expand the right hand side of the equations of motion, assuming k is small:

$$\begin{cases} \dot{k}_x = -\omega_c^* k_y \\ \dot{k}_y = \omega_c^* k_x \end{cases}$$

The solution is $k_x(t) = A \cos(\omega_c^* t) + B \sin(\omega_c^* t)$

$$k_y(t) = -\frac{1}{\omega_c^*} \dot{k}_x(t) = A \sin(\omega_c^* t) - B \cos(\omega_c^* t)$$

A and B are determined by the initial conditions:

$$k_x(0) = A \quad , \quad k_y(0) = -B$$

$$k_x(t) = k_x(0)\cos(\omega_c^* t) - k_y(0)\sin(\omega_c^* t)$$

$$k_y(t) = k_x(0)\sin(\omega_c^* t) + k_y(0)\cos(\omega_c^* t)$$

To rewrite this in a more compact form use the fact that the band energy is a constant of motion.

$$\varepsilon = \frac{\hbar^2}{2m^*}k^2 = \frac{\hbar^2}{2m^*}(k_x^2 + k_y^2) = \text{const.}$$

$$k_x^2 + k_y^2 = \frac{2m^*\varepsilon}{\hbar^2} = \text{const}$$

let $$\frac{k_x(0)}{k} = \frac{k_x(0)}{\sqrt{k_x^2+k_y^2}} = \cos\delta$$

$$\frac{k_y(0)}{k} = \sin\delta$$

$$\delta = \arctan\left(\frac{k_y(0)}{k_x(0)}\right)$$

Then the solution can be written as:

$$k_x(t) = \sqrt{\frac{2m\varepsilon}{\hbar^2}}\cos(\omega_c^* t + \delta)$$

$$k_y(t) = \sqrt{\frac{2m\varepsilon}{\hbar^2}}\sin(\omega_c^* t + \delta)$$

Problem 2

$$\sigma = \frac{e^2 \tau}{4\pi^2 \hbar} \int dl_F \, v_k$$

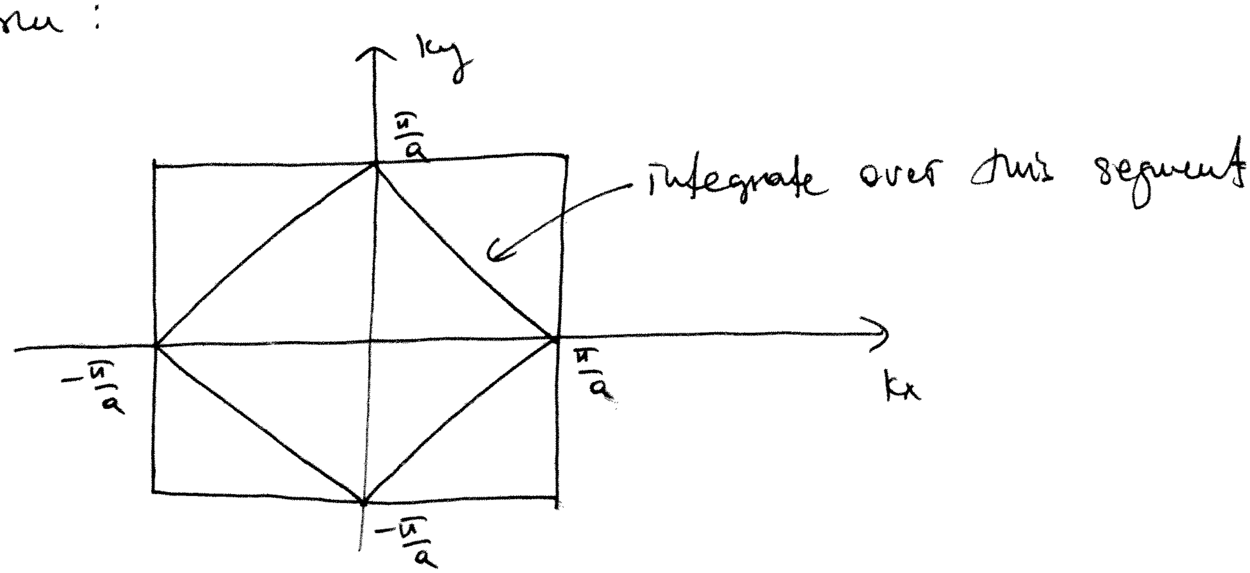
$$\vec{v} = \frac{1}{\hbar} \frac{\partial \varepsilon(\vec{k})}{\partial \vec{k}}$$

$$v_x = \frac{2\gamma a}{\hbar} \sin(k_x a)$$

$$v_y = \frac{2\gamma a}{\hbar} \sin(k_y a)$$

$$v_k = \sqrt{v_x^2 + v_y^2} = \frac{2\gamma a}{\hbar} \sqrt{\sin^2(k_x a) + \sin^2(k_y a)}$$

The fermi surface for half-filled band has the form:



Clearly, integrals over all 4 segments are equal $\Rightarrow$

$\Rightarrow$ need to integrate over 1 segment and multiply by 4.

Integrate over segment shown by arrow. Its equation is:

$$k_y = \frac{\pi}{a} - k_x \quad , \quad 0 \le k_x \le \frac{\pi}{a}$$

$$\sigma = \frac{e^2\tau}{4\pi^2\hbar}\, 4 \int_0^{\frac{\pi}{a}} \frac{dk_x}{\cos\left(\frac{\pi}{4}\right)}\, v_k =$$

$$= \frac{\sqrt{2}\, e^2\tau}{\pi^2\hbar}\, \frac{2\gamma a}{\hbar} \int_0^{\frac{\pi}{a}} dk_x \sqrt{\sin^2(k_x a) + \sin^2(\pi - k_x a)} =$$

$$= \frac{4 e^2 \tau \gamma a}{\pi^2 \hbar^2} \int_0^{\frac{\pi}{a}} dk_x\, |\sin(k_x a)| = \frac{8 e^2 \tau \gamma}{\pi^2 \hbar^2}$$

$$\sigma = \frac{8 e^2 \tau \gamma}{\pi^2 \hbar^2}$$

If one uses effective mass approximation, one obtains:

$$\sigma = \frac{n e^2 \tau}{m^*}$$

$$n = \frac{1}{a^2}, \quad m^* = \frac{\hbar^2}{2\gamma a^2}$$

$$\sigma = e^2\tau \cdot \frac{1}{a^2}\, \frac{2\gamma a^2}{\hbar^2} = \frac{2\gamma e^2 \tau}{\hbar^2}$$

~~Thus σ is more than a factor of 2 larger than the correct result.~~

Thus σ is a factor of $\frac{\pi^2}{4}$ larger than the correct result.

Trajectory for electrons near the bottom of the band.

```
Clear[kx, ky];
s = NDSolve[{kx'[t] + Sin[ky[t]] == 0, ky'[t] - Sin[kx[t]] == 0, kx[0] == 0.5, ky[0] == 0.},
  {kx[t], ky[t]}, {t, 0, 10}]
ParametricPlot[{kx[t], ky[t]} /. s, {t, 0, 10}, PlotRange → {{-Pi, Pi}, {-Pi, Pi}}]

{{kx[t] → InterpolatingFunction[{{0., 10.}}, <>][t],
  ky[t] → InterpolatingFunction[{{0., 10.}}, <>][t]}}
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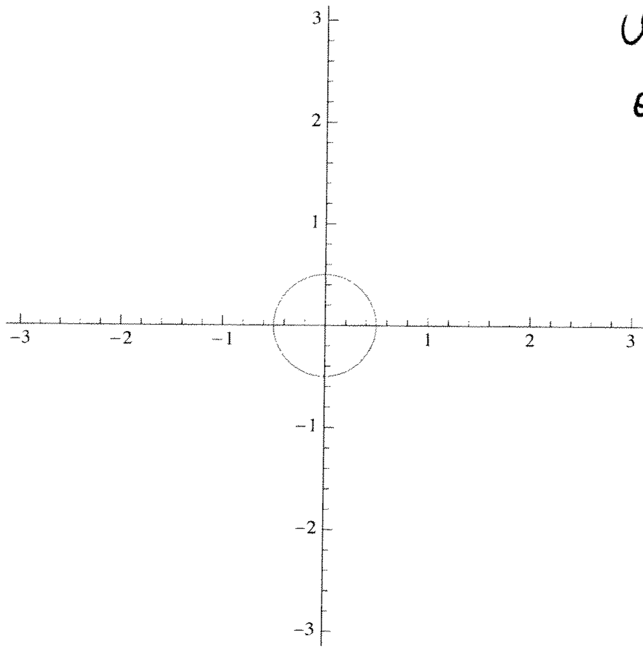

Using a as unit of length and $\frac{1}{\omega_c^*}$ as unit of time.

Trajectory at the middle of the band.

```
Clear[kx, ky];
s = NDSolve[{kx'[t] + Sin[ky[t]] == 0, ky'[t] - Sin[kx[t]] == 0, kx[0] == Pi - 0.001, ky[0] == 0.},
  {kx[t], ky[t]}, {t, 0, 100}]
ParametricPlot[{kx[t], ky[t]} /. s, {t, 0, 100}, PlotRange → {{-Pi, Pi}, {-Pi, Pi}}]
```

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{{kx[t] → InterpolatingFunction[{{0., 100.}}, <>][t],
  ky[t] → InterpolatingFunction[{{0., 100.}}, <>][t]}}
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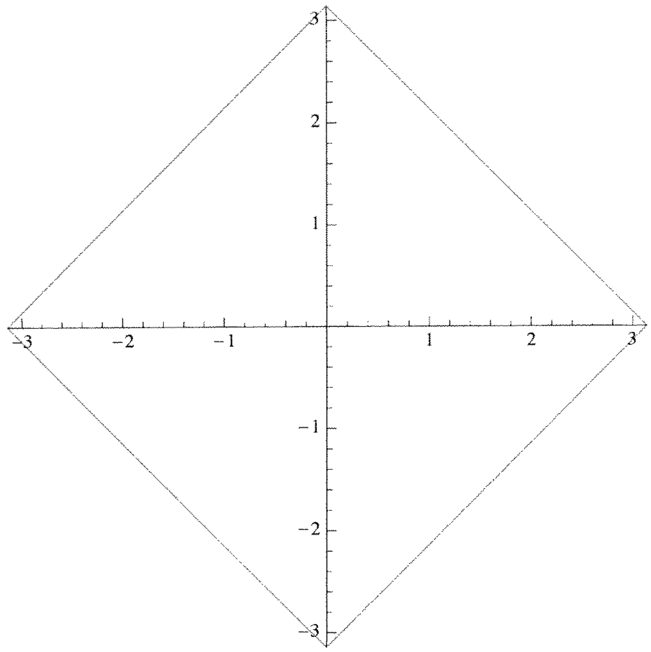

Near the top of the band.

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Clear[kx, ky];
s = NDSolve[{kx'[t] + Sin[ky[t]] == 0, ky'[t] - Sin[kx[t]] == 0, kx[0] == Pi - 0.5, ky[0] == Pi - 0.5},
  {kx[t], ky[t]}, {t, 0, 20}]
ParametricPlot[{kx[t], ky[t]} /. s, {t, 0, 20}, PlotRange → {{-Pi, Pi}, {-Pi, Pi}}]
```

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{{kx[t] → InterpolatingFunction[{{0., 20.}}, <>][t],
  ky[t] → InterpolatingFunction[{{0., 20.}}, <>][t]}}
```