PHY 491, Homework 7
October 31-November 4, 2011

Problem 7.1

Use the following equation for the drift velocity of an electron in a constant electric field oscillating with a frequency ω

$$m\left(\frac{dv}{dt}+\frac{v}{\tau}\right)=-eE$$

to show that the frequency dependent conductivity (ac conductivity) is given by

$$\sigma(\omega)=\sigma(0)\frac{1+i\omega\tau}{1+(\omega\tau)^2}$$

where $\sigma(0)=\frac{ne^2\tau}{m}$ and n is the density of electrons.

$$E(t)=E(\omega)e^{-i\omega t};v(t)=v(\omega)e^{-i\omega t};j(t)=j(\omega)e^{-i\omega t}$$

$$j(\omega)=-nev(\omega)=\sigma(\omega)E(\omega)$$

$$\sigma(\omega)=\sigma(0)\frac{1+i\omega\tau}{1+(\omega\tau)^2}$$

Problem 7.2
Consider a square lattice with lattice constant a. Draw the 1st BZ and give the coordinates of it's symmetry points (here use 4-fold rotation about the z-axis)

The 1st BZ is a square. The symmetry points are:
$(k_x, k_y) = (0,0), (\pm\pi/a, 0), (0, \pm\pi/a), (\pm\pi/a, \pm\pi/a)$

Now consider the states of an electron whose $\vec{k}$ vector corresponds to one of the corner points of the BZ.
How many plane waves have the same kinetic energy as the one corresponding to this $\vec{k}$? What are their $\vec{k}$ vectors?
(We will call these as degenerate set of plane waves, because in the absence of crystal potential these plane waves have the same kinetic energy)

There are 4 plane waves $e^{i\vec{k}\cdot\vec{r}}$ where
$\vec{k} = (\pi/a, \pi/a), (-\pi/a, -\pi/a), (\pi/a, -\pi/a), (-\pi/a, \pi/a)$

All these 4 plane waves have same kinetic energy =

$$\frac{\hbar^2}{2m}\left[\left(\frac{\pi}{a}\right)^2 + \left(\frac{\pi}{a}\right)^2\right] = \frac{\hbar^2}{m}\left(\frac{\pi}{a}\right)^2$$

Construct two stationary wave functions from the above degenerate set such that for one $[\psi_1(x, y)]$ the probability of finding the electron at the lattice sites is maximum and for the other $[\psi_2(x, y)]$ it is minimum.

Let's denote the 4 degenerate plane waves as

$$\phi_1(x,y) = e^{i\left(\frac{\pi}{a}x+\frac{\pi}{a}y\right)}; \phi_2(x,y) = e^{-i\left(\frac{\pi}{a}x+\frac{\pi}{a}y\right)}; \phi_3(x,y) = e^{i\left(\frac{\pi}{a}x-\frac{\pi}{a}y\right)}; \phi_4(x,y) = e^{-i\left(\frac{\pi}{a}x-\frac{\pi}{a}y\right)}$$

$$\psi_1(x,y) = \phi_1 + \phi_2 + \phi_3 + \phi_4 = 2\cos\left(\frac{\pi}{a}x + \frac{\pi}{a}y\right) + 2\cos\left(\frac{\pi}{a}x - \frac{\pi}{a}y\right) = 4\cos\left(\frac{\pi}{a}x\right)\cos\left(\frac{\pi}{a}y\right)$$

$$\psi_2(x,y) = \phi_1 + \phi_2 - \phi_3 - \phi_4 = 2\cos\left(\frac{\pi}{a}x + \frac{\pi}{a}y\right) - 2\cos\left(\frac{\pi}{a}x - \frac{\pi}{a}y\right) = 4\sin\left(\frac{\pi}{a}x\right)\sin\left(\frac{\pi}{a}y\right)$$

Probability of finding the electron at the lattice site is largest for ψ_1. The probability of finding the electron at the lattice site =0 for ψ_2. However there are two other states $4\cos\left(\frac{\pi}{a}x\right)\sin\left(\frac{\pi}{a}y\right)$ *and* $4\sin\left(\frac{\pi}{a}x\right)\cos\left(\frac{\pi}{a}y\right)$ which also give zero probability at the lattice sites. The probability maxima are at different points of the unit cell for these latter two states.

Problem 7.3

Now consider the case when there is a periodic potential in this square lattice given by

$$U(x,y) = -U_0\left[\cos\left(\frac{2\pi}{a}x\right) + \cos\left(\frac{2\pi}{a}y\right)\right]$$

What is the energy gap between the two states $[\psi_1(x,y)]$ and $[\psi_2(x,y)]$ given in Problem 7.2. Explain your result physically by matching the probability distribution of the Electron in these two states and the attractive regions of the potential.

$$E_1 = \frac{\langle\psi_1|U|\psi_1\rangle}{\langle\psi_1|\psi_1\rangle} = \frac{\int_0^a dx \int_0^a dy |\psi_1(x,y)|^2 U(x,y)}{\int_0^a dx \int_0^a dy |\psi_1(x,y)|^2} = -U_0$$

$$E_2 = \frac{\langle\psi_2|U|\psi_2\rangle}{\langle\psi_2|\psi_2\rangle} = \frac{\int_0^a dx \int_0^a dy |\psi_2(x,y)|^2 U(x,y)}{\int_0^a dx \int_0^a dy |\psi_2(x,y)|^2} = U_0$$

The energy gap between these two states is $2U_0$. However to find the actual gap you have to calculate the energies of the other two states given in Problem 7.2.