PHY801: Survey of Atomic and Condensed Matter Physics
Michigan State University

Homework 7 – Solution

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

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

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.

Solution:

$$\begin{aligned} E(t) &= E(\omega)e^{-i\omega t}\ , \\ v(t) &= v(\omega)e^{-i\omega t}\ , \\ j(t) &= j(\omega)e^{-i\omega t}\ . \end{aligned}$$

Consequently,

$$\begin{aligned} j(\omega) &= -nev(\omega)=\sigma(\omega)E(\omega)\ , \\ \sigma(\omega) &= \sigma(0)\frac{1+i\omega\tau}{1+(\omega\tau)^2}\ . \end{aligned}$$

7.2. (a) Consider a square lattice with lattice constant a. Draw the 1st BZ and give the coordinates of it's symmetry points (use 4-fold rotation about the z-axis here). 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 a crystal potential these plane waves have the same kinetic energy.)

(b) Construct two stationary wave functions $\psi_1(x,y)$ and $\psi_2(x,y)$ 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.

Solution:

(a) The 1st BZ is a square. The symmetry points are

$$\vec{k}=(k_x,k_y)=(0,0);\ \left(\pm\frac{\pi}{a},0\right);\ \left(0,\pm\frac{\pi}{a}\right);\ \left(\pm\frac{\pi}{a},\pm\frac{\pi}{a}\right)\ .$$

There are 4 plane waves $e^{i\vec{k}\cdot\vec{r}}$ with

$$\vec{k}=\left(+\frac{\pi}{a},+\frac{\pi}{a}\right);\ \left(-\frac{\pi}{a},-\frac{\pi}{a}\right);\ \left(+\frac{\pi}{a},-\frac{\pi}{a}\right);\ \left(-\frac{\pi}{a},+\frac{\pi}{a}\right)\ .$$

All these 4 plane waves have the same kinetic energy

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

(b) Let us denote the 4 degenerate plane waves as

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

Then,

$$\begin{aligned}
\psi_1(x,y) &= \phi_1+\phi_2+\phi_3+\phi_4 = 2\cos\left(\frac{\pi}{a}x+\frac{\pi}{a}y\right) + 2\cos\left(\frac{\pi}{a}x-\frac{\pi}{a}y\right) = 4\cos\left(\frac{\pi}{a}x\right)\cos\left(\frac{\pi}{a}y\right) ,\\
\psi_2(x,y) &= \phi_1+\phi_2-\phi_3-\phi_4 = 2\cos\left(\frac{\pi}{a}x+\frac{\pi}{a}y\right) - 2\cos\left(\frac{\pi}{a}x-\frac{\pi}{a}y\right) = 4\sin\left(\frac{\pi}{a}x\right)\sin\left(\frac{\pi}{a}y\right) .
\end{aligned}$$

Of these states, the probability of finding the electron at a lattice site is largest for ψ_1. The probability of finding an electron at a lattice site is zero for ψ_2.

However, there are two other states, $\psi_3(x,y) = 4\cos\left(\frac{\pi}{a}x\right)\sin\left(\frac{\pi}{a}y\right)$ and $\psi_4(x,y) = 4\sin\left(\frac{\pi}{a}x\right)\cos\left(\frac{\pi}{a}y\right)$, which also give zero probability to find an electron at the lattice sites. The probability maxima for ψ_3 and ψ_4 are at different points of the unit cell.

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 $\psi_2(x,y)$, defined 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.

Solution:

$$\begin{aligned}
E_1 &= \frac{<\psi_1|U|\psi_1>}{<\psi_1|\psi_1>} = \frac{\int_0^a dx \int_0^a dy |\psi_1(x,y)|^2 U(x,y)}{\int_0^a dx \int_0^a dy |\psi_1(x,y)|^2} = -U_0 ,\\
E_2 &= \frac{<\psi_2|U|\psi_2>}{<\psi_2|\psi_2>} = \frac{\int_0^a dx \int_0^a dy |\psi_2(x,y)|^2 U(x,y)}{\int_0^a dx \int_0^a dy |\psi_2(x,y)|^2} = +U_0 .
\end{aligned}$$

The energy gap between these two states is $2U_0$. To find the actual gap, however, you have to calculate also the energies of the other two states ψ_3 and ψ_4 that have been discussed in Problem 7.2.
