ECE 535
Notes for Lecture # 6

Class Outline:

• Properties of the Electron Gas - Part 2

Properties of the Electron Gas - 30

We have an interesting problem that arises when we consider the conductivity...

Recall our analysis of the Drude approach:

\[ \frac{m}{dt} \frac{dv}{dt} = qE - \frac{mv}{\tau} \]

Let's consider the steady-state: \( \frac{d}{dt}(\ldots) \to 0 \)

\[ v = \frac{q}{m} E = \mu E \]

From this, it is easy to see what the current should be:

\[ J = qnv = \frac{nq^2 \tau}{m} E = \sigma E \implies \sigma_0 = \frac{nq^2 \tau}{m} \]
We also know the response when the electric field we apply is oscillating in time...

\[ E(t) = E e^{i\omega t} \]

Which gives the Drude response as:

\[ m \frac{dv}{dt} = qE e^{i\omega t} - \frac{mv}{\tau} \]

Assuming that we have a linear response: \( v(t) = v(0) e^{i\omega t} \)

Then we arrive at:

\[ \sigma(\omega) = \frac{\sigma_0}{1 + i\omega \tau} = \frac{\sigma_0}{1 + (\omega \tau)^2} - i \frac{\omega \tau \sigma_0}{\text{Re}(\sigma(\omega))} - i \frac{\omega \tau \sigma_0}{\text{Im}(\sigma(\omega))} \]

The flow of electrons leads us to this conductivity. How can we understand the flow of electrical charges from a quantum mechanical perspective?

Let's try to formulate a quantum mechanical model for charge transport using our knowledge of the state of the system and the wavefunction...

We begin by examining how the probability density changes as a function of time:

\[ |\Psi(x, t)|^2 = \Psi^* \Psi \]

We obtain:

\[ \frac{\partial |\Psi(x, t)|^2}{\partial t} = \Psi^* \frac{\partial \Psi}{\partial t} + \frac{\partial \Psi^*}{\partial t} \Psi \]

Using the time-dependent Schrodinger equation and its conjugate:

\[ i\hbar \frac{\partial \Psi}{\partial t} = (\hat{p}^2/2m + V) \Psi \quad -i\hbar \frac{\partial \Psi^*}{\partial t} = (\hat{p}^2/2m + V) \Psi^* \]

We obtain:

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We can continue to simplify this equation:

\[
\frac{\partial |\Psi(x, t)|^2}{\partial t} = \frac{1}{2m\hbar} (\Psi^* \hat{p}^2 \Psi - \Psi \hat{p}^2 \Psi^*)
\]

But remember that we already know the operator form of the momentum:

\[
\hat{p} = -i\hbar \nabla_r
\]

This results in an interesting form of the equation:

\[
\frac{\partial |\Psi(x, t)|^2}{\partial t} = -\nabla_r \cdot \left[ \frac{1}{2m} (\Psi^* \hat{p} \Psi - \Psi \hat{p} \Psi^*) \right]
\]

This is nothing more than the continuity equation in disguise...

\[
\frac{\partial n}{\partial t} = -\nabla_r \cdot \mathbf{j}
\]

So what does this mean?

Consider this semiconductor:

• The hole current density leaving the differential area may be larger or smaller than the current density that enters the area.
• This is a result of recombination and generation.

**Net increase in hole concentration per unit time, \( \frac{dp}{dt} \), is difference between hole flux per unit volume entering and leaving, minus the recombination rate.**
How can we explain this?

The net increase in hole concentration per unit time is the difference between the hole flux entering and leaving minus the recombination rate...

\[
\frac{\Delta p}{\Delta t} = \frac{1}{q} \left( J_p(x) - J_p(x + \Delta x) \right) - \frac{\Delta p}{\tau_p}
\]

Rate of hole buildup.

Increase in hole concentration in \( \Delta x A \) per unit time.

Recombination rate

As \( \Delta x \) goes to zero, we can write the change in hole concentration as a derivative, just like in diffusion...

\[
\frac{\partial p(x,t)}{\partial t} = \frac{\partial p}{\partial t} = -\frac{1}{q} \frac{\partial J_p}{\partial x} = \frac{\Delta p}{\tau_p}
\]

Holes

\[
\frac{\partial n(x,t)}{\partial t} = \frac{\partial n}{\partial t} = \frac{1}{q} \frac{\partial J_n}{\partial x} = \frac{\Delta n}{\tau_n}
\]

Electrons

These relations form the continuity equations.

If this is indeed the continuity equation in disguise, then we can read off the quantum mechanical current density:

\[
j = \frac{1}{2m} \left( \Psi^* \hat{p} \Psi - \Psi \hat{p} \Psi^* \right)
\]

This provides us with the quantum mechanical form that we need to calculate the probability current flow. A few observations:

• If the wavefunction is real, then the current density is zero.

• Since the wavefunction has dimensions \( 1/\sqrt{\text{volume}} \), then the current density is per unit area per second.

\[
\frac{d}{dt} \left( \int_{\text{space}} d^3r \left| \Psi(x,t) \right|^2 \right) = - \int_{\text{space}} d^3r \nabla \cdot j = - \oint j \cdot dS = 0
\]

• Here we have used Gauss' theorem.

• The integral goes to zero because the wavefunction, and therefore the current density, go to zero at infinity.

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• Here we have used Gauss' theorem.

• The integral goes to zero because the wavefunction, and therefore the current density, go to zero at infinity.
What happens if then the particle number is not conserved?

\[ \int_{\text{space}} d^3r |\Psi|^2 = 1 \]

In this case, we need to add recombination (annihilation) and generation (creation) terms to our continuity equation:

\[ \frac{\partial \rho}{\partial t} = -\nabla \cdot j + (G - R) \]

What happens in the presence of a magnetic field?

\[ B = \nabla \times A \]

Make a substitution for the magnetic vector potential: \( \hat{p} \rightarrow \hat{p} + qA \)

\[ j = \frac{1}{2m} (\Psi^* \hat{p} \Psi - \Psi \hat{p} \Psi^*) + \frac{qA}{m} \Psi^* \Psi \]

We get an extra term that depends on the magnetic vector potential that is useful in explaining magnetotransport properties.

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Let’s focus on the determination of the electrical current:

\[ J = qj \]

In the absence of a magnetic field, we obtain the electric current density:

\[ J = \frac{q}{2m_e} (\Psi^* \hat{p} \Psi - \Psi \hat{p} \Psi^*) \]

Everything checks out as this has units of Amperes, but can we make this expression more useful? Examine free electrons in 1D with periodic boundary conditions.

\[ \Psi_E(x, t) = (1/\sqrt{L}) e^{ikx} e^{-iE(k)t/\hbar} \]

Current density and the current then become:

\[ J(k) = I(k) = q\hbar k/m_e L \]

\[ I(k) = q\hbar k/m_e L \rightarrow v(k) = \frac{q v(k)}{L} \rightarrow v(k) = \hbar k/m_e \]

Quantum Classical
We can generalize this to any dimension, $d$:

$$J_d = \frac{q}{L^d} \sum_{k} v_g(k) f(k)$$

- Where we have now included the Fermi-Dirac occupation probability for each state $k$.
- We can make this more general by splitting it into spin and valley degeneracies.

Spin $g_s = 2$ Valley $g_v$

Furthermore, picture the current flow moving from a "left" contact to a "right" contact and allow for the inclusion of scattering.

$$J_d = \frac{g_s g_v}{L^d} \sum_{k} v_g(k) T(k) [f_L(k) - f_R(k)]$$

The quantity $T(k)$ is the quantum mechanical transmission probability of particles moving from the left to the right contact and does not depend on the direction of the current flow.

Where does the difference in the Fermi-Dirac come from? As with the density of states, we would like to convert the $k$-space integral to an integral in energy. To do this, we use the following...

$$\sum_{k} (...) = \int \frac{d^d k}{(2\pi)^d} (...)$$

Note that now the dependence on the dimension $L$ disappears. We may now write the current density as:

$$J_d = \frac{g_s g_v}{(2\pi)^d} \int d^d k \times v_g(k) T(k) [f_L(k) - f_R(k)] \quad \Lambda/m^{d-1}$$

This expression is widely applicable:
- Any number of dimensions.
- Any transport condition: Ballistic to Diffusive.
- The group velocity is tied DIRECTLY to the bandstructure of the material.