Lecture 16

Thursday, February 25, 2010

We consider further consequences of the semi-classical EOM, with the addition of the Bohr-Sommerfeld quantization, in the case of the dHvA, SdH measurements. We discuss electrons and holes, as distinct physical entities.

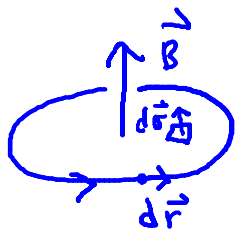
Quantum Oscillations (Landau levels; dHvA, SdH measurements)

We start where we left. We apply the Bohr-Sommerfeld quantization condition, $\oint d\vec{r}\cdot\vec{p} = (n+\gamma)h$, to the classical particle with the canonical momentum $\vec{p} = m\vec{v} + \frac{q}{c}\vec{A} = \hbar\vec{k} + \frac{q}{c}\vec{A}$.

$$\oint d\vec{r}\cdot\vec{p} = \hbar\oint d\vec{r}\cdot\vec{k} + \frac{q}{c}\oint d\vec{r}\cdot\vec{A}$$

Stoke's theorem

In the 2nd term: $\oint d\vec{r}\cdot\vec{A} = \int d\vec{\sigma}\cdot\vec{\nabla}\times\vec{A} = \int d\vec{\sigma}\cdot\vec{B} = \Phi =$ magnetic flux.



For the 1st term, recall that $d\vec{k} = \frac{q}{\hbar c}d\vec{r}\times\vec{B}$, and so $\vec{k} = \frac{q}{\hbar c}\vec{r}\times\vec{B} + const$ in the constant $\vec{B}$ field. So, the 1st term: $\hbar\oint d\vec{r}\cdot\vec{k} = \frac{q}{c}\oint d\vec{r}\cdot(\vec{r}\times\vec{B}) = \frac{q}{c}\vec{B}\cdot\oint d\vec{r}\times\vec{r} = -2\frac{q}{c}B\Sigma$ where Σ is the area enclosed by the orbit. Since $B\Sigma = \Phi$, by collecting the first and the 2nd terms we get the following quantization condition:

$$-\frac{q}{c}\Phi = (n+\gamma)h$$

For the electron, we use $q = -e$, to get

$$\Phi_n = (n+\gamma)\frac{hc}{e}$$

So, **the magnetic flux is quantized**. The flux quantum $\Phi_0 = \frac{hc}{e} = 4.14\times 10^{-7}$ gauss cm^2, and $\Phi_n = (n+\gamma)\Phi_0$

In other words, an orbit area quantization occurs, both in $\vec{r}$ space and in $\vec{k}$ space, in this semi-classical picture. Let us call the area in $\vec{r}$ space A_n, and the area in $\vec{k}$ space S_n. The above flux quantization means that $A_n B = (n+\gamma)\frac{\hbar c}{e}$. And, since $d\vec{k} = \frac{-e}{\hbar c} d\vec{r} \times \vec{B}$, we have $S_n = \left(\frac{eB}{\hbar c}\right)^2 A_n$. Therefore, we have the following quantization for the orbital area in $\vec{k}$ space.

$$S_n = 2\pi \frac{eB}{\hbar c}(n+\gamma)$$

This is the central formula that explains why the quantum oscillation phenomena occur.

Suppose one has a 2D electron gas. In the absence of the $\vec{B}$ field, the allowed $\vec{k}$ values form a practical continuum. As the $\vec{B}$ field is turned on, though, not all $\vec{k}$ values are accessible. Only those $\vec{k}$ values on a circle, whose area corresponds to S_n are available. $\vec{k}$ is not a good quantum number any more, but each circle represents a quantum number: this is the **Landau level***,* which is just the index of concentric circles in $\vec{k}$ space, or equivalently in $\vec{r}$ space. [In some conventions, the Landau level starts from $n = 1$, in which case $\gamma = -1/2$, instead of $1/2$. Here we will use $n = 0,1,2, \ldots$ and $\gamma = 1/2$.]

It is convenient to define a "magnetic length scale" $l_B = \sqrt{\frac{\hbar c}{eB}}$ to express the above results as:

$$S_n = \frac{2\pi}{l_B^2}(n+\gamma),\ A_n = l_B^4 S_n,\ A_n = 2\pi l_B^2 (n+\gamma)$$

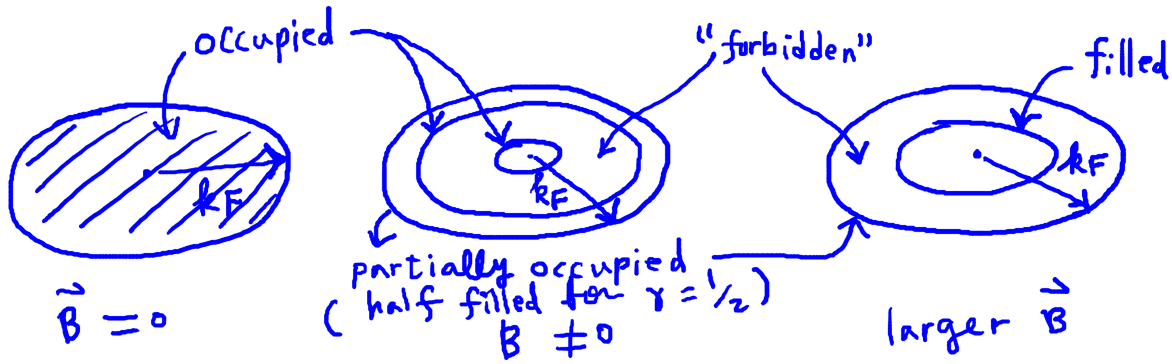
With $\gamma = 1/2$, and $n = 0,1,2, \ldots$, one sees that l_B ($1/l_B$) is the radius of the first Landau orbit in $\vec{r}$ ($\vec{k}$) space. $l_B = \frac{257}{\sqrt{B}}$ Å, if B was in unit of Tesla. So, in accessible B field range, l_B would be a few tens of Å or more, or $2\pi l_B \gtrsim 100$ Å. In terms of flux quantum Φ_0, $l_B = \sqrt{\frac{\Phi_0}{2\pi B}}$: i.e., πl_B^2 corresponds to half the flux quantum.

Landau levels have a degeneracy that increases with B. From the above equation, $\Delta S_n = \frac{2\pi}{l_B^2}$. It is reasonable to conjecture that the degeneracy of each Landau level is just this divided by the usual $(2\pi)^2/A_S$, where A_s is the area of the two dimensional crystal (or the crossectional area of the three dimensional crystal).

Not surprisingly, Quantum Mechanics proves this conjecture to be true. So, the Landau degeneracy is $D = \frac{1}{2\pi}\frac{A_S}{l_B^2} = \frac{BA_S}{\Phi_0} = \Phi_{tot}/\Phi_0$, where Φ_{tot} is the magnetic flux through the sample. Including the spin degeneracy, we get

$$D = 2\Phi_{tot}/\Phi_0$$

The physics of Landau levels underlies all quantum oscillation measurements.



In the current semi-classical picture, the above picture describes what happens as we turn on the $\vec{B}$ field. Without the $\vec{B}$ field, the states up to $\vec{k} = \vec{k}_F$ are occupied. With the $\vec{B}$ field, however, only those circles of $\vec{k}$ values are allowed (keeping in mind, of course, that, in the quantum mechanical sense, there would be only dense and sparse regions of $\vec{k}$ space, in terms of the probability density). For a given $\vec{B}$ field, there would be an outermost orbit which is partially-occupied or un-occupied while all smaller orbits are fully occupied. As $\vec{B}$ field is increased, the orbits will become large, while at the same time their Laudau degeneracy increases. Therefore, the outermost orbital will be emptied gradually, until it becomes completely empty and then the number of occupied orbitals decrease by 1. This is the origin of all quantum oscillation measurements in the $\vec{B}$ field.

How does this make it possible to measure the Fermi surface? Note that from the above diagram the emptying of the outermost orbital will come when the area of the outermost orbital is equal to the area of the Fermi surface plus $\frac{2\pi}{l_B^2}\gamma$. Thus, $S_n = \frac{2\pi}{l_B^2}(n+\gamma) = A_{FS} + \frac{2\pi}{l_B^2}\gamma$ defines the condition for the "jumps" where A_{FS} is the area of the Fermi surface. $\frac{4\pi^2 B}{\Phi_0}n = A_{FS}$, or $\frac{1}{B} = \frac{4\pi^2}{\Phi_0 A_{FS}}n$. This is the origin of oscillations in physical quantities as a function of $\frac{1}{B}$. The period in $\frac{1}{B}$ is given by $\frac{4\pi^2}{\Phi_0 A_{FS}}$.

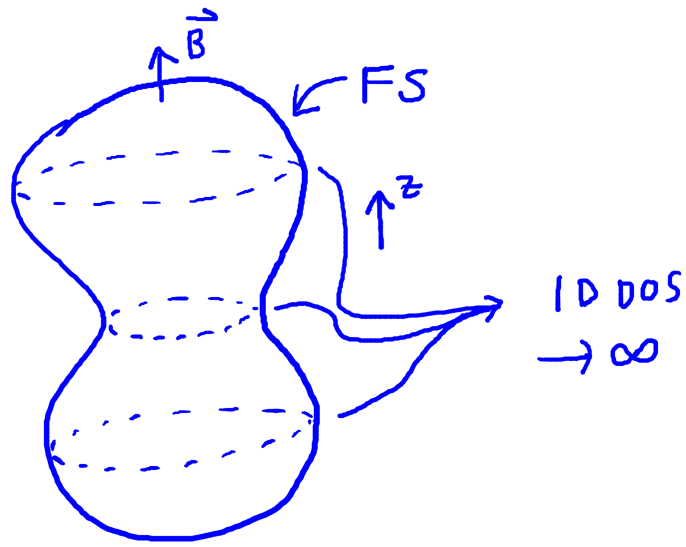
$$\Delta\left(\frac{1}{B}\right) = \frac{4\pi^2}{\Phi_0}\frac{1}{A_{FS}} = \frac{2\pi e}{\hbar c}\frac{1}{A_{FS}}$$

So, by measuring the period, A_{FS} can be measured!

It is a well-known QM result that each Landau level has the energy $\left(n+\frac{1}{2}\right)\hbar\omega_c$, where $\omega_c = \frac{eB}{mc} = \frac{\hbar}{m}\frac{1}{l_B^2}$ is the cyclotron frequency. In the above semi-classical model, this can be obtained as $\frac{p^2}{2m} = \frac{\hbar^2}{2m}\frac{S_n}{\pi} = \frac{\hbar^2}{m}\frac{1}{l_B^2}(n+\gamma) = \hbar\omega_c(n+\gamma)$.

In order for the quantum oscillation measurements to succeed, it is necessary that the sample is pure (the mean free path $l \gg l_B$) and the temperature is very low ($k_B T \ll \hbar\omega_c$).

So far, we have considered only a two dimensional case. What about three dimensions? Here the so called "one dimensional density of states (1D DOS) effect" comes in. For a given dispersion $\epsilon(\vec{k})$, consider the 1D density of states along the z direction, which is defined as the direction of the $\vec{B}$ field. For a given energy and fixed k_x, k_y vaules, one can think about the 1D DOS, in the sense of the available number of k_z values. Thus, 1D DOS $\propto \frac{1}{\left|\frac{\partial\epsilon(\vec{k})}{\partial k_z}\right|} \propto \frac{1}{|v_{g,z}|}$. The importance of this 1D DOS is that when it diverges, that k_z value will singularly contribute the response of the system.



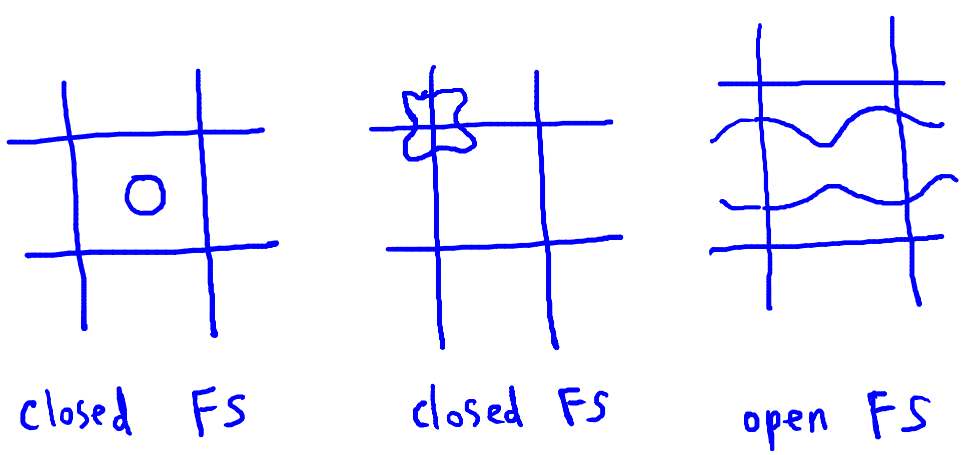
This is illustrated in the above diagram. While quantum oscillation phenomena happen at any fixed k_z value, the three **extremal Fermi surfaces** $\left(\frac{\partial\epsilon(\vec{k})}{\partial k_z} = 0\right)$ shown in the diagram are the only ones that show up in the actual measurements, since they dominate the response function, because the 1D DOS is infinite at those k_z values. In the case illustrated here, the two or three oscillation frequencies will beat.

The oscillation in $1/B$ can be measured in a variety of physical quantities (conductivity, magnetization, specific heat etc.). For instance, when the magnetization (or the magnetic susceptibility) is measured and plotted as a function of $1/B$, an oscillatory behavior can be observed. The period of that oscillation ($\frac{2\pi e}{\hbar c}\frac{1}{A_{FS}}$) gives information about the area of the extremal FS. This effect is called the **de Hass van Alphen (dHvA)** effect. When the conductivity shows an oscillatory behavior, then it is called the **Schbnikov de Hass (SdH)** effect. These are very important techniques in probing the Fermi surface.

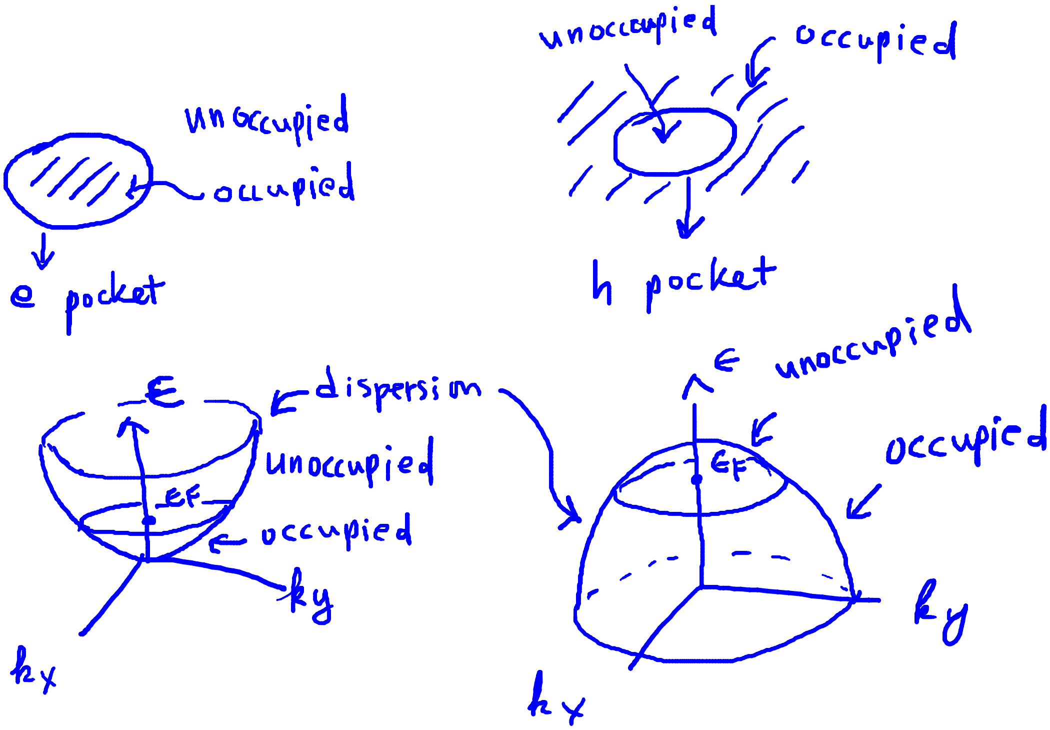
Holes and Electrons

The flux quantization discussed above has some connection to so called topological effects in physics. The flux quantization in superconductors and the Aharanov-Bohm effect are well-known topological effects. Now, an even simpler topological effect in solid state physics is the emergence of the hole as a physical entity in semi-conductors.

Let us recall how we defined the electron pocket and the hole pocket in relation to a Fermi surface. We assume that we have a closed Fermi surface, as an open Fermi surface leaves the electron or the hole nature poorly defined or dependent on the direction.

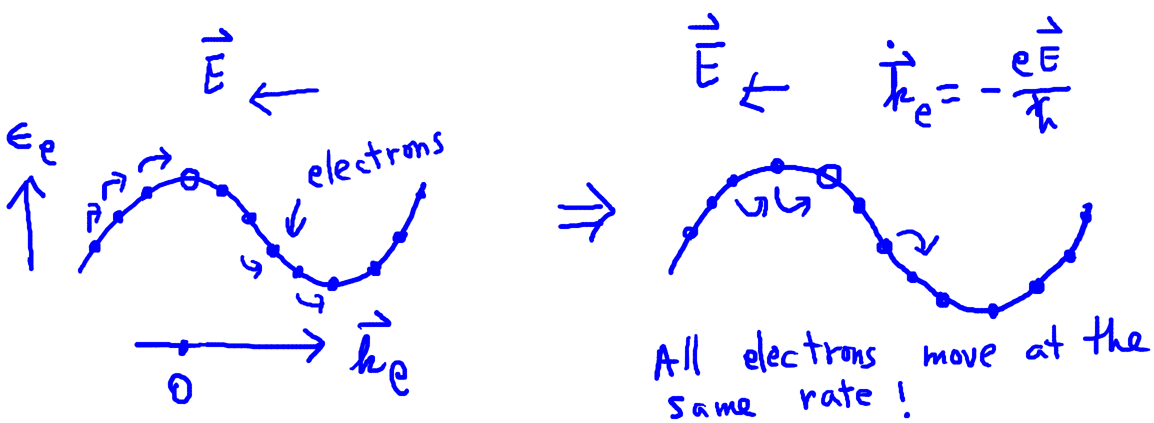


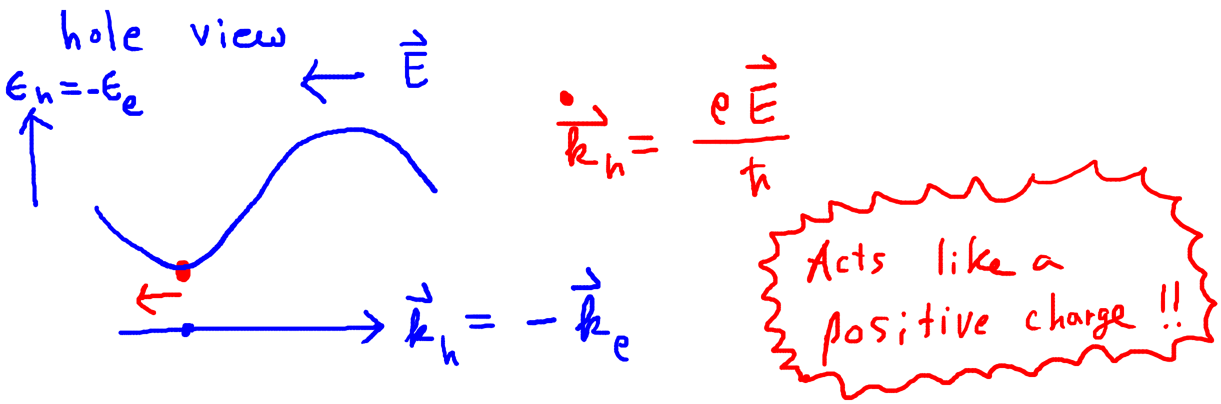
For a given closed Fermi surface, if the band dispersion that gives rise to that Fermi surface is occupied in the interior of the Fermi surface, then that is an electron pocket. If the interior is un-occupied, then that is a hole pocket.



Why is this -- e-pocket or a h-pocket -- a topological property? This is because, it is not possible to continuously deform an e-pocket to a h-pocket, and vice versa. (This topological argument is valid only in dimensions higher than one.)

By studying the following diagrams carefully, one can grasp what we really mean by "hole." The most important fact is that the concept "hole" considers the completely filled band as the reference state, or the vacuum state if you like. Thus energy of the hole = (total energy of the N - 1 state) - (total energy of the N state), where the N state corresponds to the completed filled band. The wave vector of the hole = (total wave vector of the N - 1 state) - (total wave vector of the N state). **So, to go from the electron diagram to the hole diagram, both the energy and the wave vector (momentum) need to be flipped in sign**. The same holds for the spin/orbital angular momentum. But, note that the group velocity remains the same.





Note, by the way, that the above diagram shows that in a completely filled band, each electron will move exactly the same way in $\vec{k}$ space. So, there is no net change. This is why materials with completely filled bands acts as though nothing happens (like no conductivity), since the overall state is not changing at all.